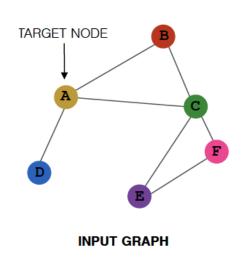
IT5429E-1-24 (24.1A01)(Fall 2024): Graph Analytics for Big Data

Week 10: Graph Transformer

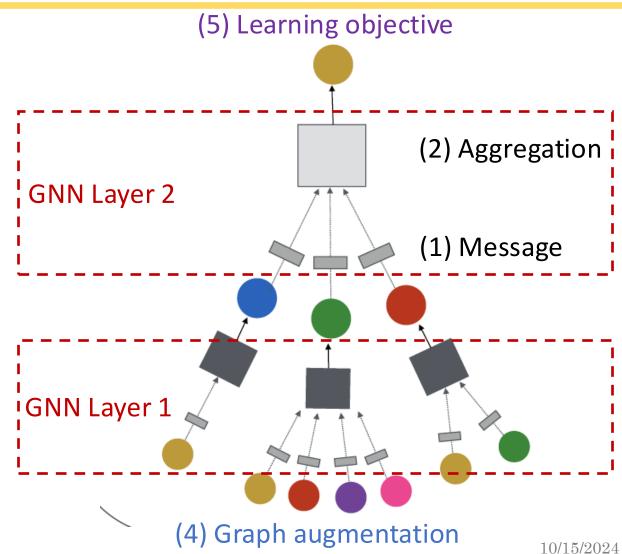
Instructor: Thanh H. Nguyen

Many slides are adapted from https://web.stanford.edu/class/cs224w/

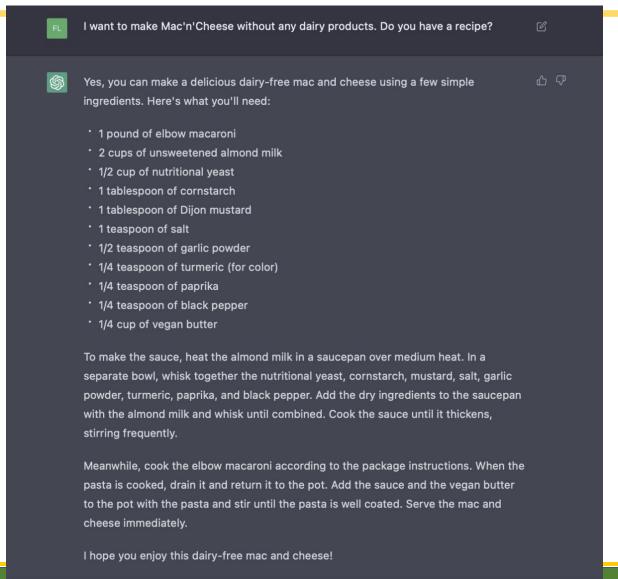
Recap: A General GNN Framework



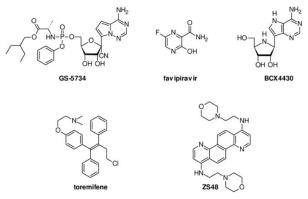
(3) Layer connectivity



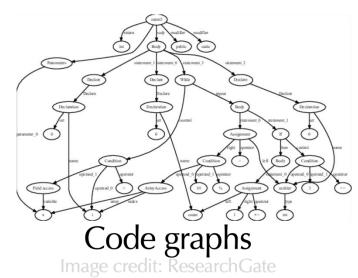
Transformers: The Backbone of Generative Al

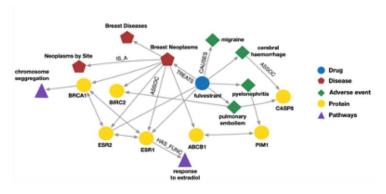


Goal: Bring Power of Transformer to Graphs

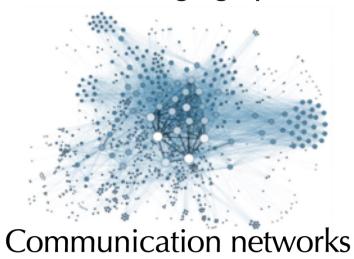


Small molecules





Knowledge graphs



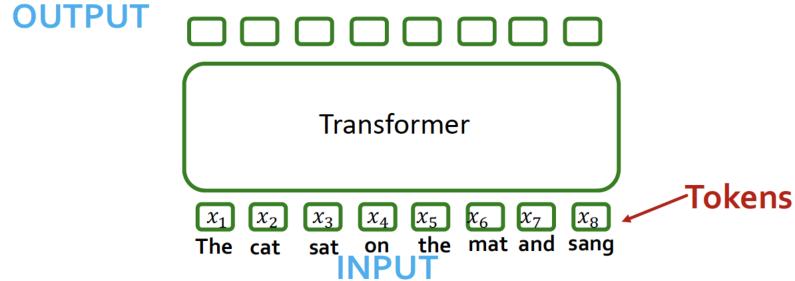
Χ

Outline

- Part 1:
 - Introducing Transformers
 - Relation to message passing GNNs
- Part 2:
 - A new design landscape for graph Transformers
- Part 3:
 - Sign invariant Laplacian positional encodings for graph Transformers

Transformer Ingest Tokens

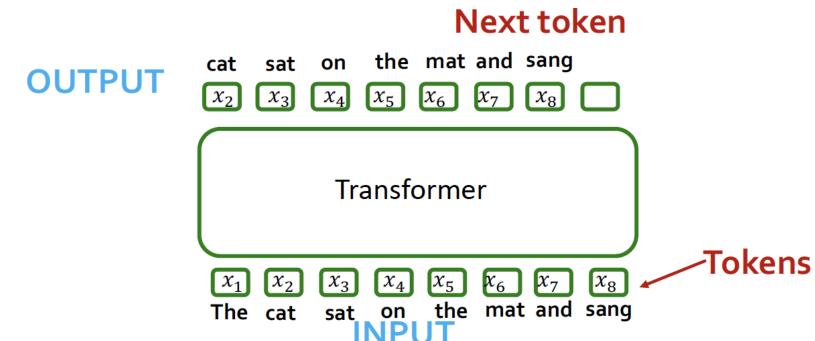
• Transformers map 1D sequences of vectors to 1D sequences of vectors



 g_{024} (6)

Transformer Ingest Tokens

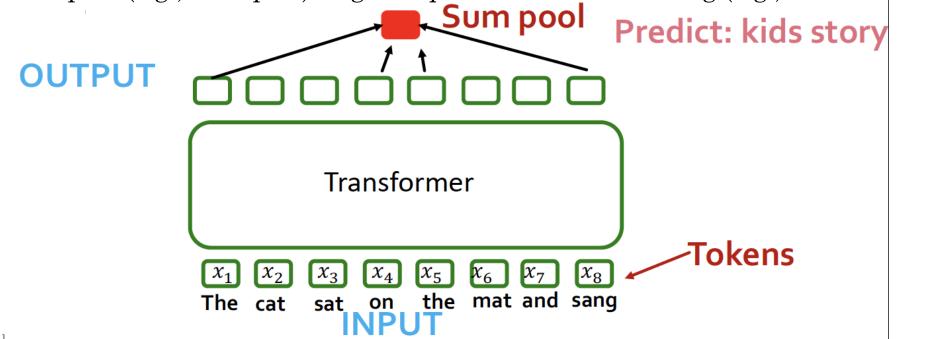
- Transformers map 1D sequences of vectors to 1D sequences of vectors
 - Tokens describe a "piece" of data e.g., a word
- What output sequence?
 - Option 1: next token => GPT



Thanh H. Nguy ... 10/15/2024

Transformer Ingest Tokens

- Transformers map 1D sequences of vectors to 1D sequences of vectors
 - Tokens describe a "piece" of data e.g., a word
- What output sequence?
 - Option 1: next token => GPT
 - Option 2:-pool (e.g., sum-pool) to get sequence level-embedding (e.g., for classification task)



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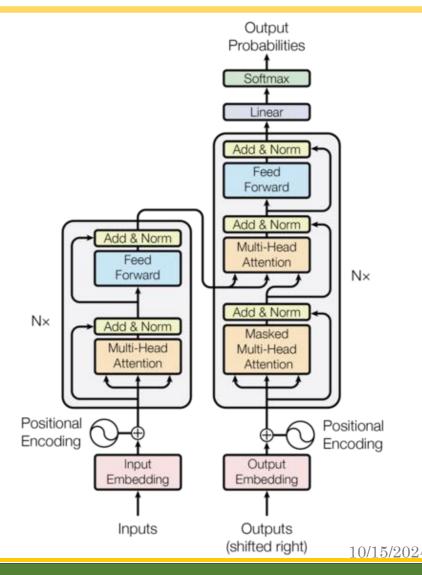
Thanh H. Ngu, ...

Transformer Blueprint

• How are tokens processed?

- Lots of components
 - Normalization
 - Feed forward networks
 - Positional encoding
 - Multi-head self-attention

• What does self-attention block do?



Intuition

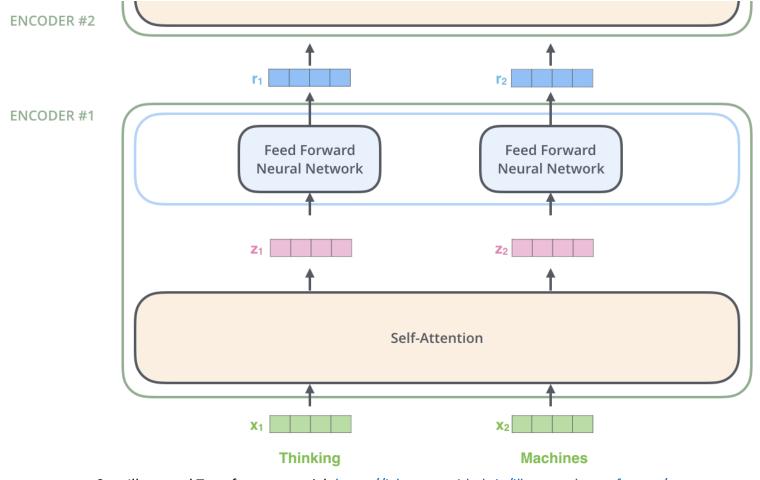
• As the model processes each word, self attention allows it to look at other positions in the input sequence for clues that can help lead to a better encoding for this word.

• Example:

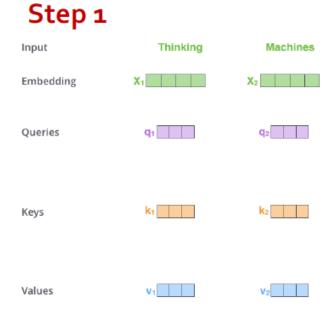
The animal didn't cross the street because it was too tired.

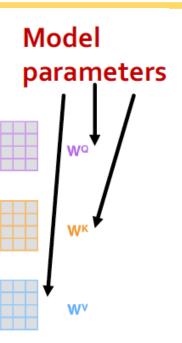
• When a model processes the word "it", self-attention allows it to associate "it" with "animal".

■ Before "multi-head" self-attention, what is "single head" self-attention?

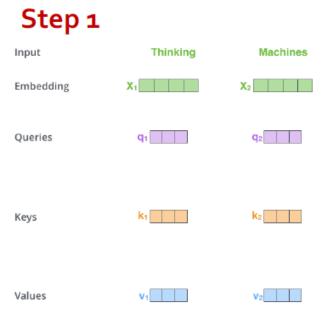


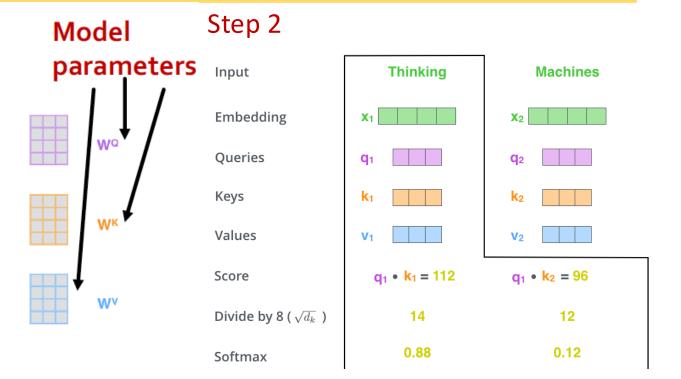
• Step 1: compute "key, value," query" for each input





- Step 1: compute "key, value, query" for each input
- Step 2 (just for x₁): compute scores between pairs, turn into probabilities (same for x₂)

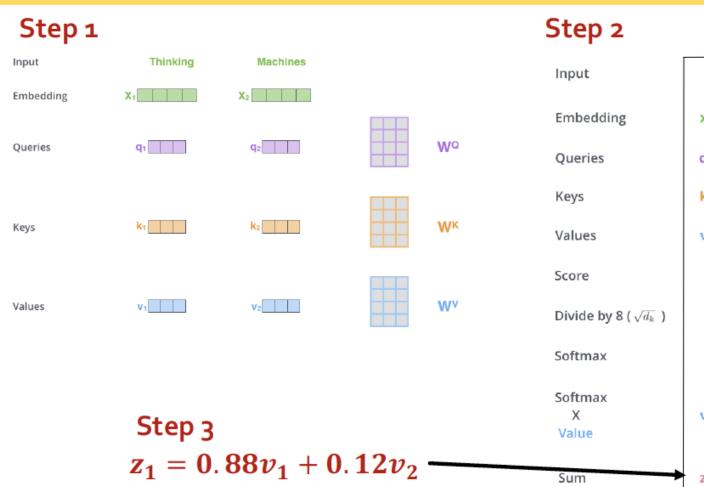


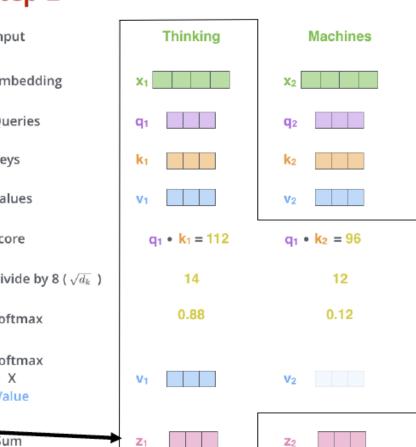


• Step 1: compute "key, value, query" for each input

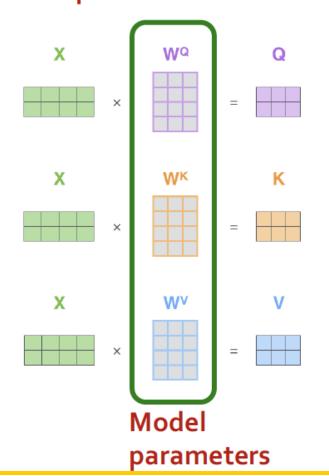
■ Step 2 (just for x_1): compute scores between pairs, turn into probabilities (same for x_2)

• Step 3: get new embedding z_1 by weighted sum of v_1, v_2





Same calculation in matrix formStep 1

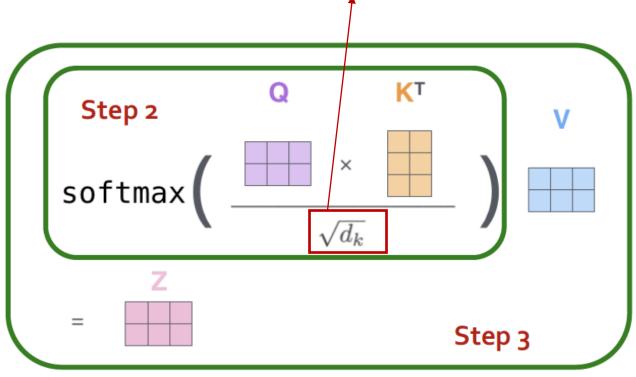


Large similarities will cause softmax to saturate and give vanishing gradients.

Recall a . b = |a||b| cos(angle)

Suppose that a and b are constant vectors of dimension D.

Then $|a| = (\sum_{i} a^{2})^{\frac{1}{2}} = a\sqrt{D}$



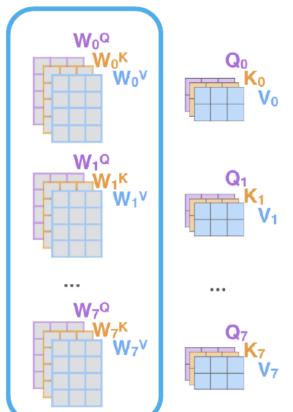
Multi-Head Self-Attention

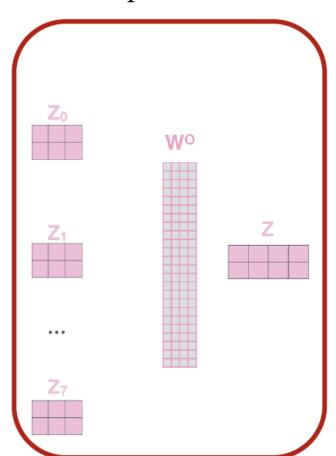
- Do many self-attentions in parallel, and combine
- Different heads can learn different "similarities" between inputs

Each has own set of parameters

Thinking Machines





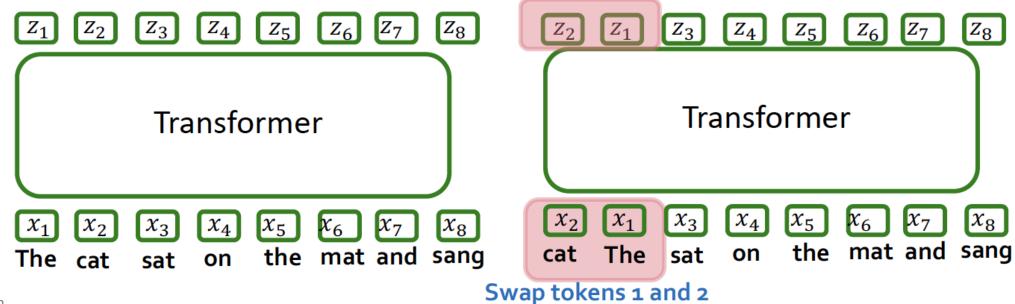




- First recall update formula: $z_1 = \sum_{j=1}^n softmax(q_1^T k_j)v_j$ Key Observation: order of tokens does not matter!!!

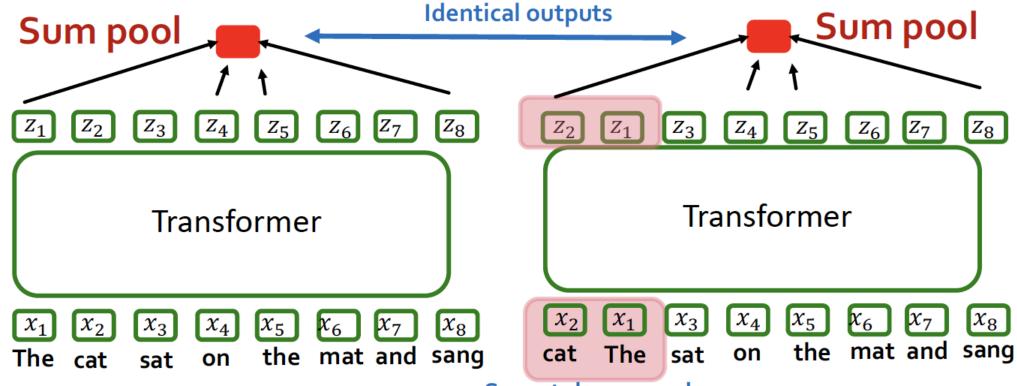


- First recall update formula: $z_1 = \sum_{j=1}^n softmax(q_1^T k_j)v_j$ Key Observation: order of tokens does not matter!!!



Outputs swap, but do not otherwise change

- This is a problem
- Same predictions no matter what order the words are in!
 - How to fix?

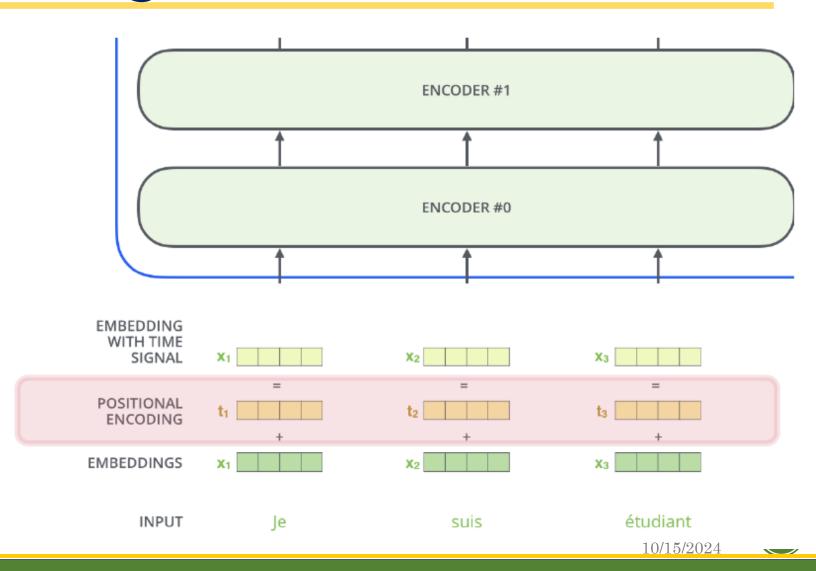


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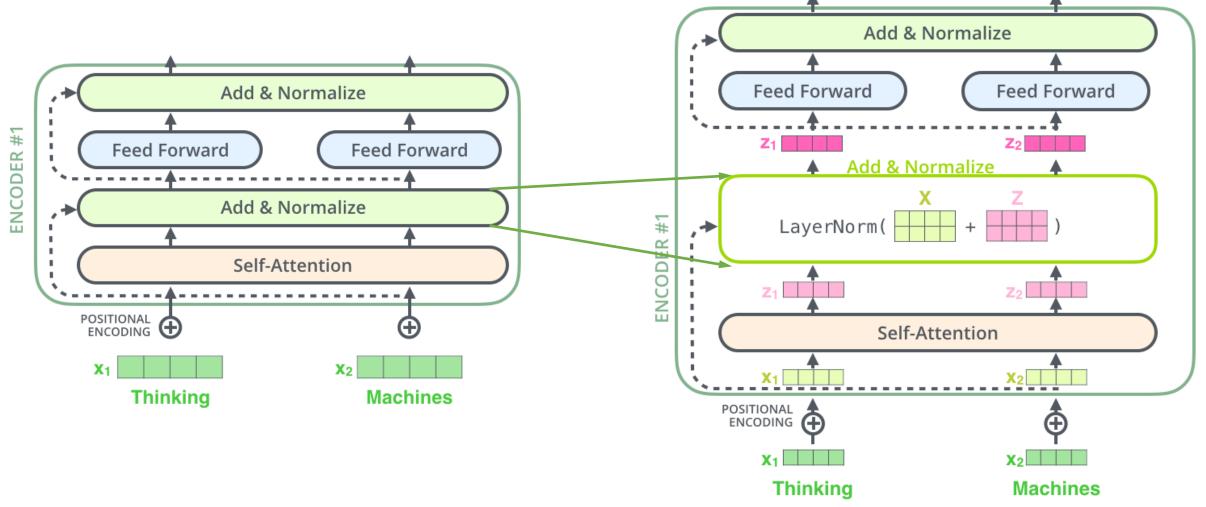
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Positional Encodings

- Transformer doesn't know order of inputs
- Extra positional features needed so it knows that
 - Je = word 1,
 - suis = word 2
 - etc.
- For NLP, positional encoding vectors are learnable parameters

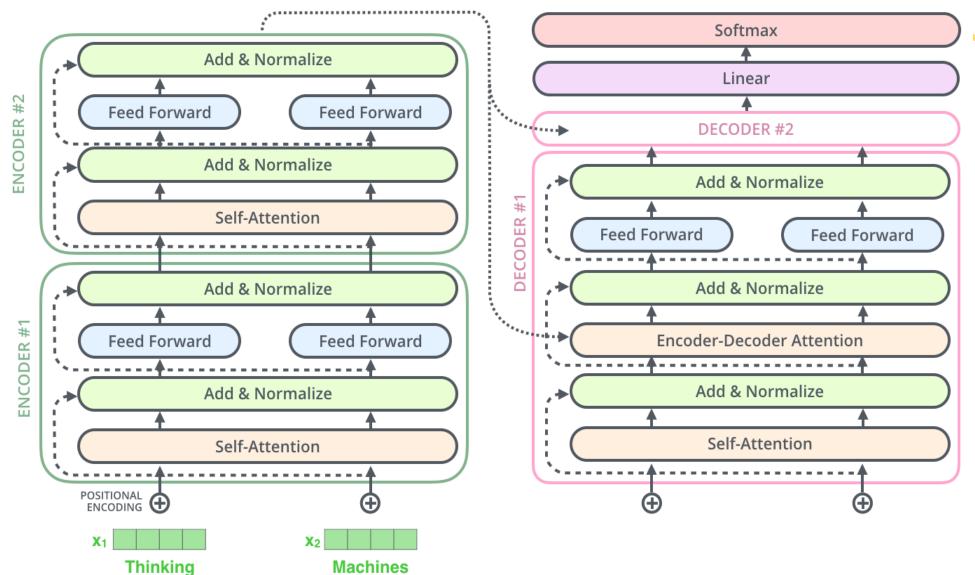


Residual Connection & Normalization

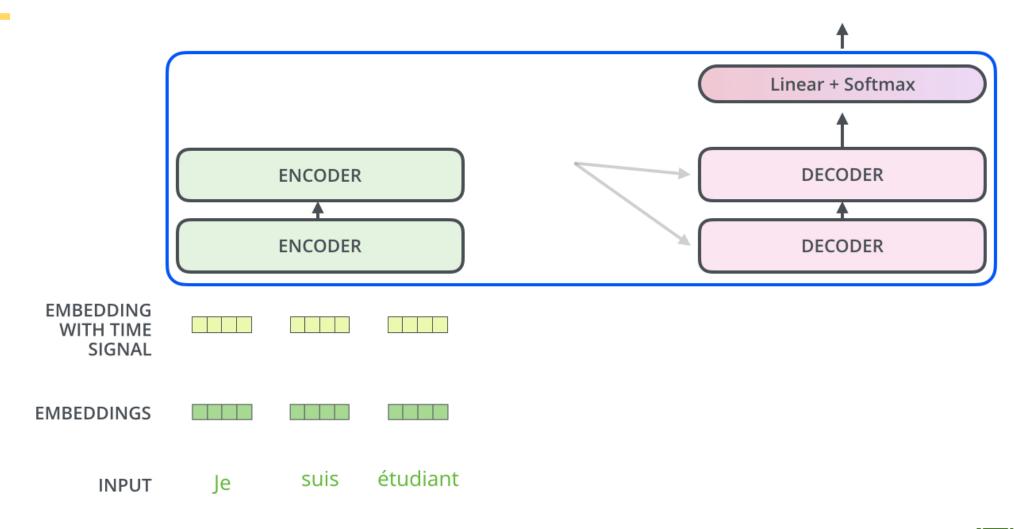


Transformer: Encoder

Transformer: Decoder



Decoder

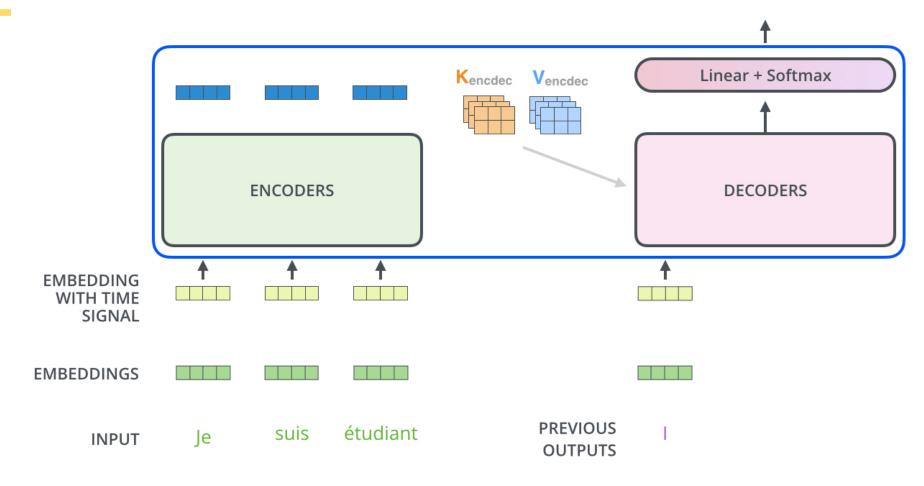


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Decoding time step: 1 2 3 4 5 6

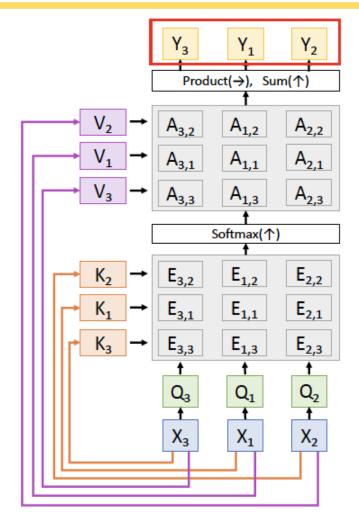
OUTPUT

Decodei

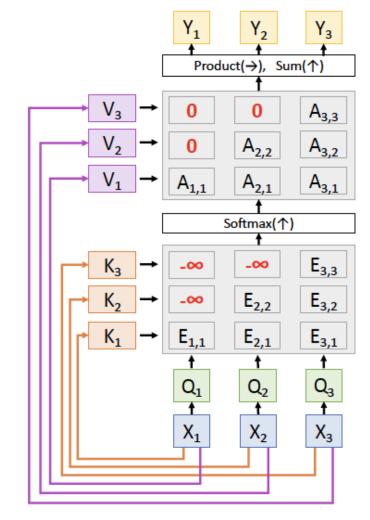




Decoder: Masked Self-Attention Layer





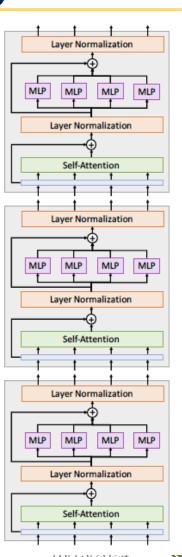


(26)

The Transformer: Transfer Learning

• "ImageNet Moment for Natural Language Processing"

- Pretraining:
 - Download a lot of text from the internet
 - Train a giant Transformer model for language modeling
- Finetuning:
 - Fine-tune the Transformer on your own NLP task



Scaling Up Transformers

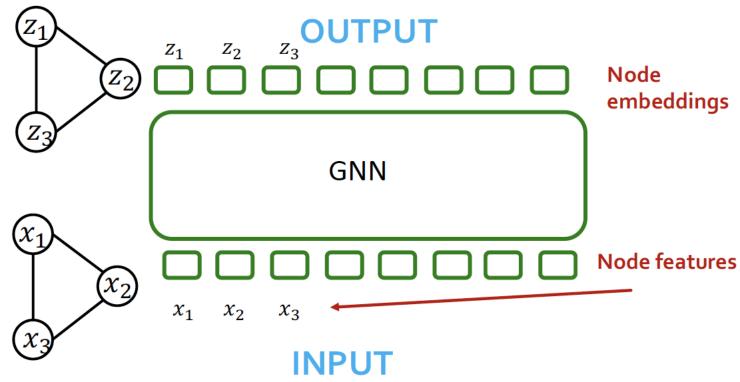
Model	Layers	Width	Heads	Params	Data	Training
Transformer-Base	12	512	8	65M		8x P100 (12 hours)
Transformer-Large	12	1024	16	213M		8x P100 (3.5 days)
BERT-Base	12	768	12	110M	13 GB	
BERT-Large	24	1024	16	340M	13 GB	
XLNet-Large	24	1024	16	~340M	126 GB	512x TPU-v3 (2.5 days)
RoBERTa	24	1024	16	355M	160 GB	1024x V100 GPU (1 day)
GPT-2	48	1600	?	1.5B	40 GB	
Megatron-LM	72	3072	32	8.3B	174 GB	512x V100 GPU (9 days)
Turing-NLG	78	4256	28	17B	?	256x V100 GPU
GPT-3	96	12,288	96	175B	694GB	?
Gopher	80	16,384	128	280B	10.55 TB	4096x TPUv3 (38 days)

Transformers for Graph Data



Comparing Transformers with GNN

- Similarity: GNNs also take in a sequence of vectors (in no particular order) and output a sequence of embeddings
- Difference: GNNs use message passing, Transformer uses self-attention

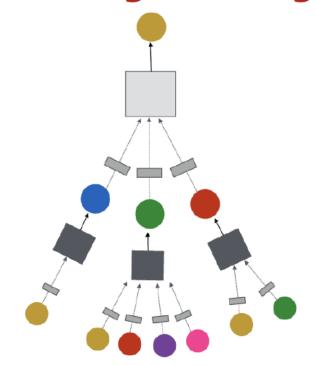


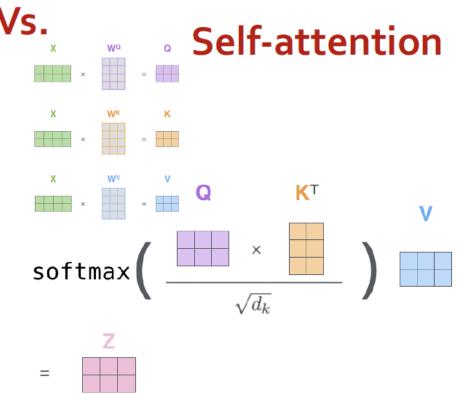
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Comparing Transformers with GNN

- Difference: GNNs use message passing, Transformer uses self-attention
- Are self-attention and message passing really different?

Message Passing





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Self-Attention versus Message Passing



Interpreting the Self-Attention Update

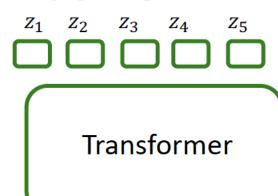
Recall formula for attention update

$$Att(X) = \operatorname{softmax}(K^{T}Q)V$$
$$= \operatorname{softmax}((XW^{K})^{T}(XW^{Q}))(XW^{V})$$

Input stored row-wise

$$X = [\cdots x_i \cdots]$$

OUTPUT





 x_1 x_2 x_3 x_4 x_5

Input tokens



Interpreting the Self-Attention Update

Recall formula for attention update

$$Att(X) = \operatorname{softmax}(K^{T}Q)V$$
$$= \operatorname{softmax}((XW^{K})^{T}(XW^{Q}))(XW^{V})$$

Input stored row-wise

$$X = [\cdots x_i \cdots]$$

- This formula gives the embedding for all tokens simultaneously
- What if we simplify to just token x_1 ?

$$z_1 = \sum_{j=1}^{5} softmax_j(q_1^T k_j)v_j$$
 How to interpret this?

- Steps for computing new embedding for token 1:
 - 1. Compute message from j: $MSG(x_j) = (v_j, k_j) = (W^V x_j, W^K x_j)$
 - 2. Compute query for 1: $q_1 = W^Q x_1$
 - 3. Aggregate all messages: $Agg(\{MSG(x_j):j\},q_1) = \sum_{j=1}^n softmax(q_1^Tk_j)v_j$

Self-Attention as Message Passing

- Takeaway: Self-attention can be written as message + aggregation i.e., it is a GNN!
- But so far there is no graph just tokens.
 - So what graph is this a GNN on?
- Clearly tokens = nodes, but what are the edges?
- Key observation:
 - Token 1 depends on (receives "messages" from) all other tokens
 - ➤ The graph is fully connected!
- Alternatively: if you only sum over $j \in N(i)$, you get \sim GAT

$$\frac{1}{\sum_{n=1}^{n} \operatorname{softmax}(a^{T}k)n}$$

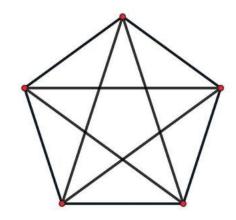
 $z_1 = \sum_{j=1}^{n} softmax(q_1^T k_j) v_j$

- Steps for computing new embedding for token 1:
 - 1. Compute message from j: $MSG(x_j) = (v_j, k_j) = (W^V x_j, W^K x_j)$
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 - 3. Aggregate all messages: $Agg(\{MSG(x_j):j\},q_1) = \sum_{j=1}^n softmax(q_1^Tk_j)v_j$



Self-Attention as Message Passing

- Takeaway 1: Self-attention is a special case of message passing
- Takeaway 2: It is message passing on the fully connected graph
- Takeaway 3: Given a graph *G*, if you constrain the self-attention softmax to only be over *j* adjacent to *i* nodes, you get ~GAT!



- Steps for computing new embedding for token 1:
 - 1. Compute message from j: $MSG(x_j) = (v_j, k_j) = (W^V x_j, W^K x_j)$
 - 2. Compute query for 1: $q_1 = W^Q x_1$
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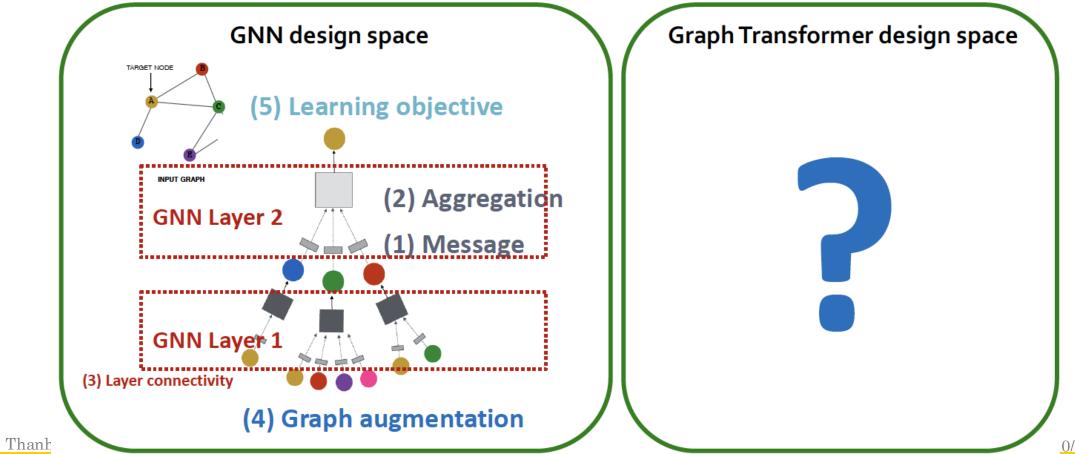


A New Design Landscape for Graph Transformer

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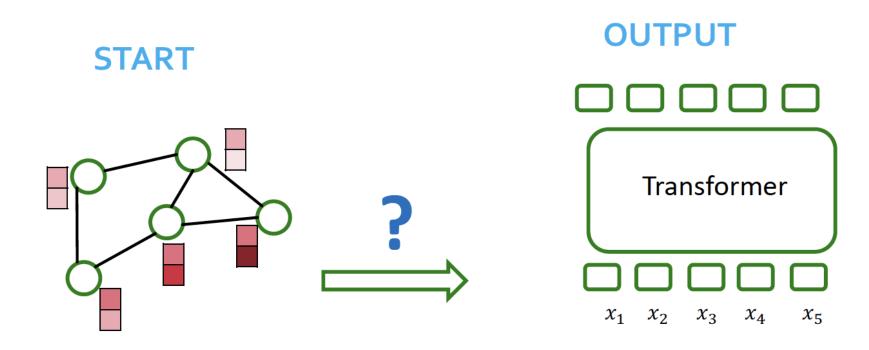
Recap: A General GNN Framework

- We know a lot about the design space of GNNs
- What does the corresponding design space for Graph Transformers look like?



Processing Graphs with Transformer

- We start with graph(s)
- How to input a graph into a Transformer?



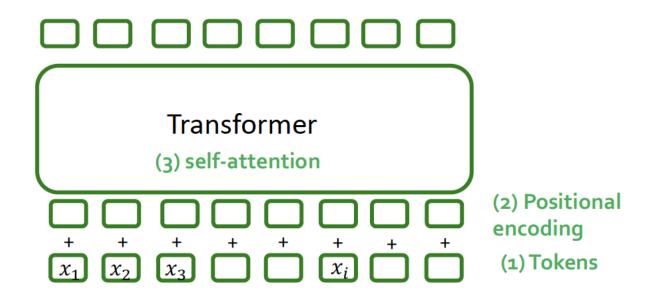
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Components of a Transformer

- Key components of Transformer
 - 1. tokenizing
 - 2. positional encoding
 - 3. self-attention

How to chose these for graph data?

• Key question: What should these be for a graph input?



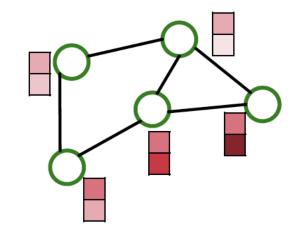
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Processing Graphs with Transformers

- A graph Transformer must take the following inputs:
 - 1. Node features?
 - 2. Adjacency information?
 - 3. Edge features?

- Key components of Transformer
 - 1. tokenizing
 - 2. positional encoding
 - 3. self-attention

- There are many ways to do this
- Different approaches correspond to different "matchings" between graph inputs (1), (2), (3) transformer components (1), (2), (3)



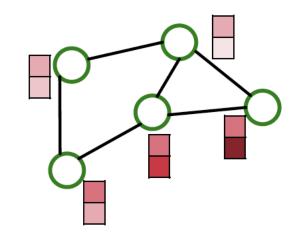
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Processing Graphs with Transformers

• A graph Transformer must take the following inputs:

- Key components of Transformer
- 1. Node features?

 1. tokenizing
- 2. Adjacency information? ← 2. positional encoding
- 3. Edge features? ← 3. self-attention Today
- There are many ways to do this
- Different approaches correspond to different "matchings" between graph inputs (1), (2), (3) transformer components (1), (2), (3)



Nodes as Tokens

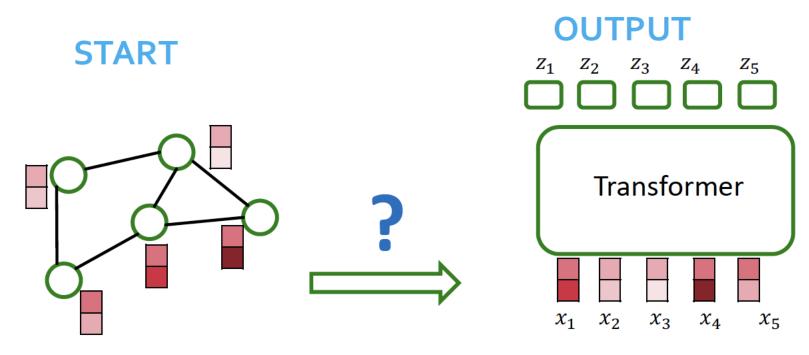
- Q1: what should our tokens be?
- Sensible Idea: node features = input tokens
- This matches the setting for the "attention is message passing on the fully connected graph" observation

(1) Input tokens = Node features

 $\left(43\right)$

Processing Graphs with Transformers

- Problem? We completely lose adjacency info!
- How to also inject adjacency information?

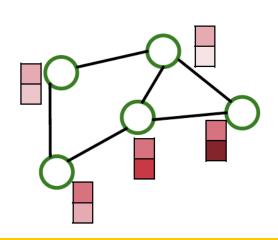


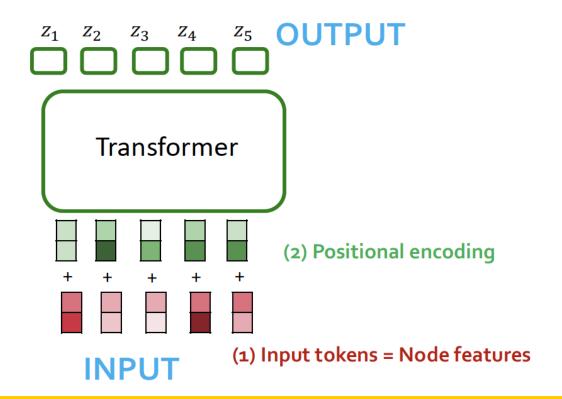
(1) Input tokens = Node features

How to Add Back Adjacency Info?

- Idea: Encode adjacency info in the positional encoding for each node
- Positional encoding describes where a node is in the graph

How to design a good positional encoding?

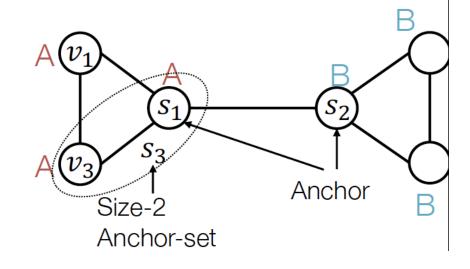




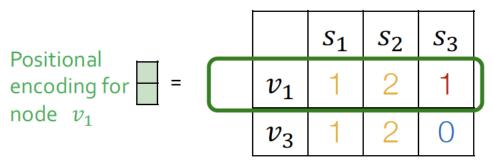
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Option 1: Relative Distances

- Last lecture: positional encoding based on relative distances
- Similar methods based on random walks
- This is a good idea! It works well in many cases
- Especially strong for tasks that require counting cycles



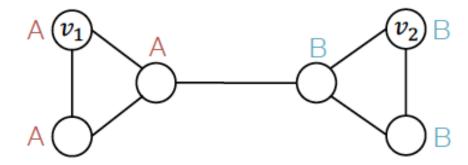
Relative Distances



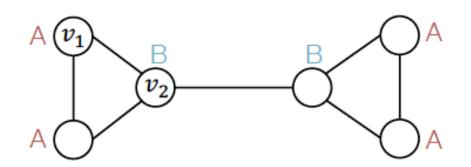
Anchor s_1 , s_2 cannot differentiate node v_1 , v_3 , but anchor-set s_3 can

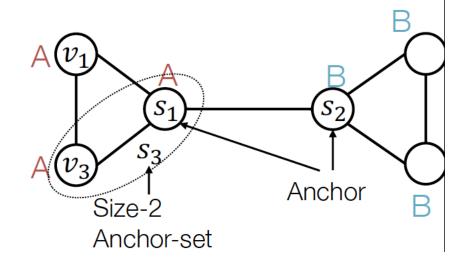
Option 1: Relative Distances

 Last lecture: Relative distances useful for position-aware task

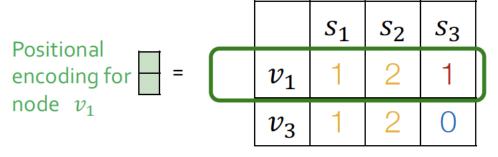


But not suited to structure-aware tasks





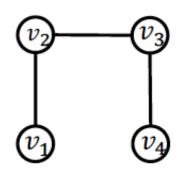
Relative Distances



Anchor s_1 , s_2 cannot differentiate node v_1 , v_3 , but anchor-set s_3 can

Option 2: Laplacian Eigenvector Positional Encodings

- What other ways to make positional encoding?
- Draw on knowledge of Graph Theory (many useful and powerful tools)
- Key object: Laplacian Matrix L = Degrees Adjacency
 - Each graph has its own Laplacian matrix
 - Laplacian encodes the graph structure
 - Several Laplacian variants that add degree information differently



L =

1	0	0	0
0	2	0	0
0	0	2	0
0	0	0	1

Degree of each node

0	1	0	0
1	0	1	0
0	1	0	1
0	0	1	0

Adjacency

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Laplacian Eigenvector Positional Encodings

- Laplacian matrix captures graph structure
- Its eigenvectors inherit this structure
- This is important because eigenvectors are vectors (!) and so can be fed into a Transformer

• Eigenvectors with small eigenvalue = local structure, large eigenvalue

= global symmetries

Refresher

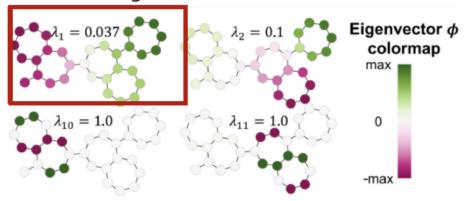
Eigenvector: v such that $Lv = \lambda v$

 $L: n \times n$ matrix

v: n dimensional vector

 λ : Scalar eigenvalue

Visualize one eigenvector

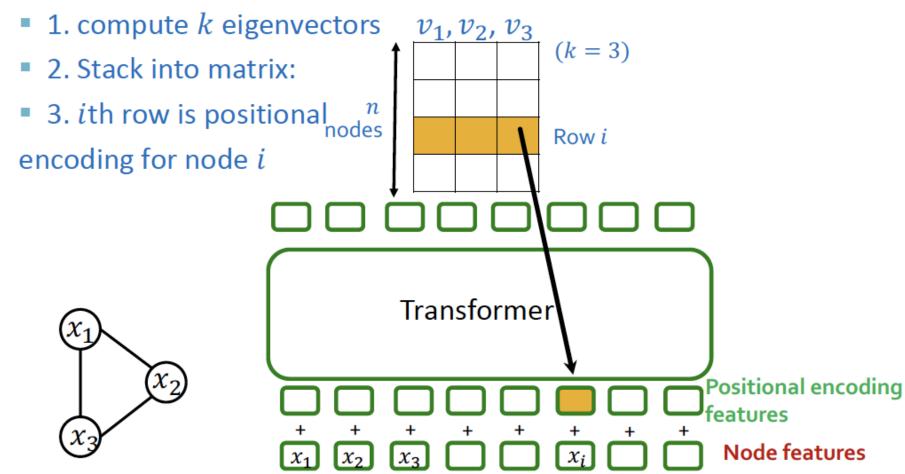


(Figure from Kreuzer* and Beaini* et al. 2021)



Laplacian Eigenvector Positional Encodings

Positional encoding steps:



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Summary: Laplacian Eigenvector Positional Encodings

- Laplacian Matrix L = Degrees Adjacency

 Eigenvector: v such that $Lv = \lambda v$ Positional encoding steps:

 1. compute k eigenvectors

 2. Stack into matrix:

 3. ith row is positional encoding for node i• NPUT
 - Laplacian Eigenvector positional encodings can also be used with message-passing GNNs
 - This helps for same reasons as relative-distance based positional encodings in previous lecture

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Laplacian Eigenvectors in Practice

- Task: given a graph, predict YES if it has a cycle, NO otherwise
- Recall, message-passing cannot solve this task!
- "PE" indicates using Laplacian Eigenvector Pos. Enc.

Train s	$ ext{samples} ightarrow$	200	500	1000	5000
$\mathbf{Model} \; \big \; L \; \big \; \# \mathbf{Param} \; \big $		Test Acc \pm s.d.			
GIN 4	100774	70.585 ± 0.636	74.995 ± 1.226	$\begin{array}{c c} 78.083 \pm 1.083 \\ 97.998 \pm 0.300 \end{array}$	86.130±1.140
GIN-PE 4	102864	86.720 ± 3.376	95.960±0.393		99.570±0.089
GatedGCN 4	103933	50.000 ± 0.000	50.000 ± 0.000	50.000 ± 0.000	50.000±0.000
GatedGCN-PE 4	105263	95.082 ± 0.346	96.700 ± 0.381	98.230 ± 0.473	99.725±0.027

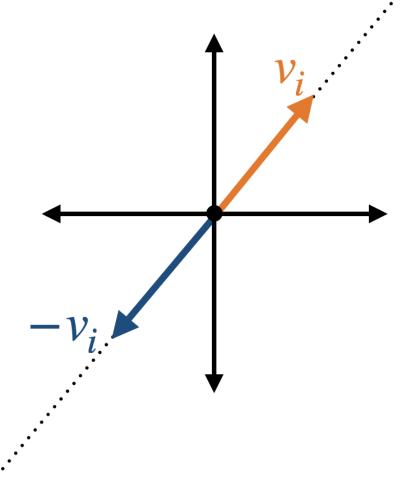
Laplacian Eigenvector Positional Encodings

- Laplacian Eigenvector positional encodings work!
- But is this the best we can do?
 - Hint: no
- Q: What is the problem with the current approach?
 - A1: Eigenvectors are not arbitrary vectors
 - A2: They have special structure that we have been ignoring!
- To use eigenvectors properly we must account for their structure in our models



Eigenvector Sign Ambiguity

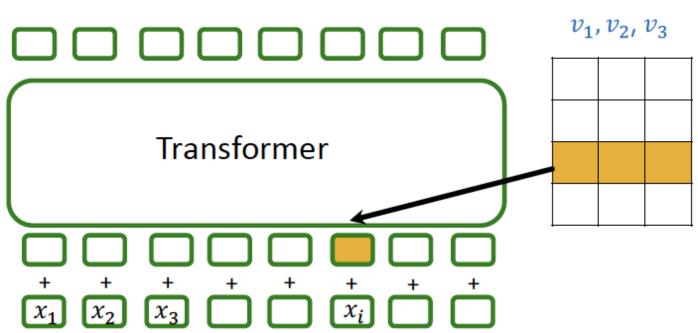
- Suppose v is a Laplacian eigenvector
 - So $Lv = \lambda v$
- But this means:
 - Also $L(-v) = \lambda(-v)$
- So -v is also a Laplacian eigenvector
- The choice of sign is arbitrary!



Sign Ambiguity is a Problem

- Both
- But when we use them as positional encodings we pick one arbitrarily
- Why does this matter for positional encodings?

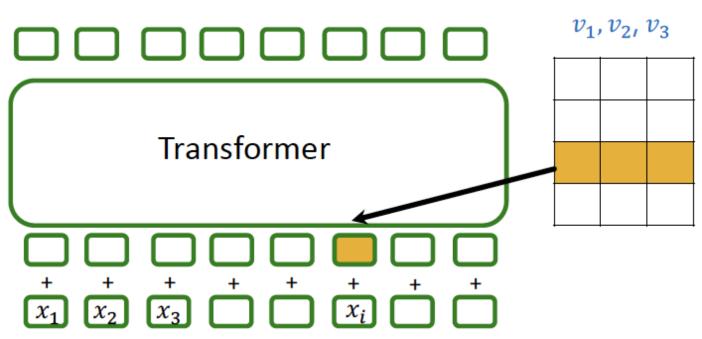
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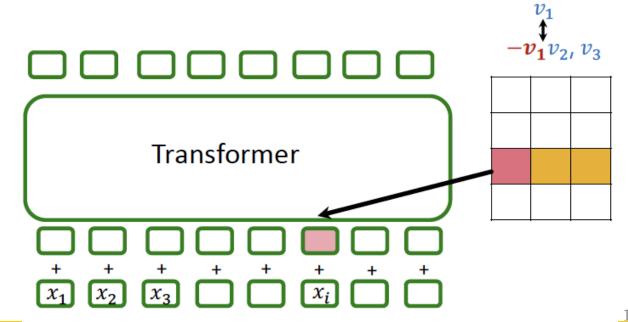
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Sign Ambiguity is a Problem

- What if we picked the other sign choice?
- Then the input PE changes
- •=> The models predictions will change!
- For k eigenvectors there are 2^k sign choices

2^k different predictions for the same input graph!



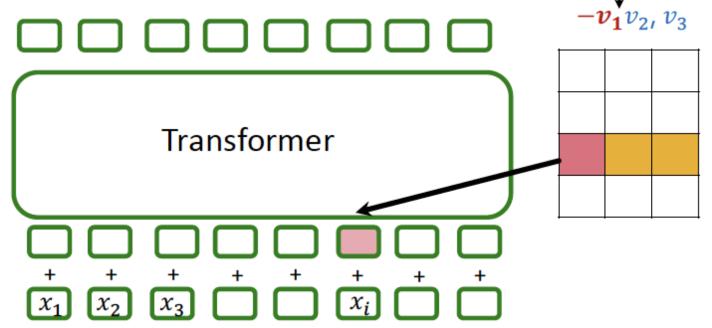
How to Fix Sign Ambiguity

- Simple Idea: randomly flip the signs of eigenvectors during training
 - I.e., data augmentation
 - Model will learn to not use the sign information
 - Issue: exponentially many sign choices is very difficult to learn

How to Fix Sign Ambiguity

• Better Idea: build a neural network that is invariant to sign choices!

•Since it is invariant, the predictions will no longer depend on the sign choice v_1



- Goal: design a neural network $f(v_1, v_2, ... v_k)$ such that:
 - $f(v_1, v_2, ... v_k) = f(\pm v_1, \pm v_2, ... \pm v_k)$ for all \pm choices
 - f is "expressive": note that $f(v_1, v_2, ... v_k) = 0$ is sign invariant... but it's a terrible neural network architecture
- Warmup: one eigenvector
 - What about $f(v_1)$ such that $f(v_1) = f(-v_1)$?

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- Warmup: one eigenvector
- Goal: design a neural network $f(v_1)$ such that $f(v_1) = f(-v_1)$
- Proposition: f satisfies $f(v_1) = f(-v_1)$ if and only if there is a ϕ such that $f(v_1) = \phi(v_1) + \phi(-v_1)$

- Warmup: one eigenvector
- •Goal: design a sign invariant neural network $f(v_1, v_2, ... v_k)$ in two steps:
 - Step 1: sign invariant $f_i(v_i)$ for each i
 - Step 2: COMBINE individual eigenvector embeddings into one:

$$f(v_1, v_2, ... v_k) = AGG(f_1(v_1), ..., f_k(v_k))$$

5/2024 (62)

- Warmup: one eigenvector
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Use model for one eigenvector

$$f(v_1,v_2,\dots v_k)\\ = AGG(\phi_1(v_1),+\phi_1(-v_1),\dots,\phi_k(v_k),+\phi_k(-v_k))\\ \text{Combine using another neural net } AGG = \rho$$



•Overall model:

$$f(v_1, v_2, \dots, v_k) = \rho((\phi_1(v_1), +\phi_1(-v_1), \dots, \phi_k(v_k), +\phi_k(-v_k))$$

- Introducing *k* distinct neural nets is costly...
- Let's minimize extra parameters by sharing one ϕ

```
f(v_1, v_2, ... v_k)
= \rho(\phi(v_1), +\phi(-v_1), ..., \phi(v_k), +\phi(-v_k))
\rho, \phi = \text{any neural network}
(MLP, GNN etc.)
```



- Recall Goal: design a neural network $f(v_1, v_2, ... v_k)$ such that:
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 - SignNet is sign invariant.
 - f is "expressive"
 - Is SignNet expressive?

$$f(v_1, v_2, ... v_k)$$

= $\rho(\phi(v_1), +\phi(-v_1), ..., \phi(v_k), +\phi(-v_k))$
 ρ, ϕ = any neural network SignNet (MLP, GNN etc.)

10/15/2024 65

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 - SignNet is sign invariant.
 - f is "expressive"
 - Is SignNet expressive?

Theorem: if f is sign invariant, then there exist functions ρ , ϕ such that

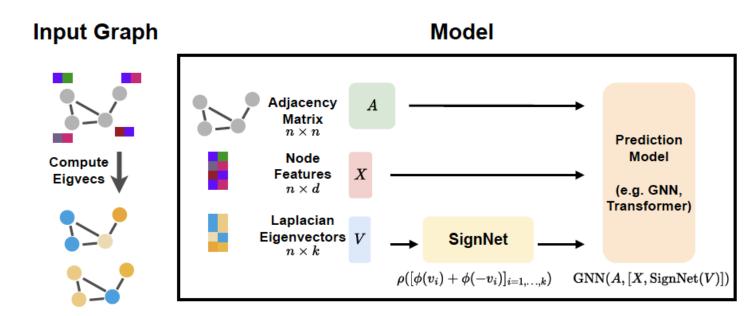
$$\begin{split} f(v_1, v_2, \dots v_k) \\ &= \rho(\phi(v_1), +\phi(-v_1), \dots, \phi(v_k), +\phi(-v_k)) \end{split}$$

SignNet can express all sign invariant functions!!

10/15/2024 (66)

SignNet in Practice

- How to use SignNet in practice?
 - Step 1: Compute eigenvectors
 - Step 2: get eigenvector embeddings using SignNet
 - Step 3: concatenate SignNet embeddings with node features X
 - Step 4: pass through main GNN/Transformer as usual.
 - Step 5: Backpropagate gradients to train SignNet + Prediction model jointly.



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Processing Graphs with Transformers

A graph Transformer must take the following inputs:

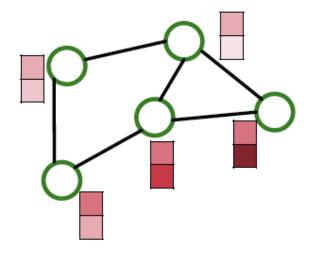
Key components of Transformer

```
    (1) Node features?
    (2) Adjacency information?
    (3) self-attention
```

• (3) Edge features?

So far

- There are many ways to do this
- Different approaches correspond to different "matchings" between graph inputs (1), (2),
 (3) transformer components (1), (2), (3)



Processing Graphs with Transformers

A graph Transformer must take the following inputs:

Key components of Transformer

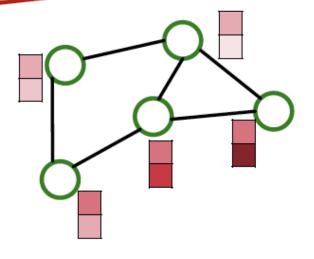
■ (1) Node features?

(2) Adjacency information?

- (3) Edge features?

Left to do

- There are many ways to do this
- Different approaches correspond to different "matchings" between graph inputs (1), (2),
 (3) transformer components (1), (2), (3)



(1) tokenizing

(3) self-attention

(2) positional encoding

Edge Features in Self-Attention

- Not clear how to add edge features in the tokens or positional encoding
- How about in the attention? $Att(X) = softmax(K^TQ)V$
- $[k_{ij}] = K^T Q$ is an n x n matrix. Entry k_{ij} describes "how much" token j contributes to the update of token i

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Implementation:

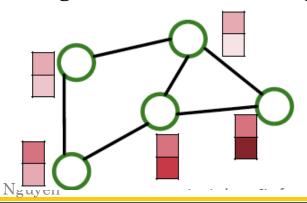
Learned parameters w₁

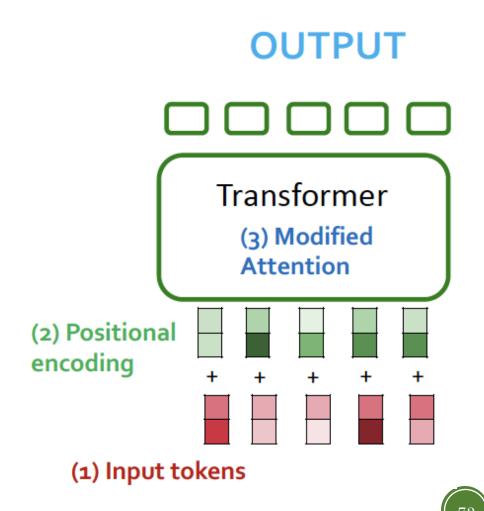
- If there is an edge between i and j with features e_{ij} , define $c_{ij} = w_1^T e_{ij}$
- If there is no edge, find shortest edge path between i and j $\left(e^{1},e^{2},...e^{N}\right)$ and define $c_{ij}=\sum_{n}w_{n}^{T}e^{n}$

Learned parameters w_1, \dots, w_N

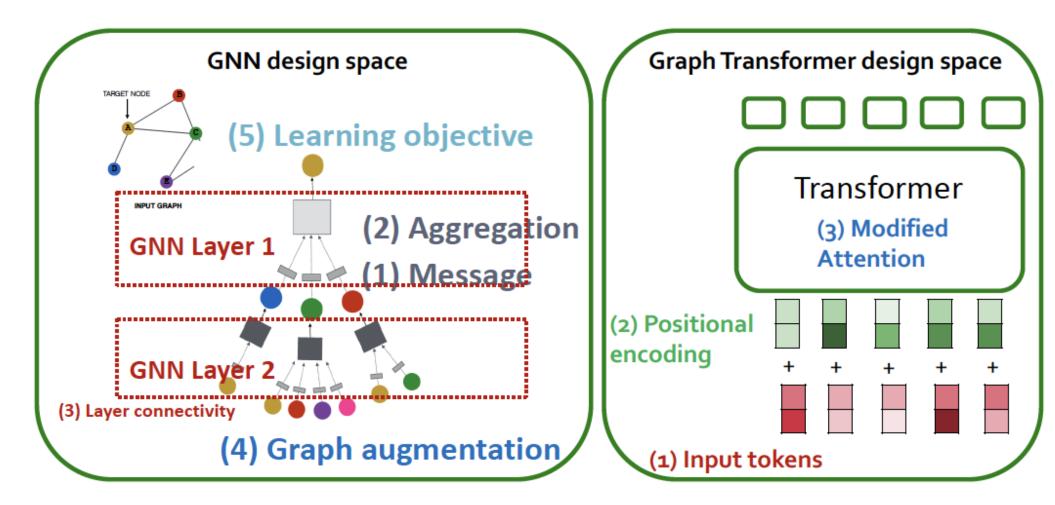
Summary: Graph Transformer Design Space

- (1) Tokenization
 - Usually node features
 - Other options, such as subgraphs, and node + edge features (not discussed today)
- (2) Positional Encoding
 - Relative distances, or Laplacian eigenvectors
 - Gives Transformer adjacency structure of graph
- (3) Modified Attention
 - Reweight attention using edge features





Summary: Graph Transformer Design Space



Class Project



List of Project Proposals (23 Students?)

- 1. Le Xuan Nam, Do Ngoc Trung. "Substructure-substructure interactions for drug-drug interaction prediction".
- 2. Dao Phan Khai, Dang Quang Thang, Nguyen Doan Hieu. "A Graph-based Approach for Android Malware Detection".
- 3. Le Ngoc Lam, Dao Duc Manh. "Completing a Temporal Knowledge Base Graph on Diachronic Entity Embedding and Applications".
- 4. Philippe Dufresne. "Application of Graph Neural Networks in Media Content Recommendation Systems".
- 5. Tran Tien Bang, Nguyen Duc Manh. "Recommender Systems".
- 6. Nguyen Tieu Anh. "Friend Recommendation".
- 7. Do Hoang Dung, Nguyen Thanh Son. "Stock Price Prediction".
- 8. Tong Ngoc Anh, Phung Thu Hang. "Book Recommendation System with Graph-Based Models".
- 9. Tran Xuan Tung. "Graph Neural Network For Receipt Information Extraction".
- 10. Uvin Wijesinghe. "Enhancing Temporal Relational Graph Neural Networks for Stock Prediction".
- 11. Nguyen Tuan Dung, Nguyen Minh Chau. "Temporal Health Event Prediction with Dynamic Disease Graphs Modelling".
- 12. Dao Minh Tuan, Nguyen Danh Phuc. "Recommender Systems".
- 13. Vu Duc Anh, Nguyen Duc Manh. "Applying Collaborative Filtering Graph Neural Network (CF-GNN) for recommender system of video social media platforms".



Class Projects: Components

- Project proposal (10%)
 - Deadline: has already passed
- Project report (60%)
 - Deadline: October 21st, 2024.

- Project presentation (20%)
 - Tuesdays, October 22nd and October 29th.

Class Projects: Project report

- Writing (40 points): 10-15 pages
 - Motivation & explanation of data/task (9 points)
 - Appropriateness & explanation of model(s) (9 points)
 - Insights + results (9 points)
 - Figures (9 points)
 - Code snippets (4 points)
- Submission:
 - Format: NeurIPS2024 LaTeX style
 - Message me the file on the class Slack channel.
- Colab (20 points)
 - Code: correctness, design (10 points)
 - Documentation: class/function descriptions, comments in code (10 points)



Class Projects: Project presentation

Present at class with Q&A

- Time:
 - Group of 1 student: 15-20 minutes
 - Group of 2 students: 25 minutes
 - Group of 3 students: 30 minutes

(79)