Stanford CS224W: Graph Transformers

CS224W: Machine Learning with Graphs

Joshua Robinson, Stanford University

http://cs224w.stanford.edu

Announcements

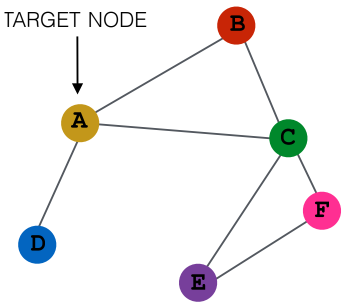
- **Homework 3** due this Thursday
  - Late submissions accepted until end of day Monday, 11/20
- **Regrade request deadlines**
  - **Homework 2**: Saturday, 11/18
    - Solutions and statistics released on Ed

Announcements

- **Thanksgivings office hours**
  - Wednesday, 11/22
    - 2pm-4pm, Thorton Center 207
    - **Also on Zoom** (link found under the Office Hours tab on the course website)
- **We are collecting feedback at https://tinyurl.com/cs224w-feedback**

J. You, R. Ying, J. Leskovec. Design Space of Graph Neural Networks, NeurIPS 2020c

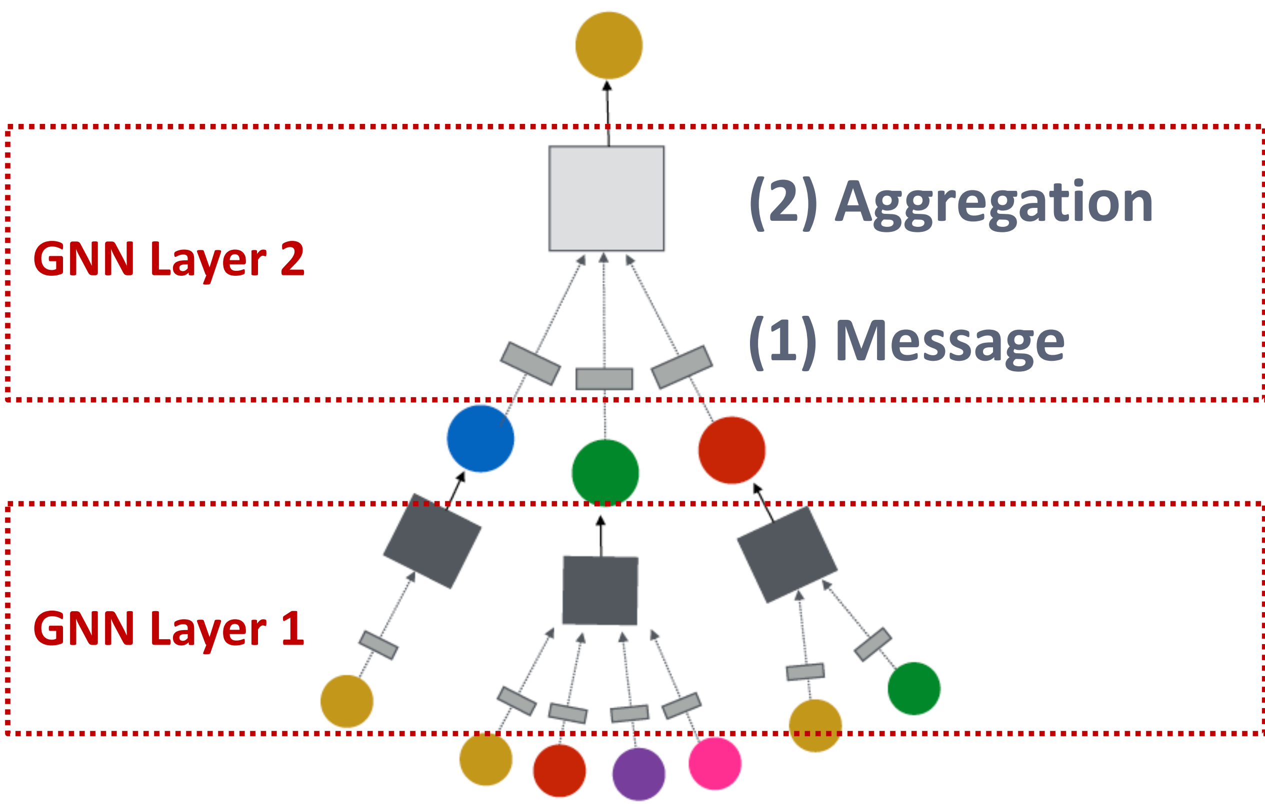
Recap: A General GNN Framework



INPUT GRAPH

(5) Learning objective

(3) Layer connectivity



(4) Graph augmentation

Stanford CS224W: Intro to Transformers

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The Backbone of Generative AI

FL I want to make Mac'n'Cheese without any dairy products. Do you have a recipe?

Yes, you can make a delicious dairy-free mac and cheese using a few simple ingredients. Here's what you'll need:

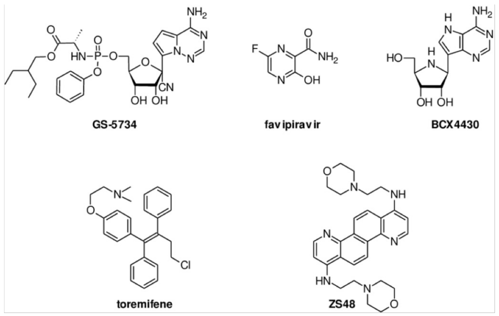
- 1 pound of elbow macaroni
- 2 cups of unsweetened almond milk
- 1/2 cup of nutritional yeast
- 1 tablespoon of cornstarch
- 1 tablespoon of Dijon mustard
- 1 teaspoon of salt
- 1/2 teaspoon of garlic powder
- 1/4 teaspoon of turmeric (for color)
- 1/4 teaspoon of paprika
- 1/4 teaspoon of black pepper
- 1/4 cup of vegan butter

To make the sauce, heat the almond milk in a saucepan over medium heat. In a separate bowl, whisk together the nutritional yeast, cornstarch, mustard, salt, garlic powder, turmeric, paprika, and black pepper. Add the dry ingredients to the saucepan with the almond milk and whisk until combined. Cook the sauce until it thickens, stirring frequently.

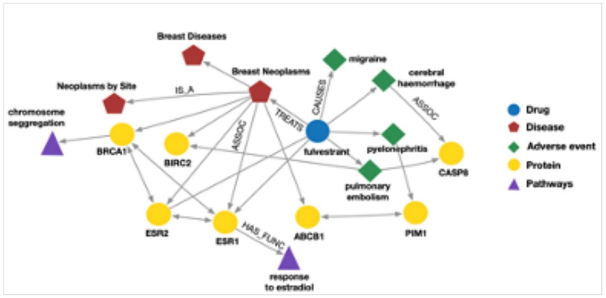
Meanwhile, cook the elbow macaroni according to the package instructions. When the pasta is cooked, drain it and return it to the pot. Add the sauce and the vegan butter to the pot with the pasta and stir until the pasta is well coated. Serve the mac and cheese immediately.

I hope you enjoy this dairy-free mac and cheese!

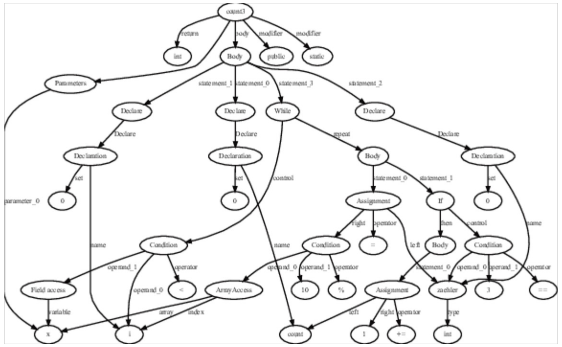
Goal: Bring Power of Transformers to Graphs



Small molecules



Knowledge graphs



Code graphs

Image credit: ResearchGate

Communication networks

Image credit: Lumen Learning

x

- **There is lots of multi-billon node/graph scale data to learn from**

Plan for Today

- **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

Stanford CS224W: Transformers

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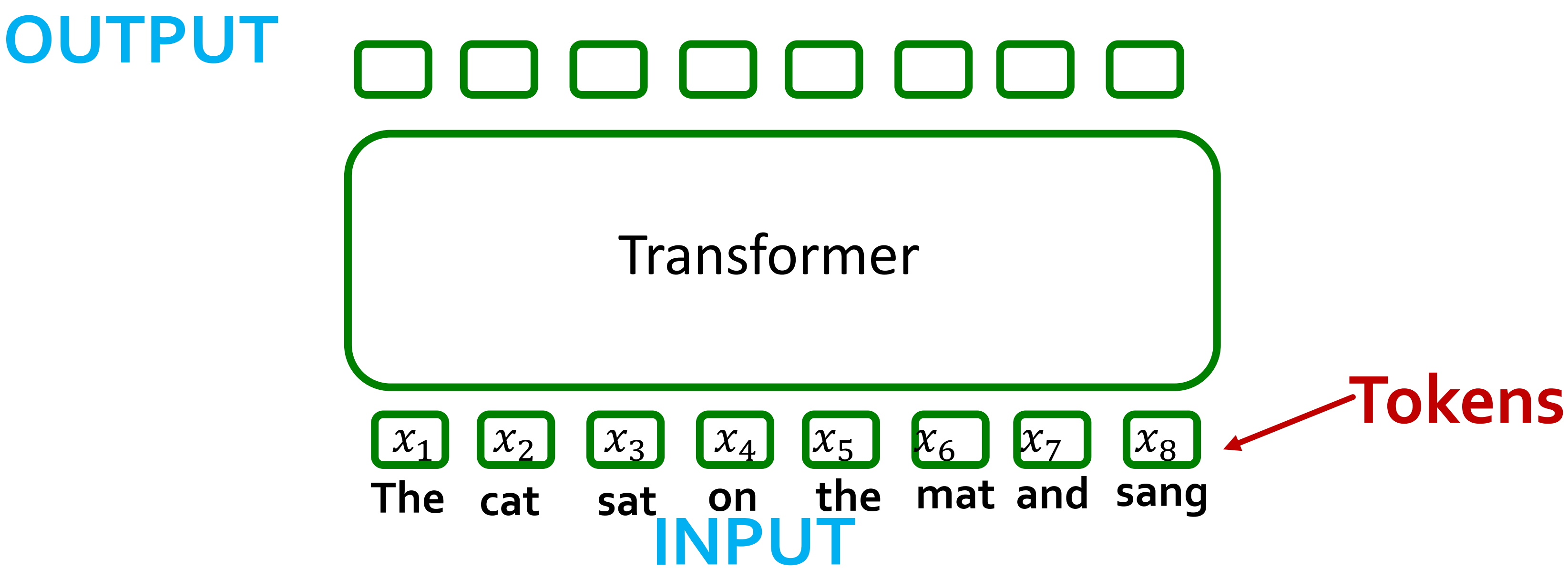
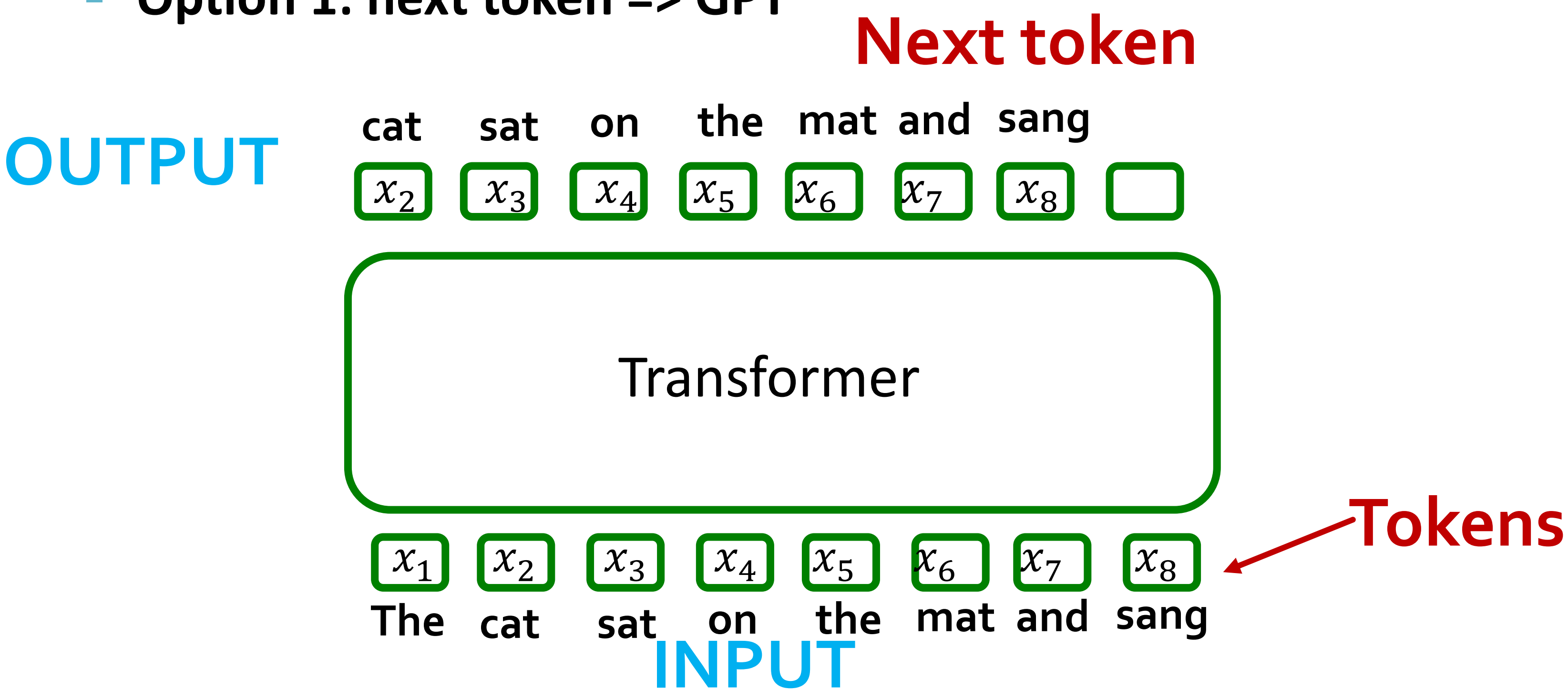
Transformers Ingest Tokens

- **Transformers map 1D sequences of vectors to 1D sequences of vectors**



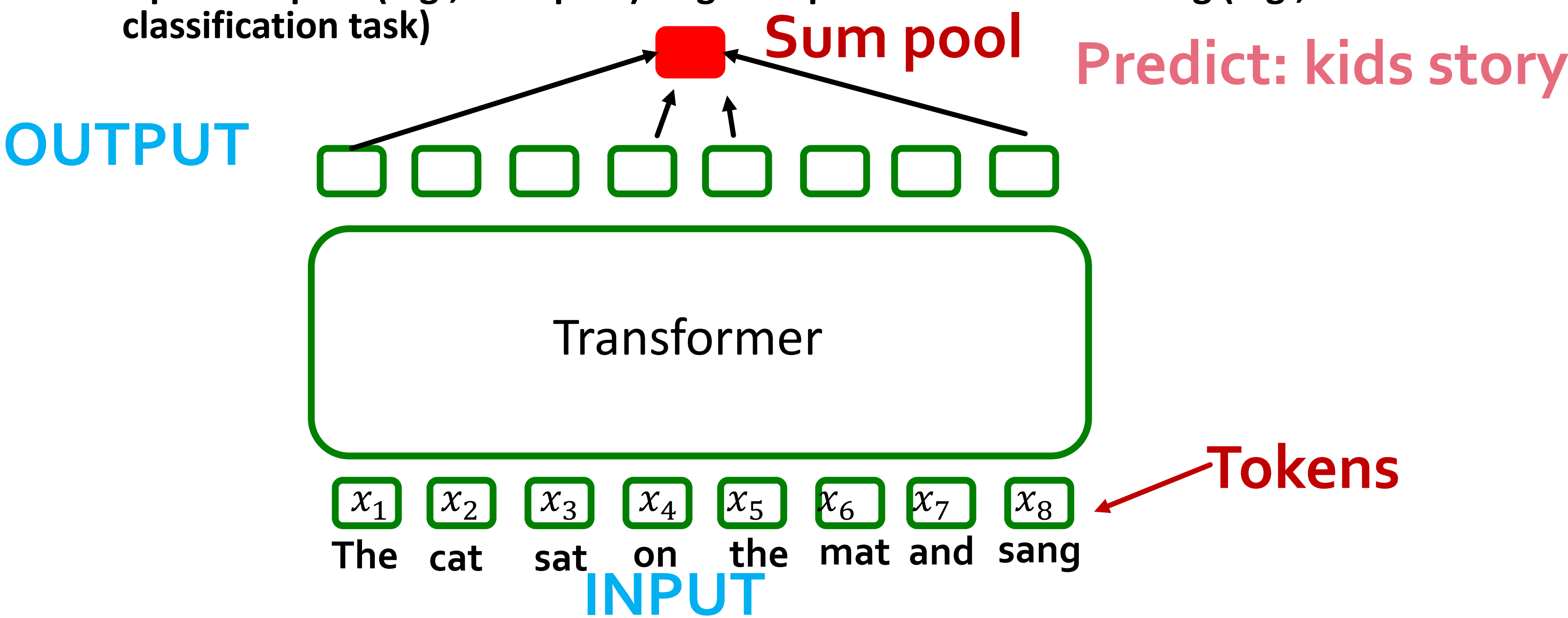
Transformers Ingest Tokens

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



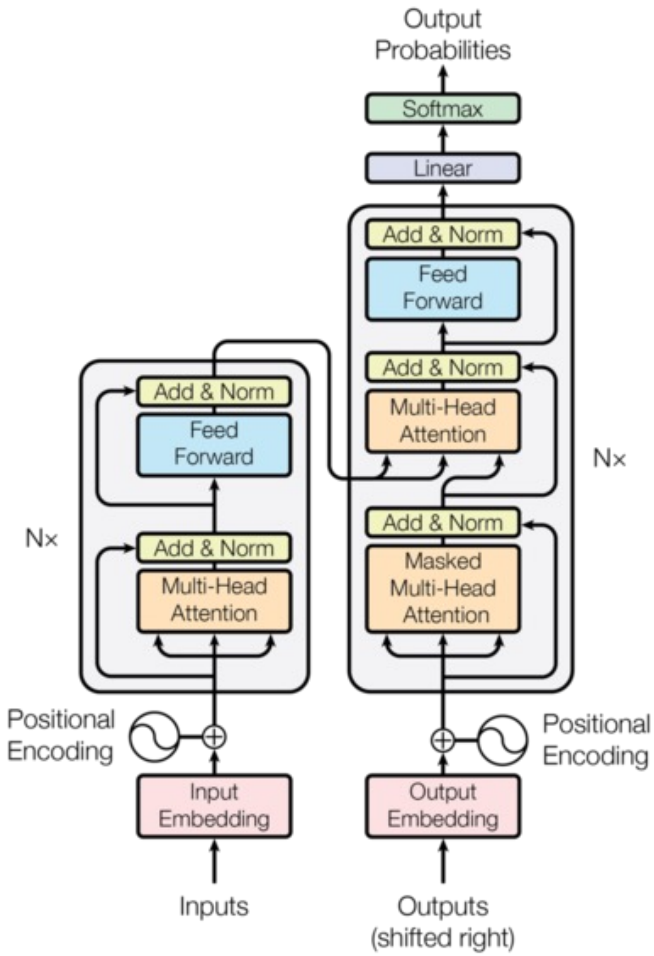
Transformers Ingest Tokens

- Transformers map 1D sequences of vectors to 1D sequences of vectors known as tokens
  - 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)



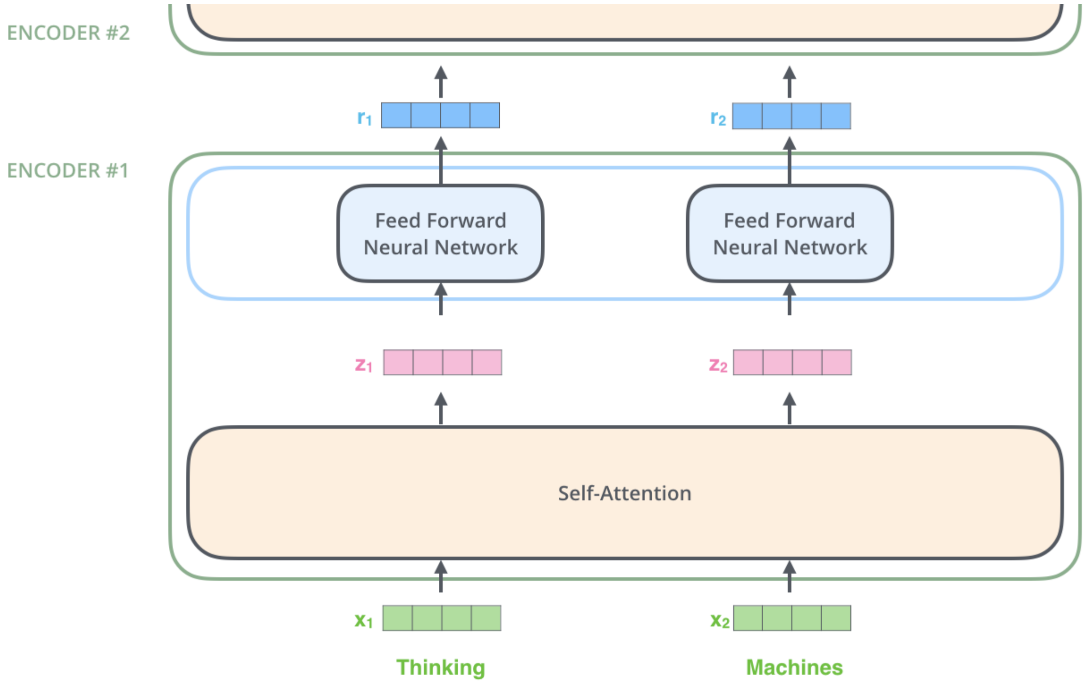
Transformer Blueprint

- **How are tokens processed?**
- **Lots of components**
  - **Normalization**
  - **Feed forward networks**
  - **Positional encoding (more later)**
  - **Multi-head self-attention**
- **What does self-attention block do?**



Self-attention

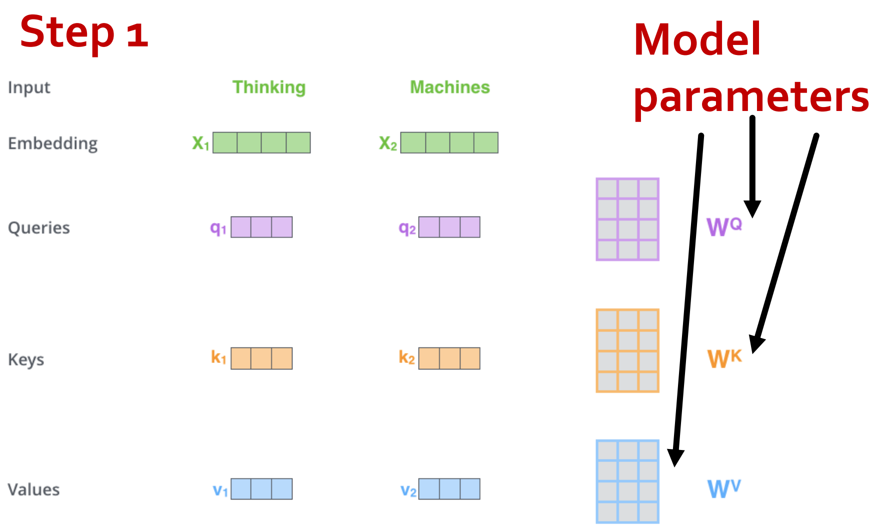
- **Before "multi-head" self-attention, what is "single head" self-attention?**



See: Illustrated Transformer tutorial, https://jalammar.github.io/illustrated-transformer/

Self-attention

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



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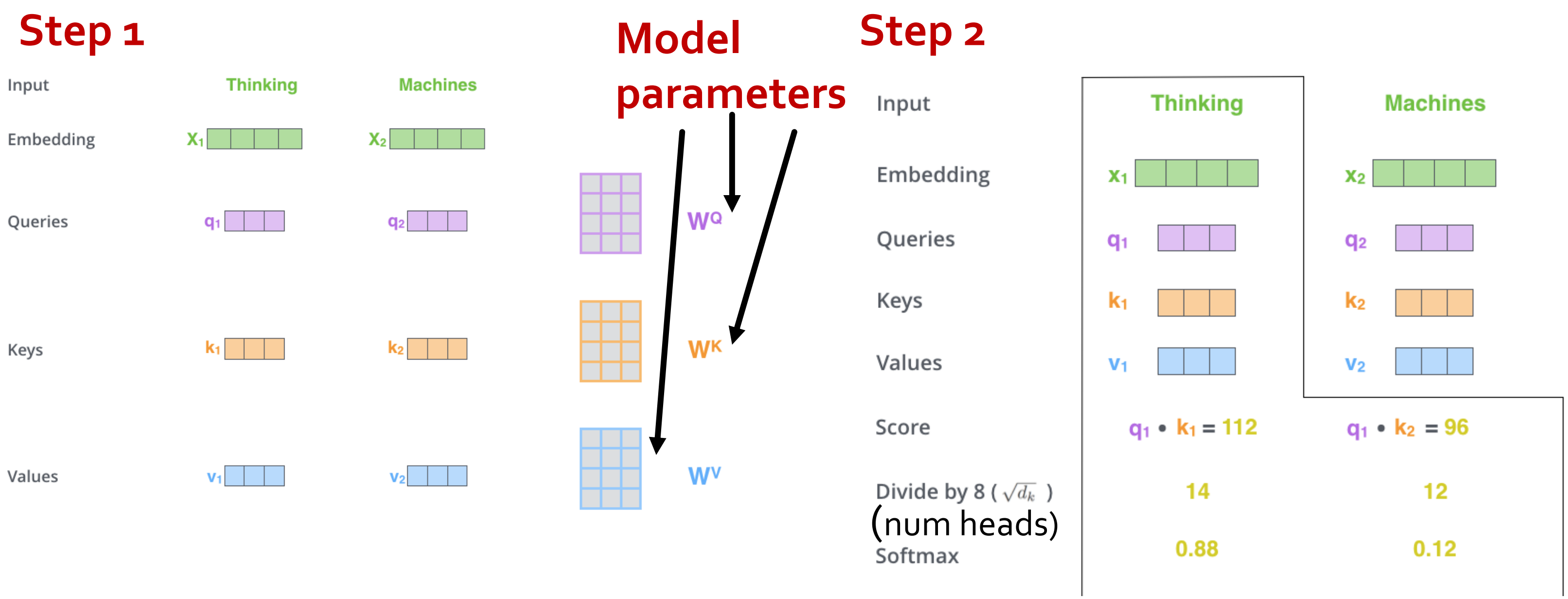
Self-attention

- **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)



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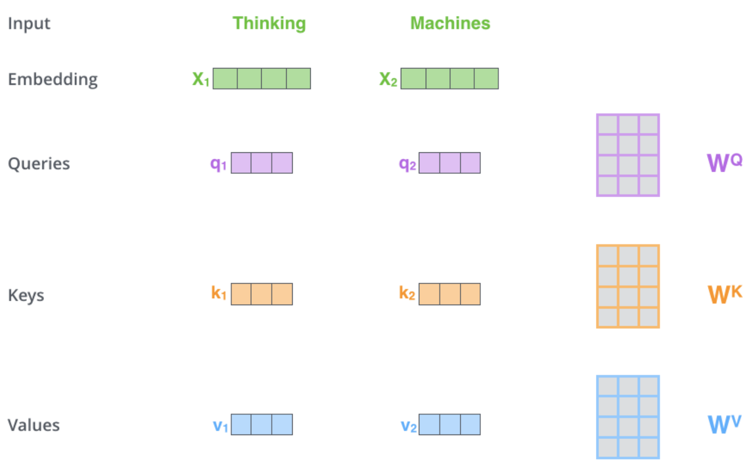
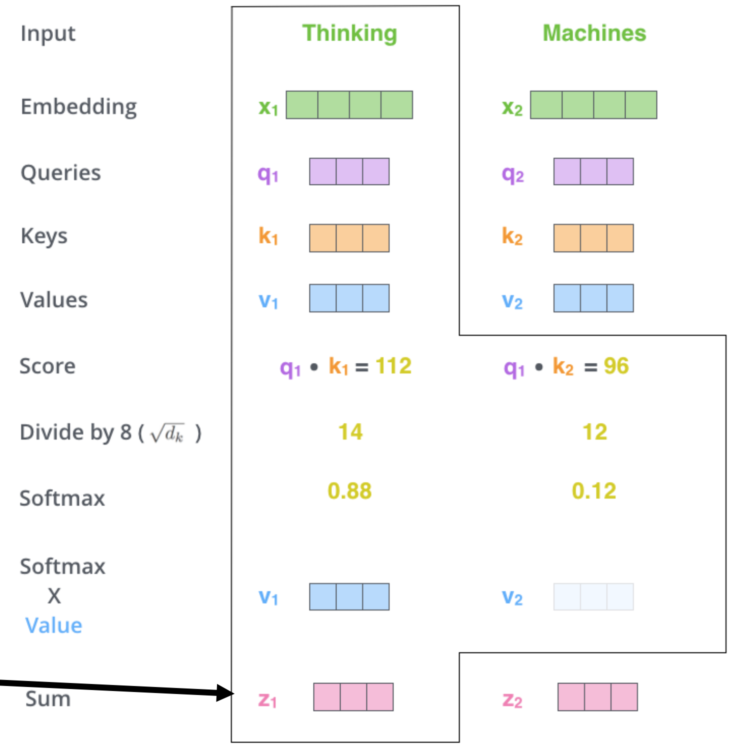
Self-attention

- **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

Step 1



Step 2



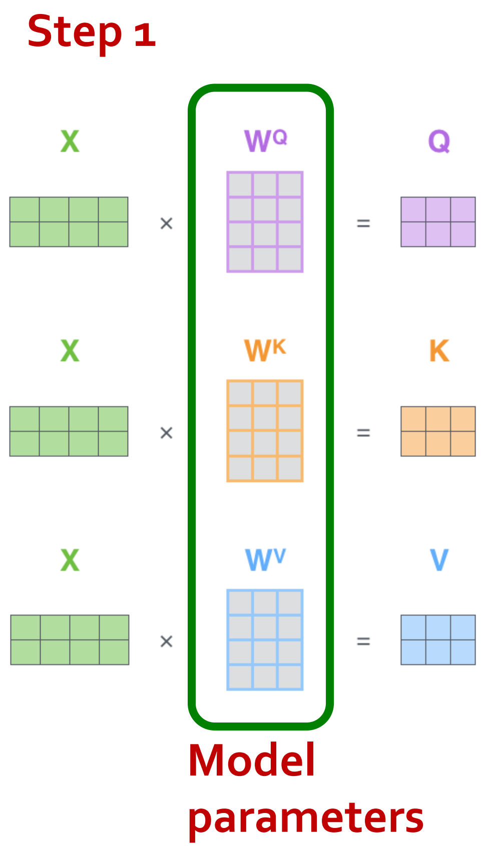
Step 3

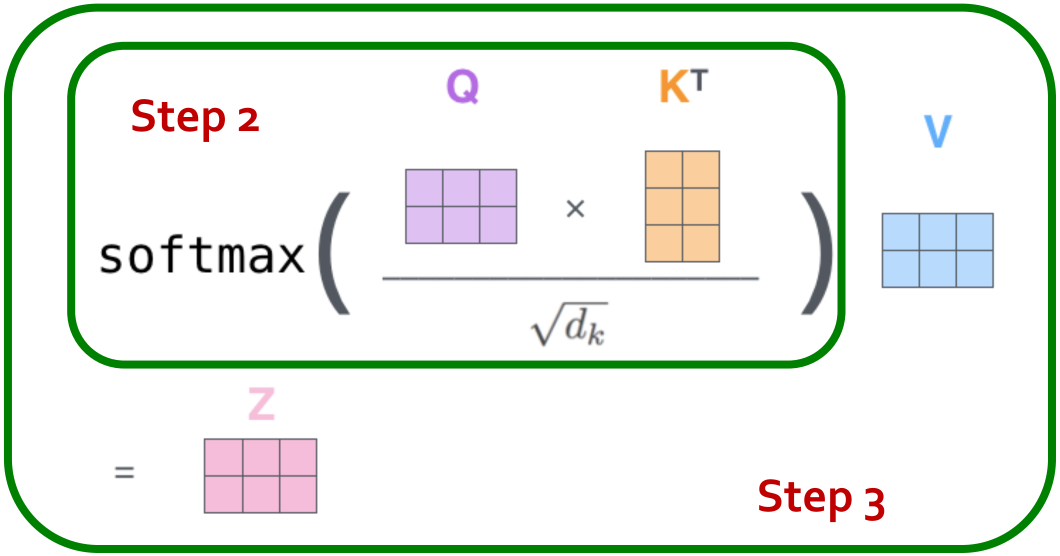
$$z_1 = 0.88 v_1 + 0.12 v_2$$

See: Illustrated Transformer tutorial, https://jalammar.github.io/illustrated-transformer/

Self-attention

- **Same calculation in matrix form**





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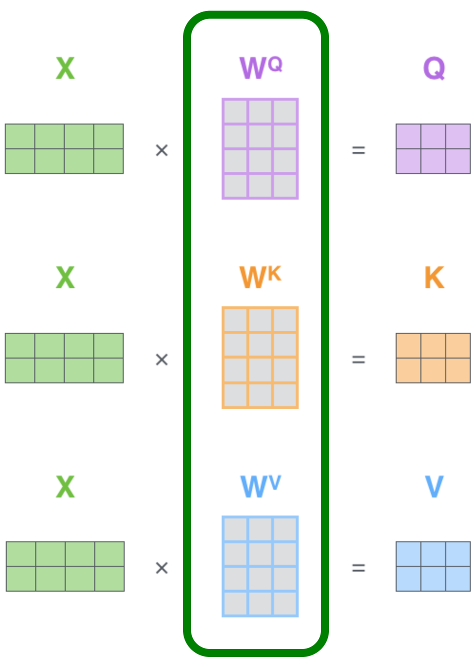
Self-attention

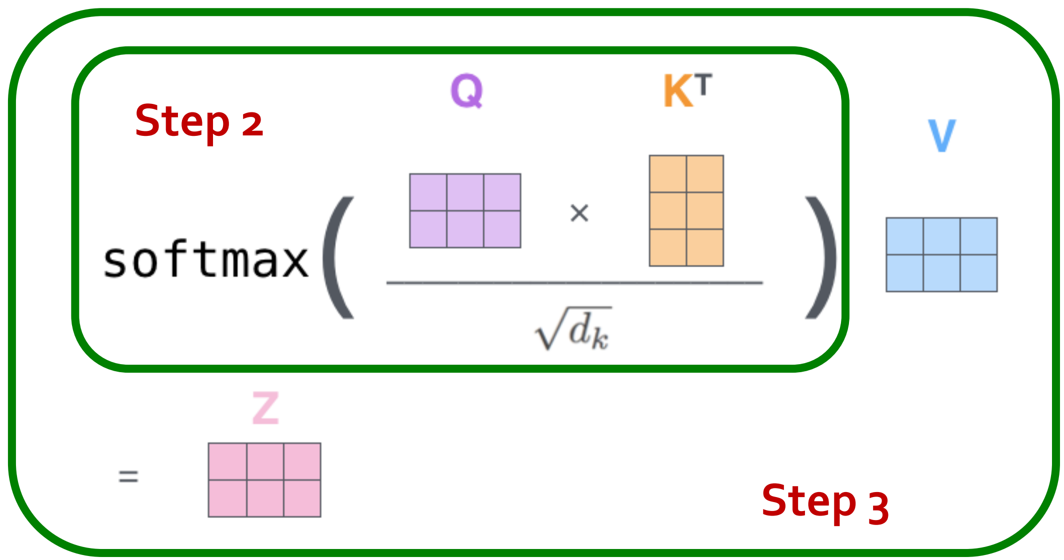
Jure: This slide is duplicated. Probably delete.

- **Same calculation in matrix for**

Step 1



Model parameters



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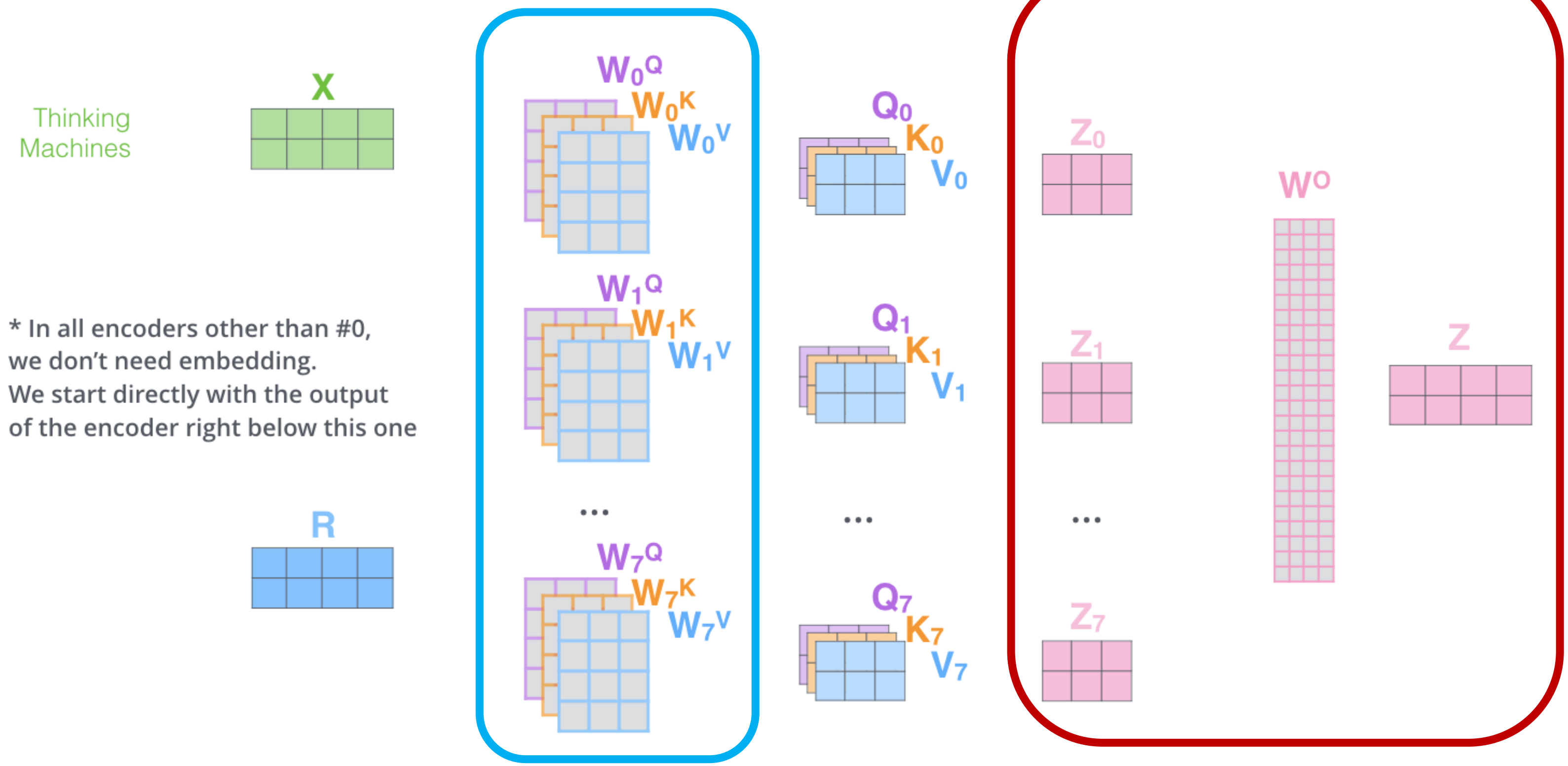
Multi-head self-attention

- Do many self-attentions in parallel, and combine
- Different heads can learn different “similarities” between inputs
- Each has own set of parameters



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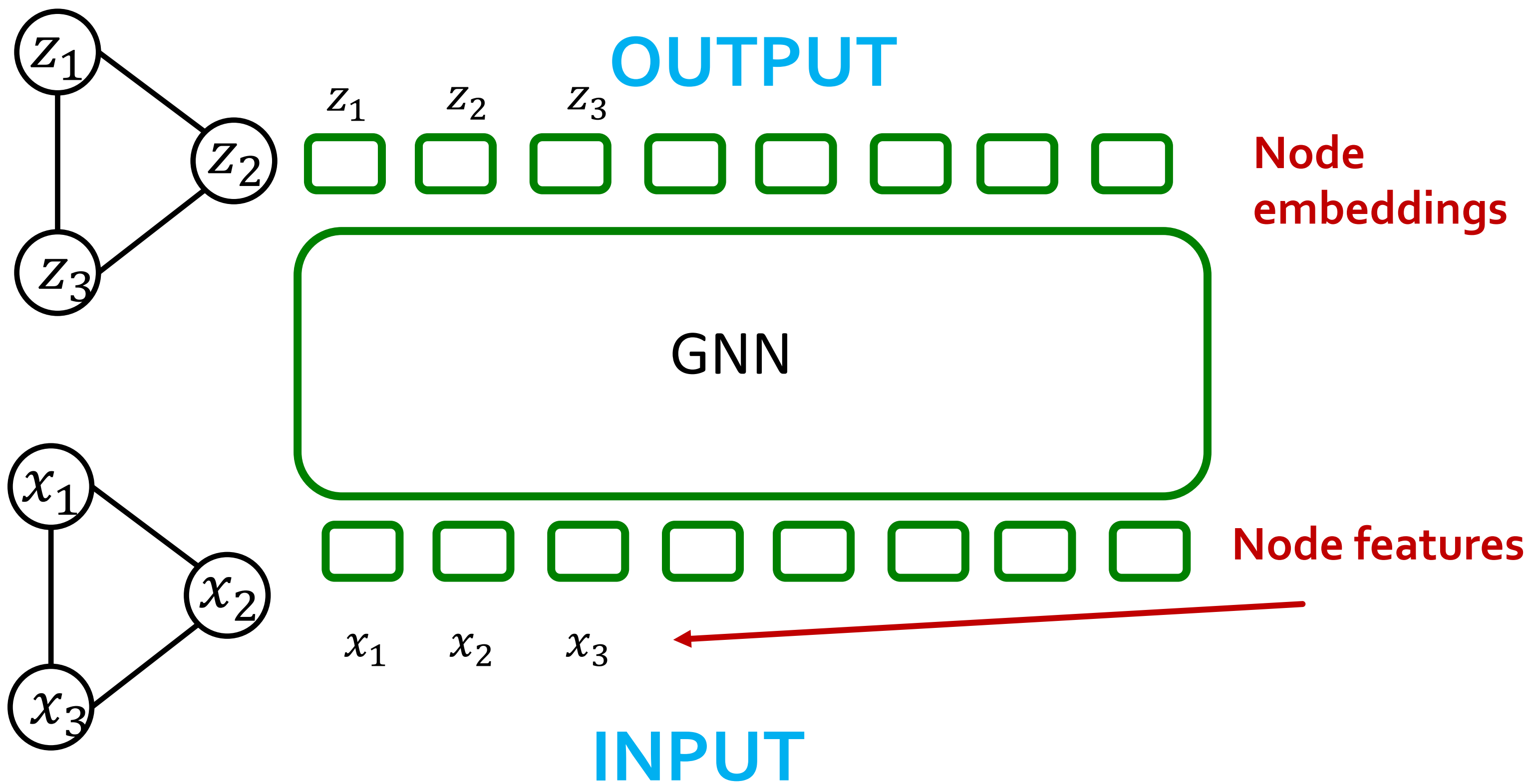
Comparing Transformers and GNN

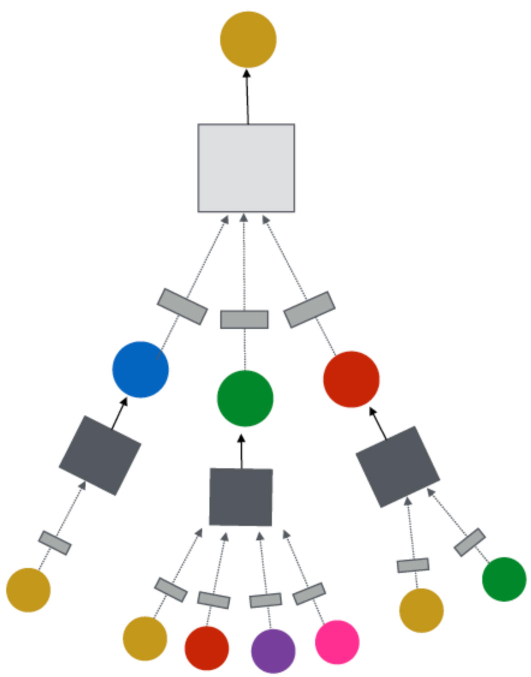
- **Similarity:** GNNs also take in a sequence of vectors (in no particular order) and output a sequence of embeddings
- **Difference:** GNNs use **message passing**, Transformer uses **self-attention**



Comparing Transformers and GNN

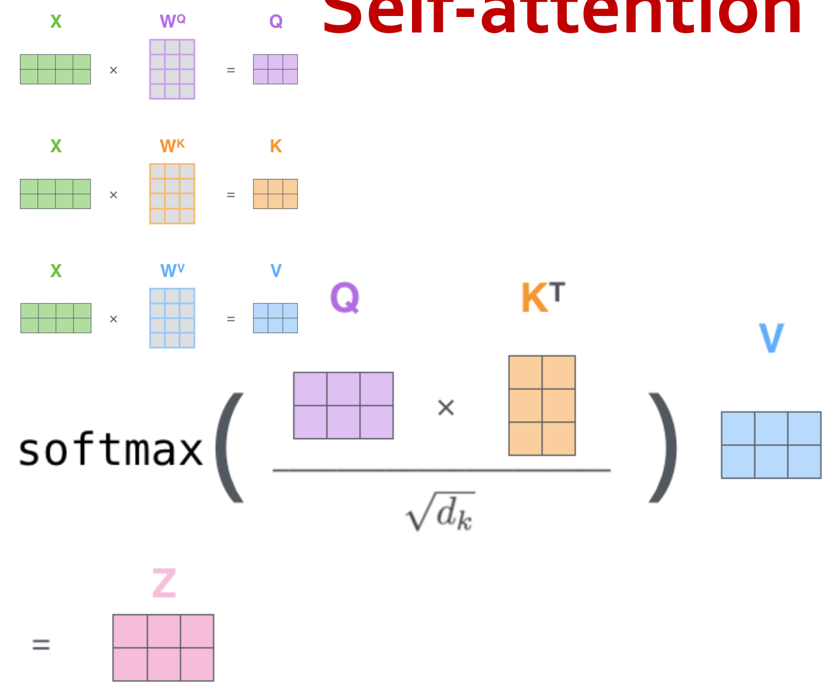
- **Difference:** GNNs use **message passing**, Transformer uses **self-attention**
- **Are self-attention and message passing really different?**

Message Passing



Vs.

Self-attention



Stanford CS224W: Self-attention vs. message passing

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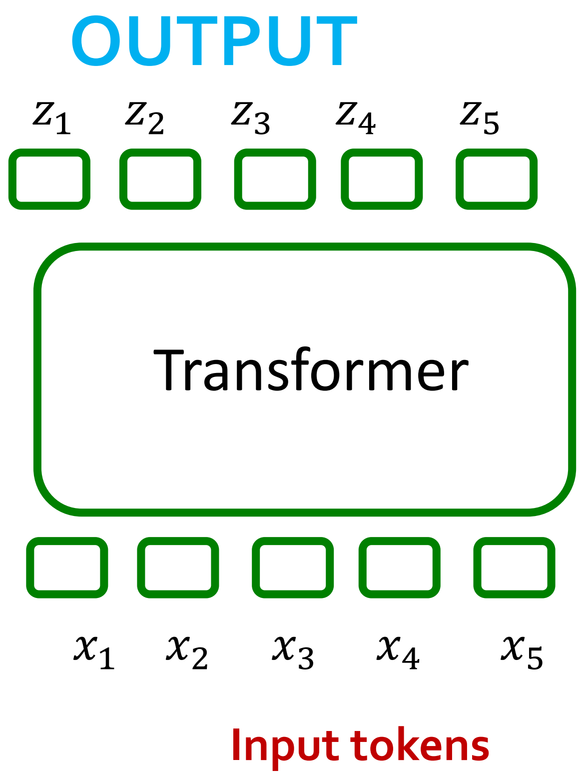
Interpreting the Self-Attention Update

- Recall Formula for attention update:

$$Att(X) = softmax(K^T Q)V$$
$$= softmax\left((XW^K)^T (XW^Q)\right) XW^V$$

Inputs stored row-wise

$$X = \left[— x_i — \right]$$



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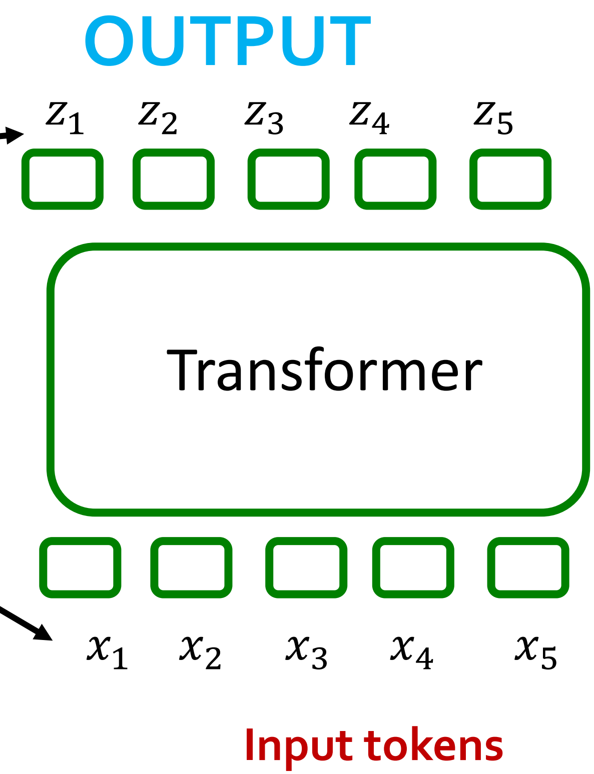
- This formula gives the embedding for **all tokens** simultaneously
- What if we simplify to just token x_1?



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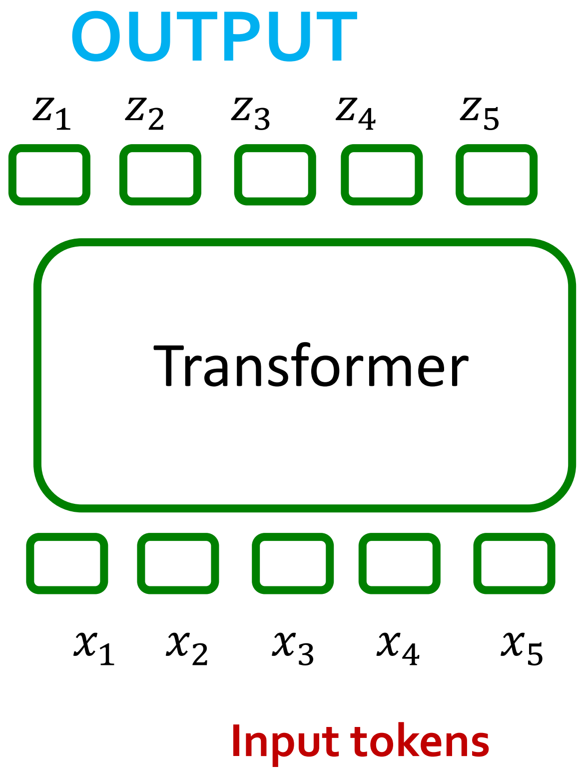
$$z_1 = \sum_{j=1}^{5} softmax_j(q_1^T k_j)v_j$$

How to interpret this?



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Inputs stored row-wise

$$X = \left[- x_i - \right]$$

- This formula gives the embedding for **all tokens** simultaneously
- If we simplify to just token x_1 what does the update look like?

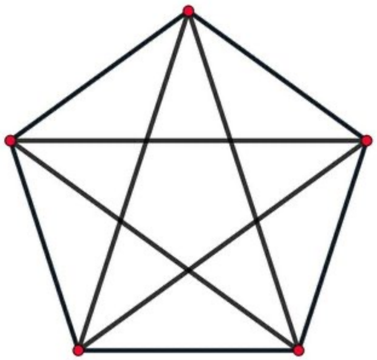
$$z_1 = \sum_{j=1}^{5} softmax_j\left(q_1^T k_j\right) v_j$$

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:** $Agg\left(\{MSG(x_j): j\}, q_1\right) = \sum_{j=1}^{n} softmax_j\left(q_1^T k_j\right) v_j$

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 ~GAT**



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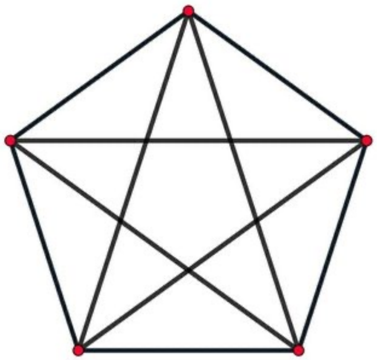
Self-Attention as Message Passing

- **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:
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  - **2. Compute query for 1:** $q_1 = W^Q x_1$
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Plan for Today

- **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

Stanford CS224W: A New Design Landscape for Graph Transformers

CS224W: Machine Learning with Graphs

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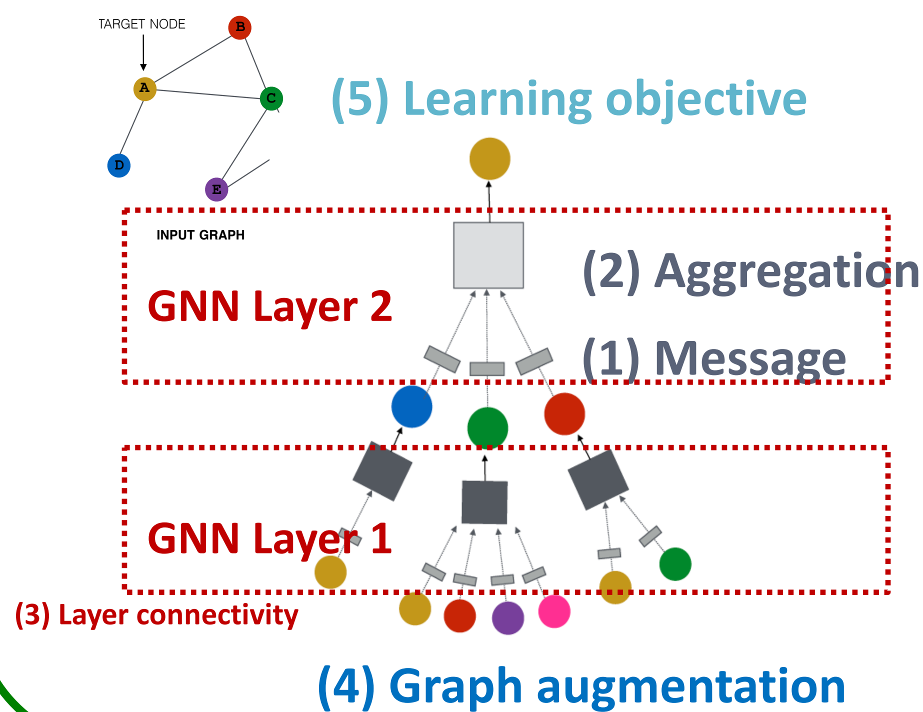
Recap: A General GNN Framework

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

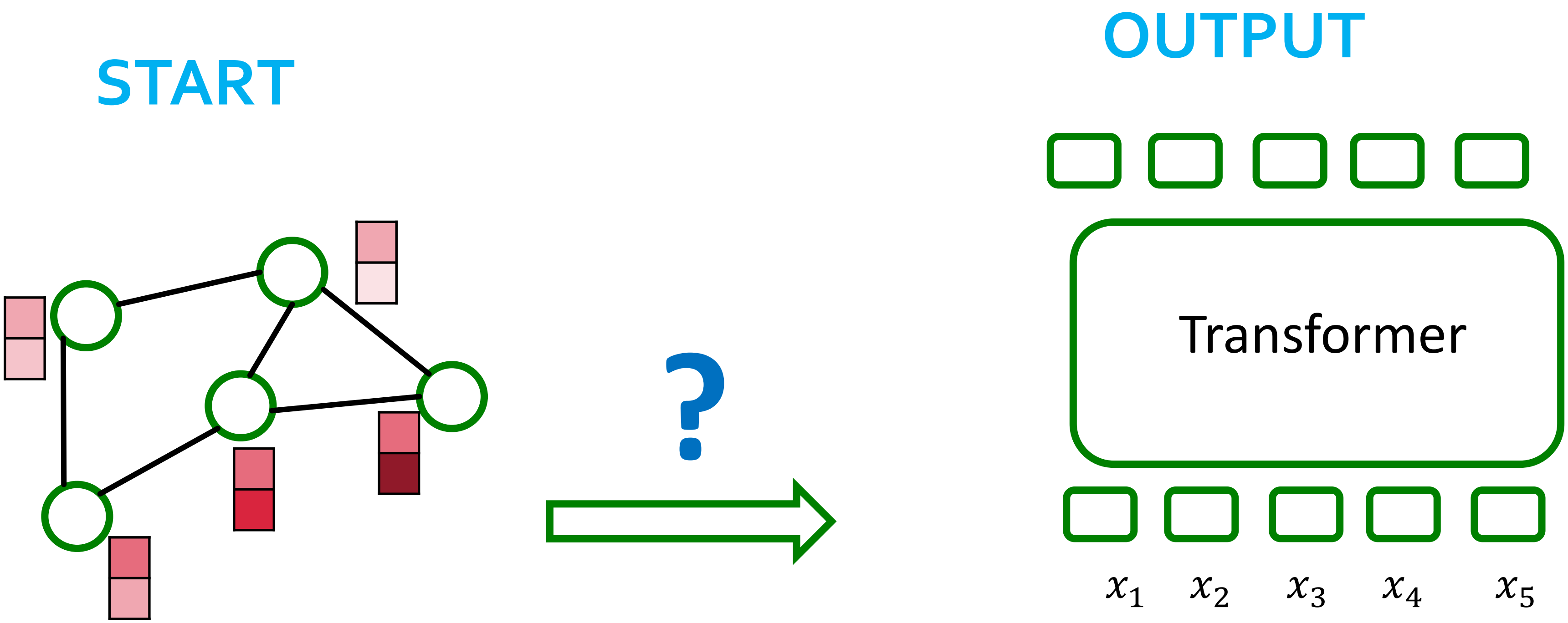
GNN design space



Graph Transformer design space

Processing Graphs with Transformers

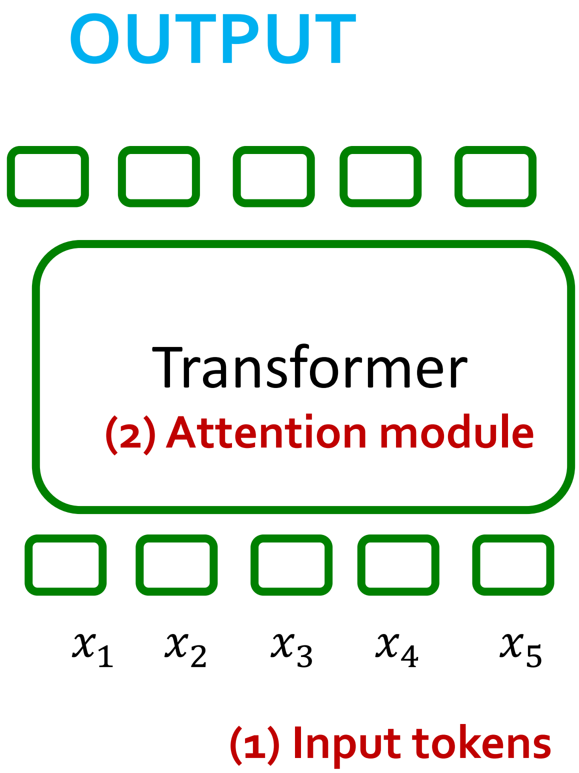
- We start with graph(s)
- How to input a graph into a Transformer?



J. You, R. Ying, J. Leskovec. [Design Space of Graph Neural Networks](), NeurIPS 2020c

Components of a Transformer

- To understand how to process graphs with Transformers we must:
  - Understand the key components of the Transformer. Seen already:
    - 1) tokenizing,
    - 2) self-attention
  - Decide how to make suitable **graph versions** of each



A final key piece: token ordering

- There is one other key missing piece we have not yet discussed…

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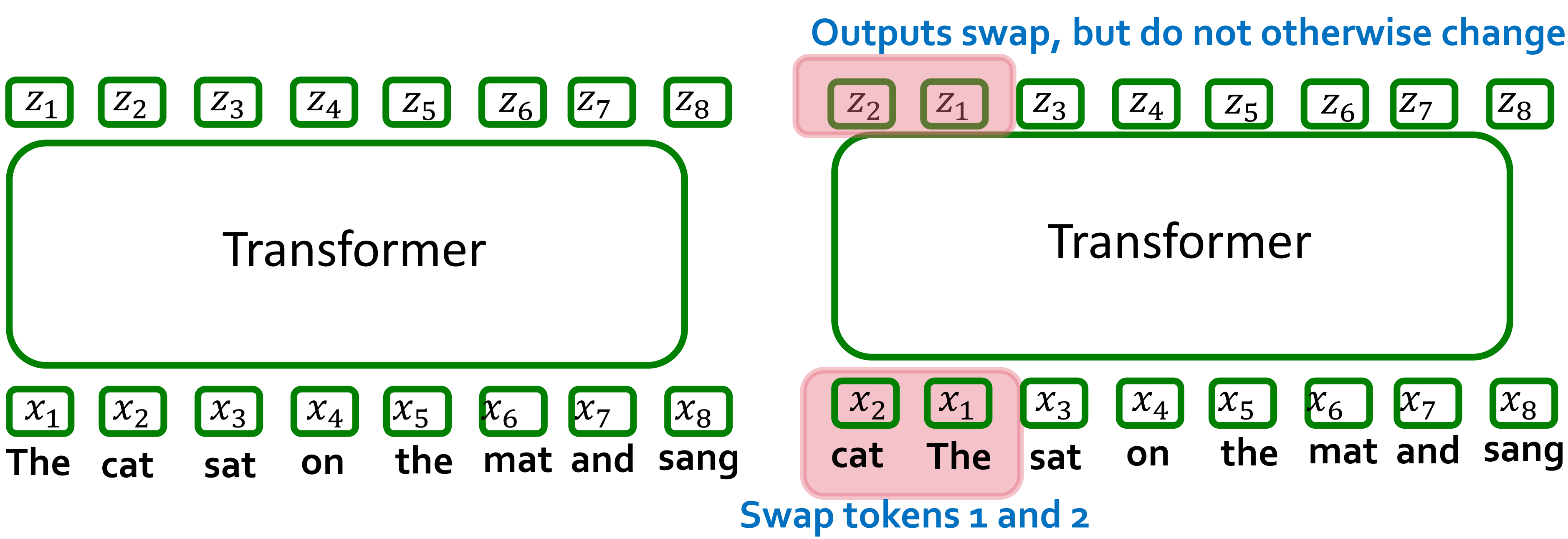
- **First recall update formula**

$$z_1 = \sum_{j=1}^{5} softmax_j\left(q_1^T k_j\right) v_j$$

- **Key Observation: order of tokens does not matter!!!**

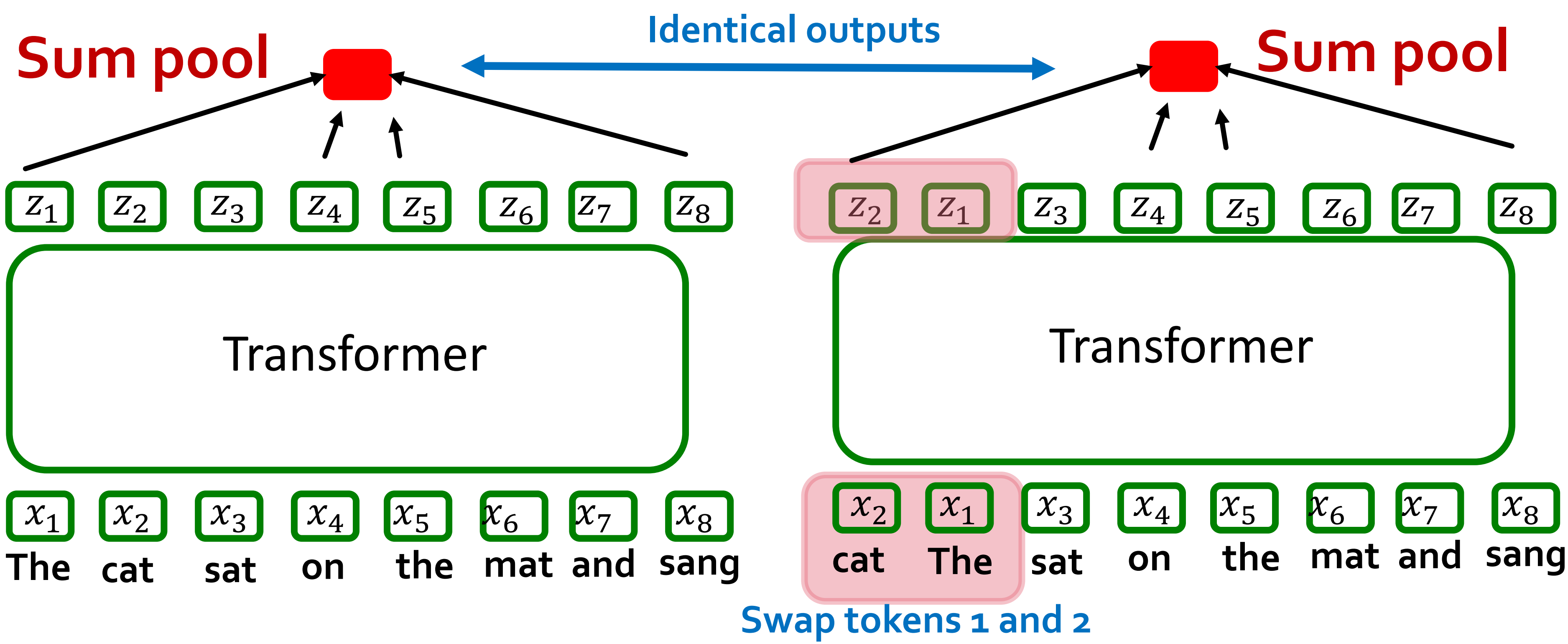
A final key piece: token ordering

- There is one other key missing piece we have not yet discussed …
- **First recall update formula** $$z_1 = \sum_{j=1}^{5} softmax_j(q_1^T k_j) v_j$$
- **Key Observation: order of tokens does not matter!!!**



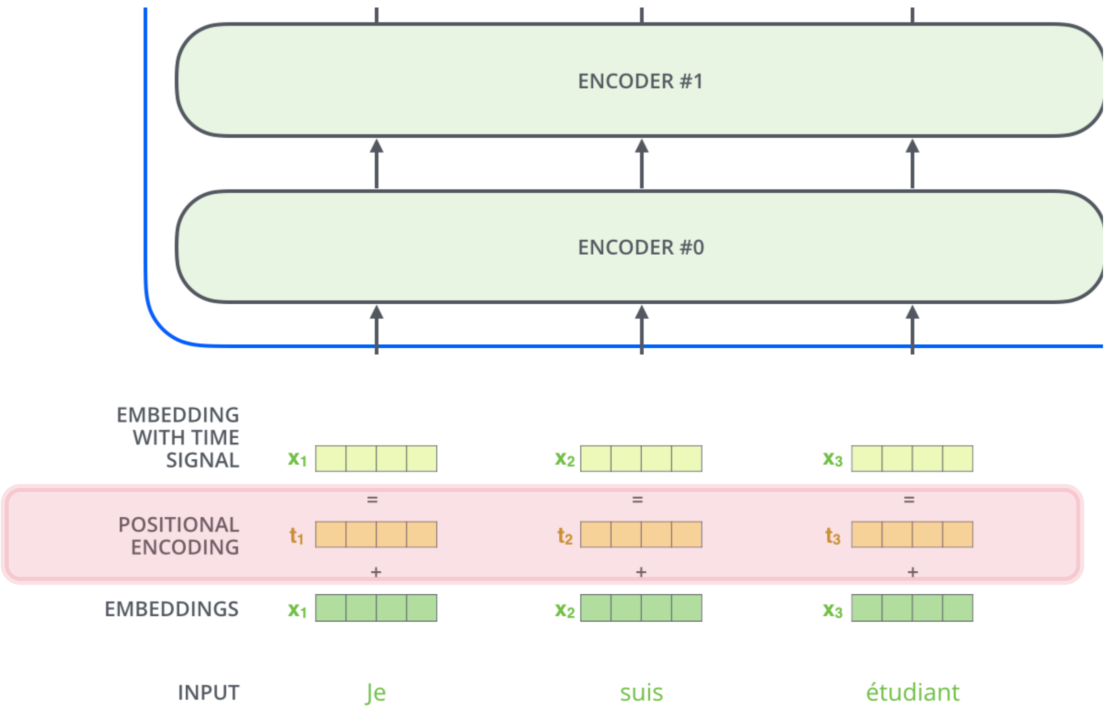
A final key piece: Token ordering

- **This is a problem**
- **Same predictions** no matter what order the words are in!
  (A "bag of words" prediction model)...
  - How to fix?



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

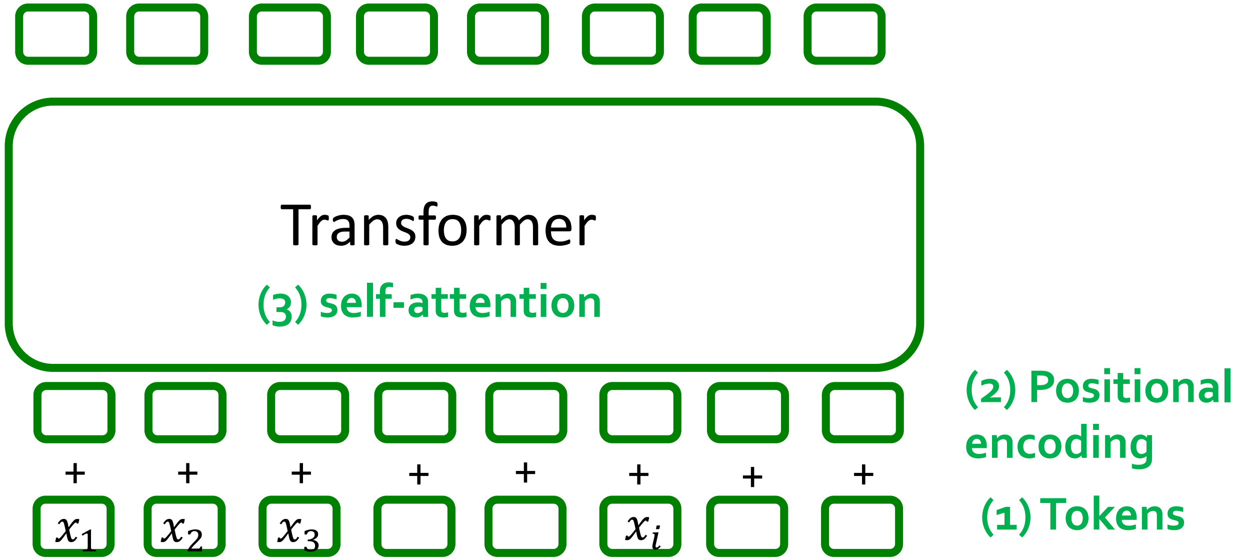


Components of a Transformer

- 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?



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
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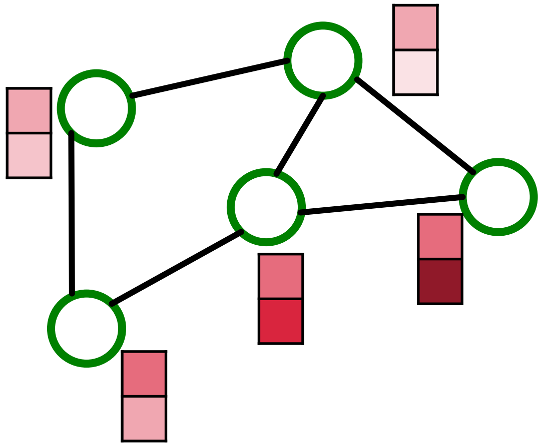

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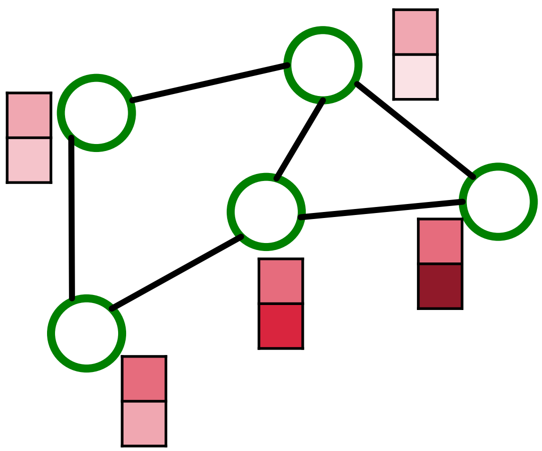


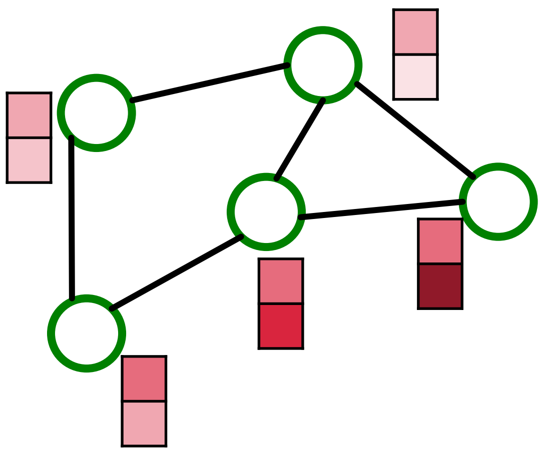
- There are many ways to do this
- Different approaches correspond to different "matchings" between graph inputs **(1), (2), (3)** transformer components **(1), (2), (3)**

Processing Graphs with Transformers

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

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

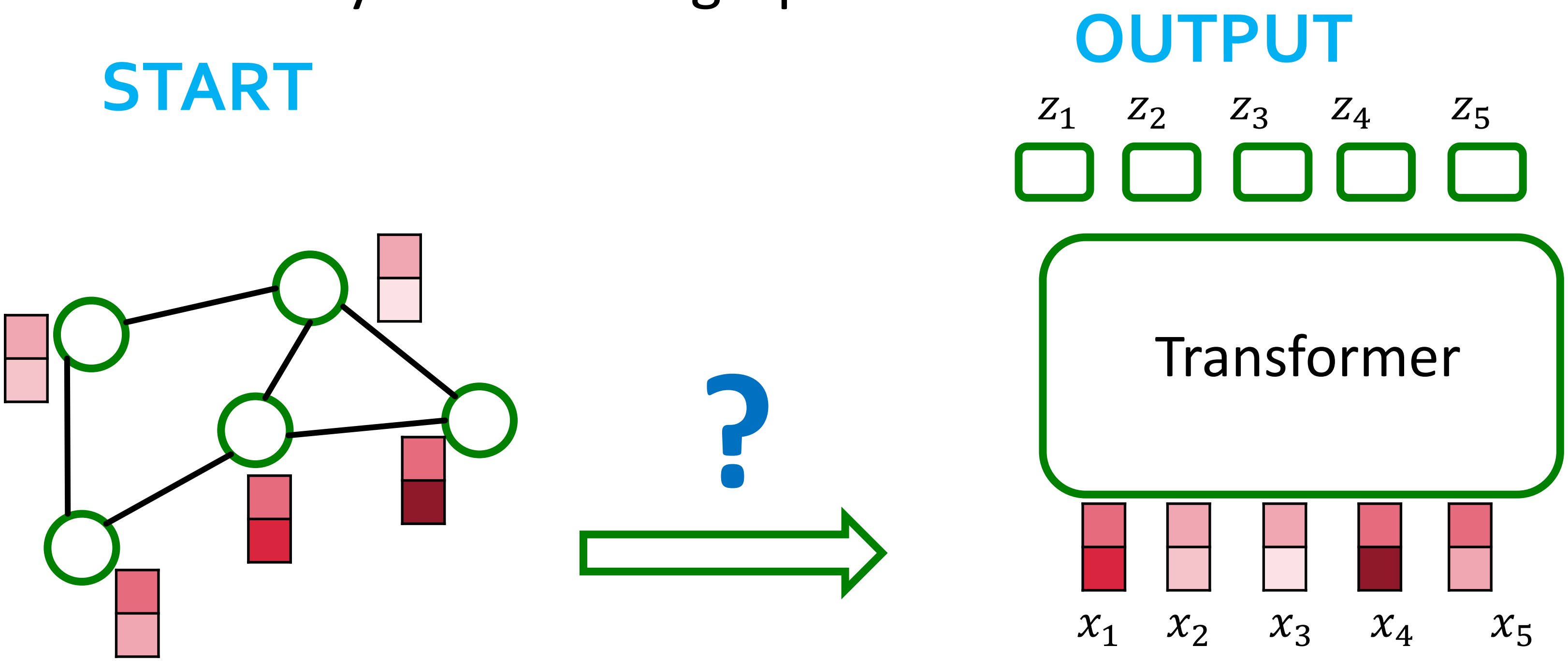
Today



- 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

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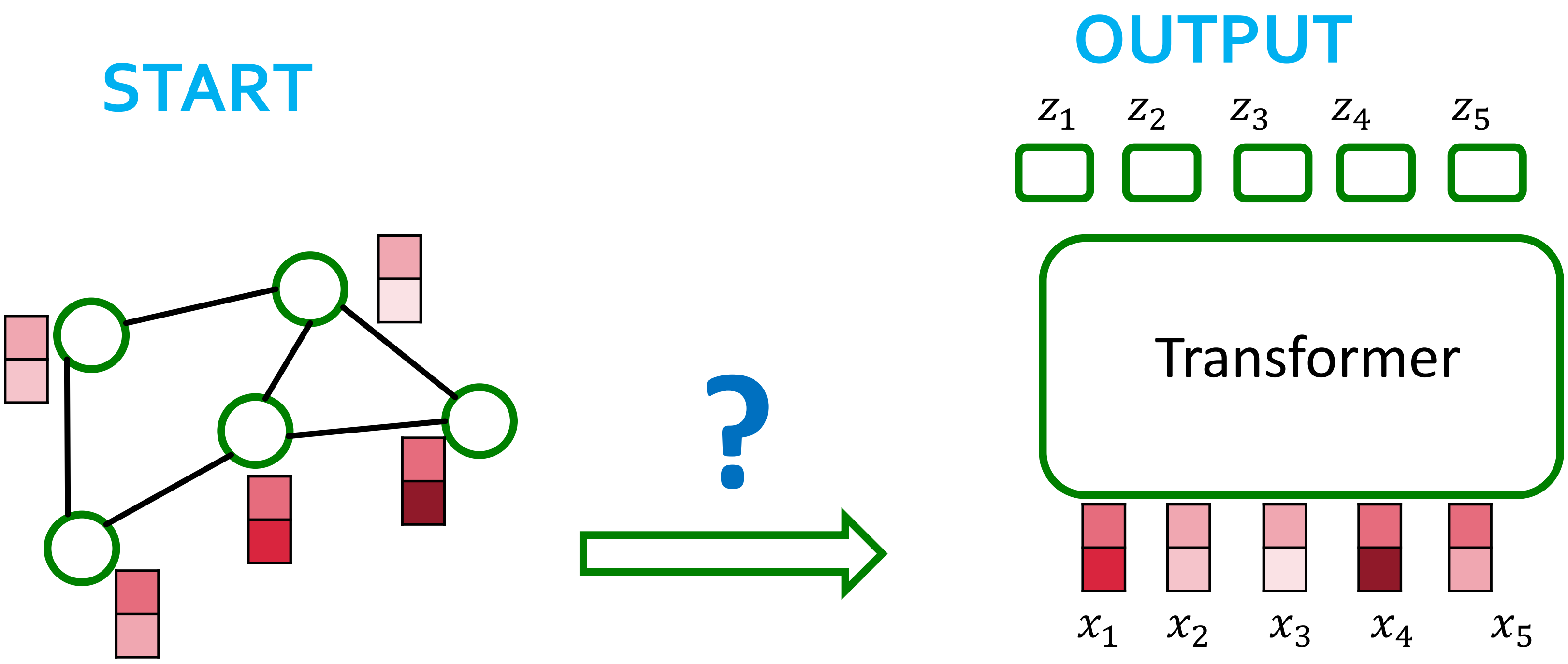
Processing Graphs with Transformers

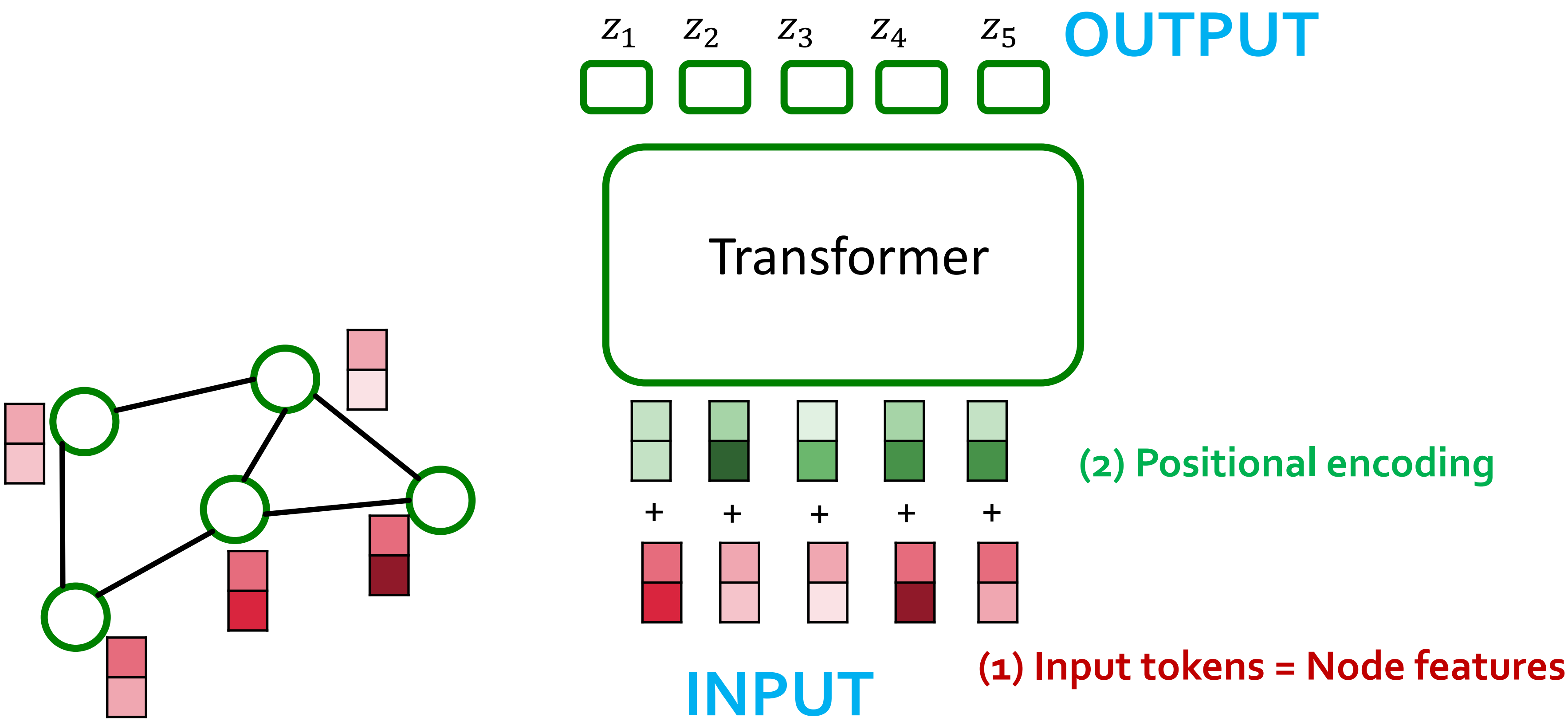
- **Problem? We completely lose adjacency info!**
- **How to also inject adjacency information?**



(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 Add Back Adjacency Info?

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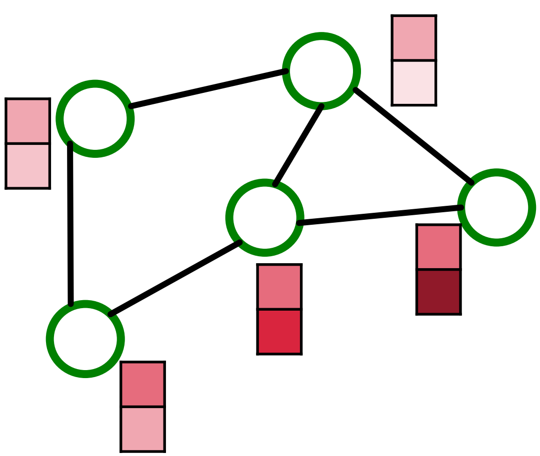
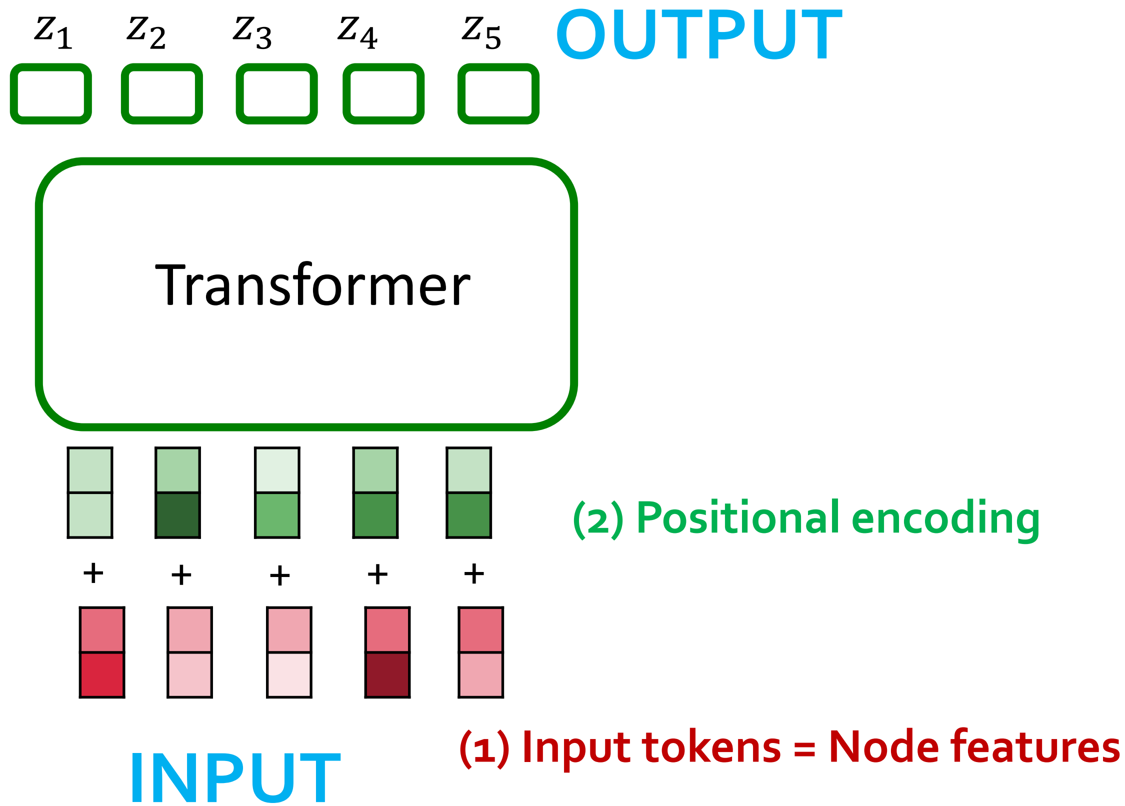
- Positional encoding describes **where** a node is in the graph

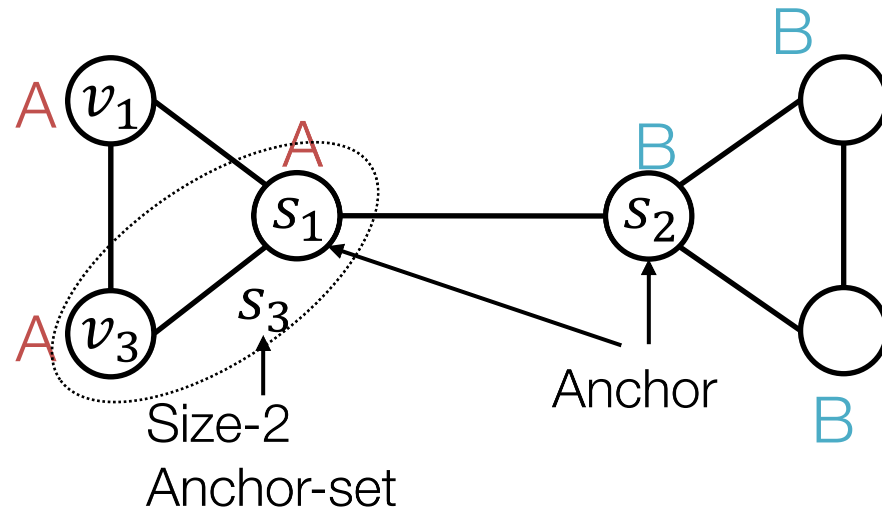
Q2: How to design a good positional encoding?





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

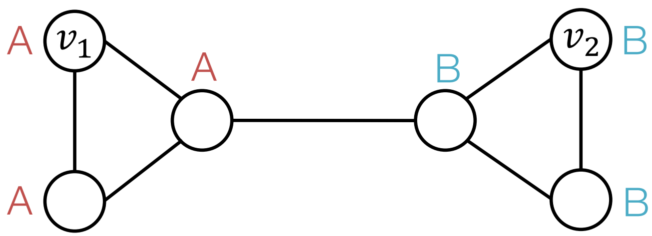
Positional encoding for node v_1 =

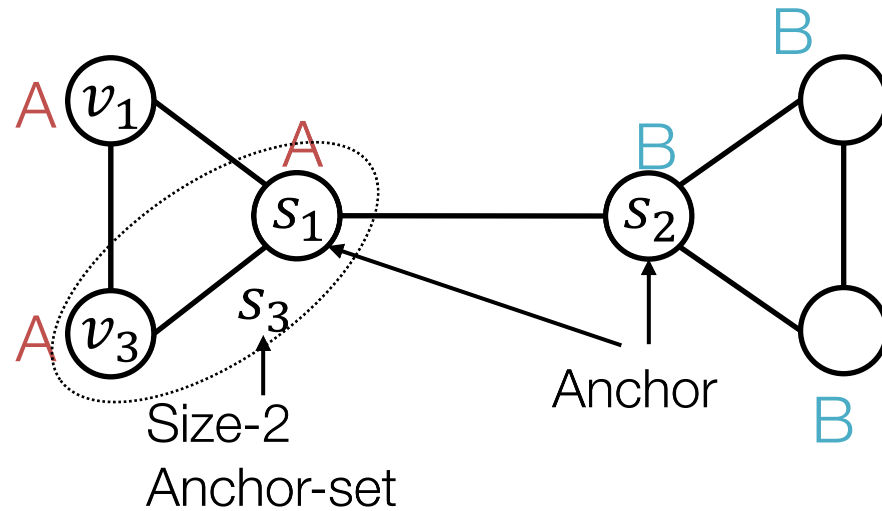
	s_1	s_2	s_3
v_1	1	2	1
v_3	1	2	0

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

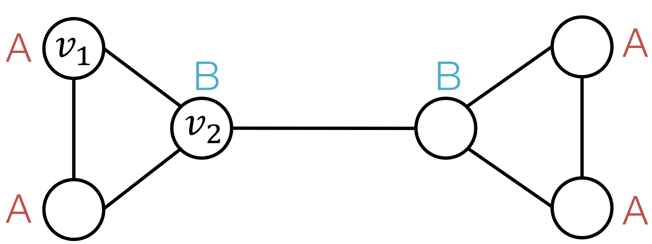
Option 1: Relative distances

- **Last lecture:** Relative distances useful for position-aware task





- But not suited to structure-aware tasks



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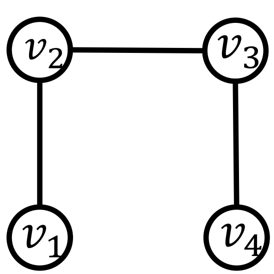
Option 2: Laplacian Eigenvector Positional Encodings

- What other ways to make positional encoding?

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



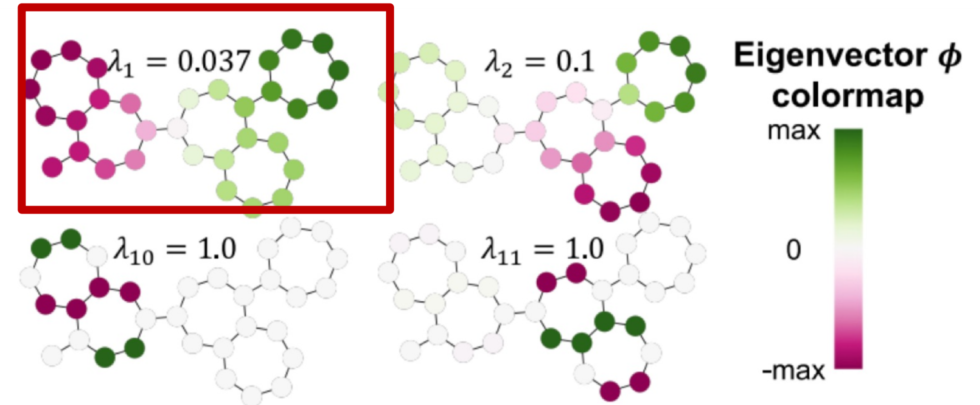
$$L = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 2 & 0 & 0 \\ 0 & 0 & 2 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix} - \begin{bmatrix} 0 & 1 & 0 & 0 \\ 1 & 0 & 1 & 0 \\ 0 & 1 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{bmatrix}$$

Degree of each node **Adjacency**

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

Visualize one eigenvector



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

Refresher

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

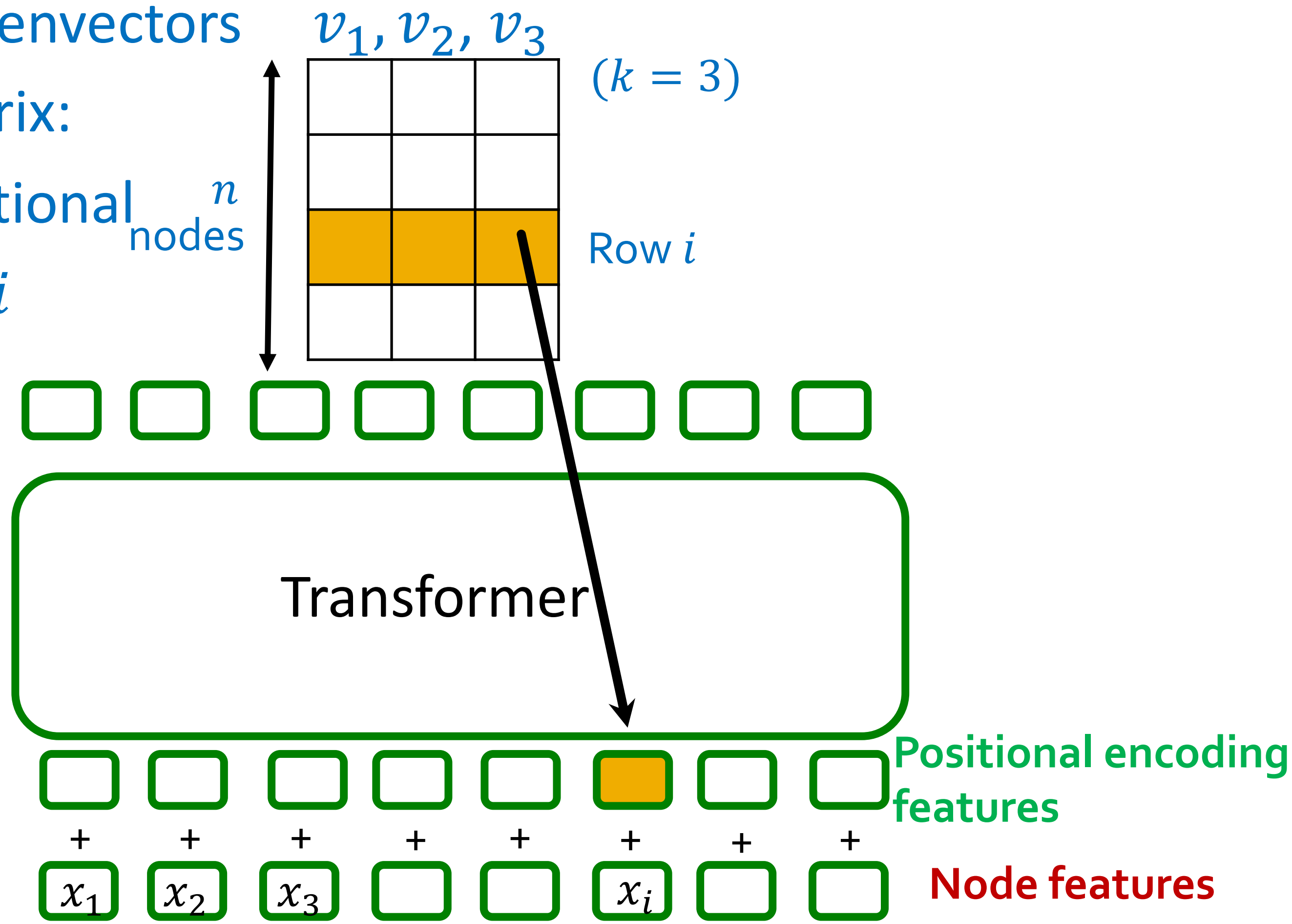
$L: n \times n$ matrix

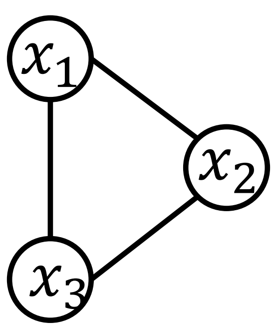
$v: n$ dimensional vector

λ: Scalar eigenvalue

Laplacian Eigenvector Positional Encodings

- **Positional encoding steps:**
  - 1. compute k eigenvectors
  - 2. Stack into matrix:
  - 3. ith row is positional encoding for node i





Summay: Laplacian Eigenvector Positional Encodings

- Laplacian Matrix **L = Degrees – Adjacency**
- $\boxed{\text{Eigenvector: } v \text{ such that } Lv = \lambda v}$
- **Positional encoding steps:**
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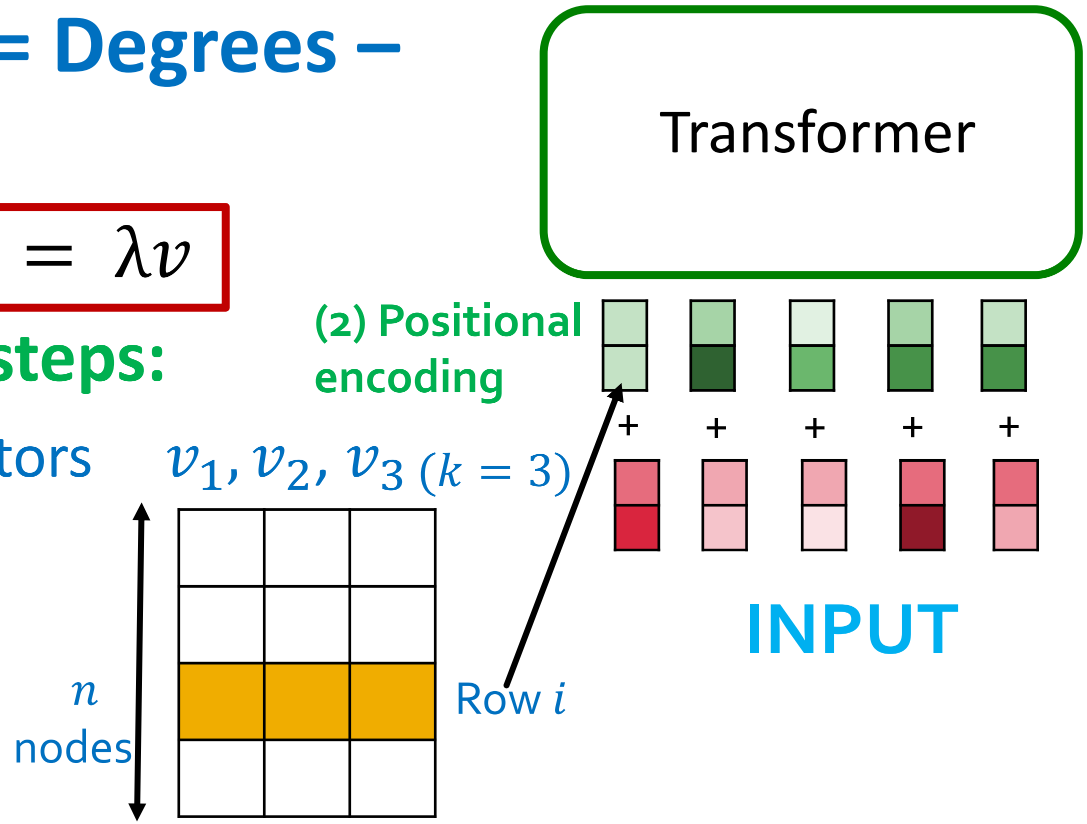


- Laplacian Eigenvector positional encodings can also be used with message-passing GNNs
  - **This helps for same reasons as relative-distance based positional encodings in previous lecture**

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.

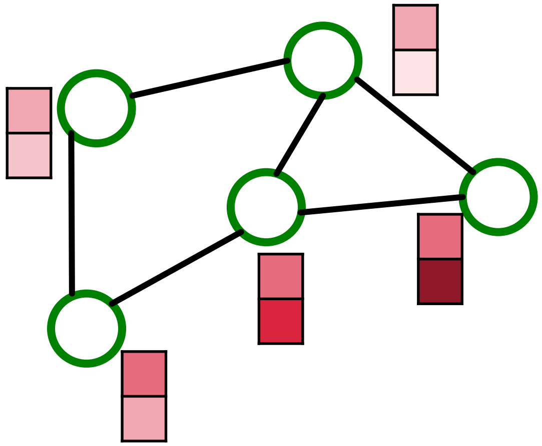
Train samples →			200	500	1000	5000
Model	L	**#Param**	**Test Acc±s.d.**			
GIN	4	100774	70.585±0.636	74.995±1.226	78.083±1.083	86.130±1.140
GIN-PE	4	102864	**86.720±3.376**	**95.960±0.393**	**97.998±0.300**	**99.570±0.089**
GatedGCN	4	103933	50.000±0.000	50.000±0.000	50.000±0.000	50.000±0.000
GatedGCN-PE	4	105263	**95.082±0.346**	**96.700±0.381**	**98.230±0.473**	**99.725±0.027**

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

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:
  - **(1) Node features?**
  - **(2) Adjacency information?**
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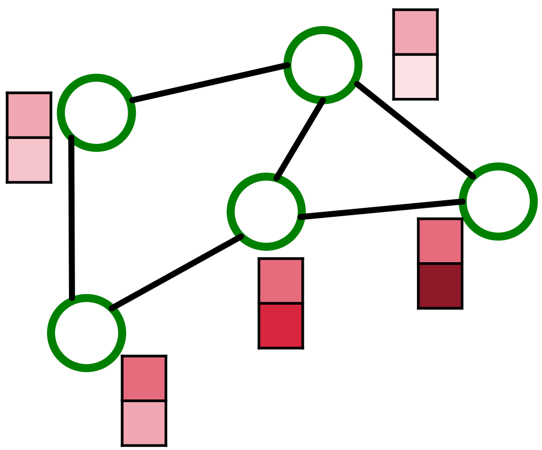
  - **(1) tokenizing**
  - **(2) positional encoding**
  - **(3) self-attention**

Left to do



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- Different approaches correspond to different "matchings" between graph inputs **(1), (2), (3)** transformer components **(1), (2), (3)**

Edge Features in Self-Attention

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

[Do Transformers Really Perform Bad for Graph Representation?](#) Ying et al. NeurIPS 2021

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- **Idea: adjust $\boldsymbol{k_{ij}}$ based on edge features. Replace with $\boldsymbol{k_{ij} + c_{ij}}$ where $\boldsymbol{c_{ij}}$ depends on the edge features**
- **Implementation:**

  Learned parameters $\boldsymbol{w_1}$

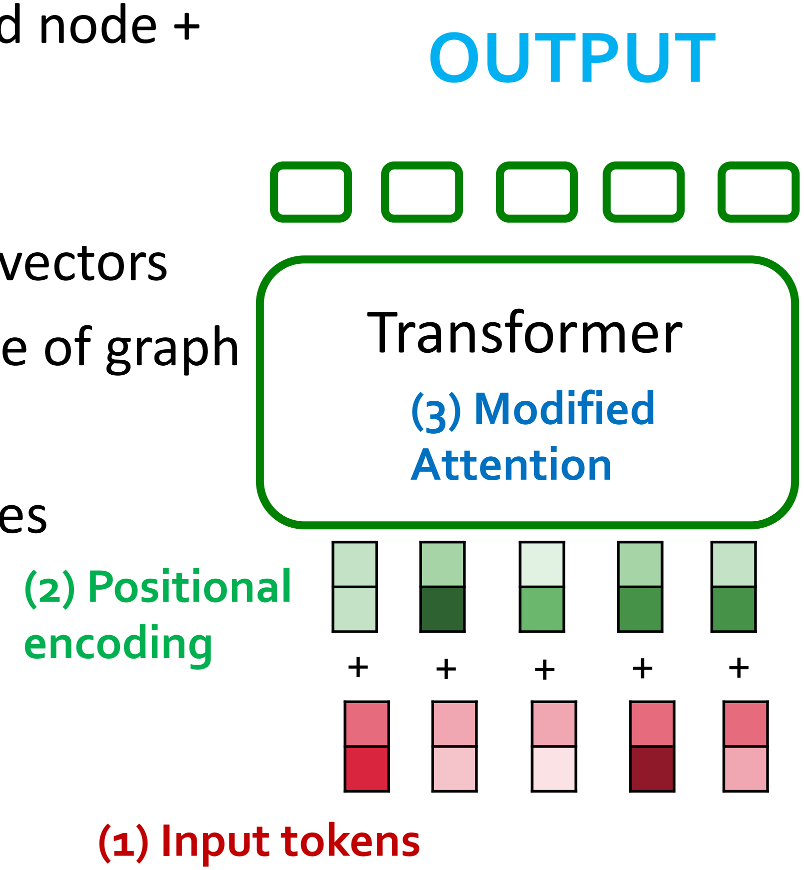
  - **If there is an edge between i and j with features $\boldsymbol{e_{ij}}$, define $\boldsymbol{c_{ij} = w_1^T e_{ij}}$**
  - **If there is no edge, find shortest edge path between i and j $\boldsymbol{(e^1, e^2, \ldots e^N)}$ and define $\boldsymbol{c_{ij} = \sum_n w_n^T e^n}$**

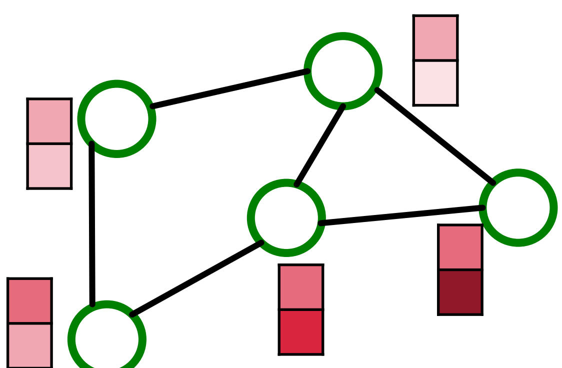
  Learned parameters $\boldsymbol{w_1, \ldots, w_N}$

Do Transformers Really Perform Bad for Graph Representation? Ying et al. NeurIPS 2021

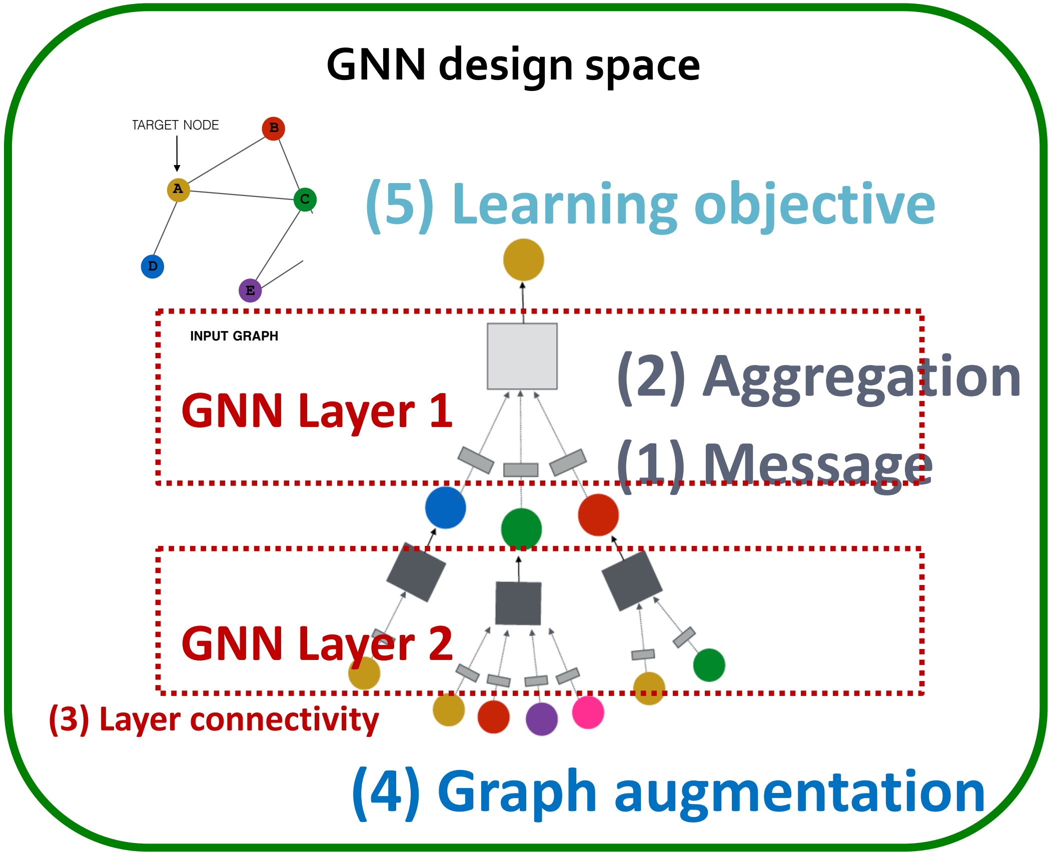
Summary: Graph Transformer Design Space

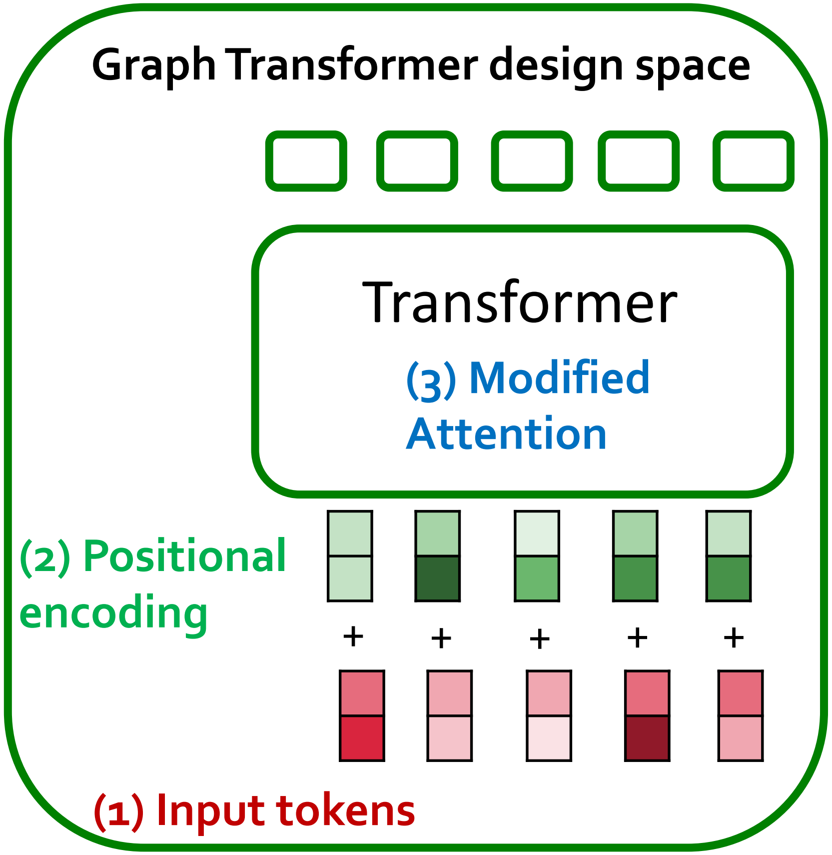
- **(1) Tokenization**
  - Usually node features
  - Other options, such as subgraphs, and node + edge features (not discussed today)
- **(2) Positional Encoding**
  - Relative distances, or Laplacian eigenvectors
  - Gives Transformer adjacency structure of graph
- **(3) Modified Attention**
  - Reweight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





Summary: Graph Transformer Design Space





Plan for Today

- **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

Jure:
The lecture is great! I like how nicely you explain the concepts and connect them!
My sense is that you have a lot of material. If you cover the material till here (finish the lecture here) it will be plenty.

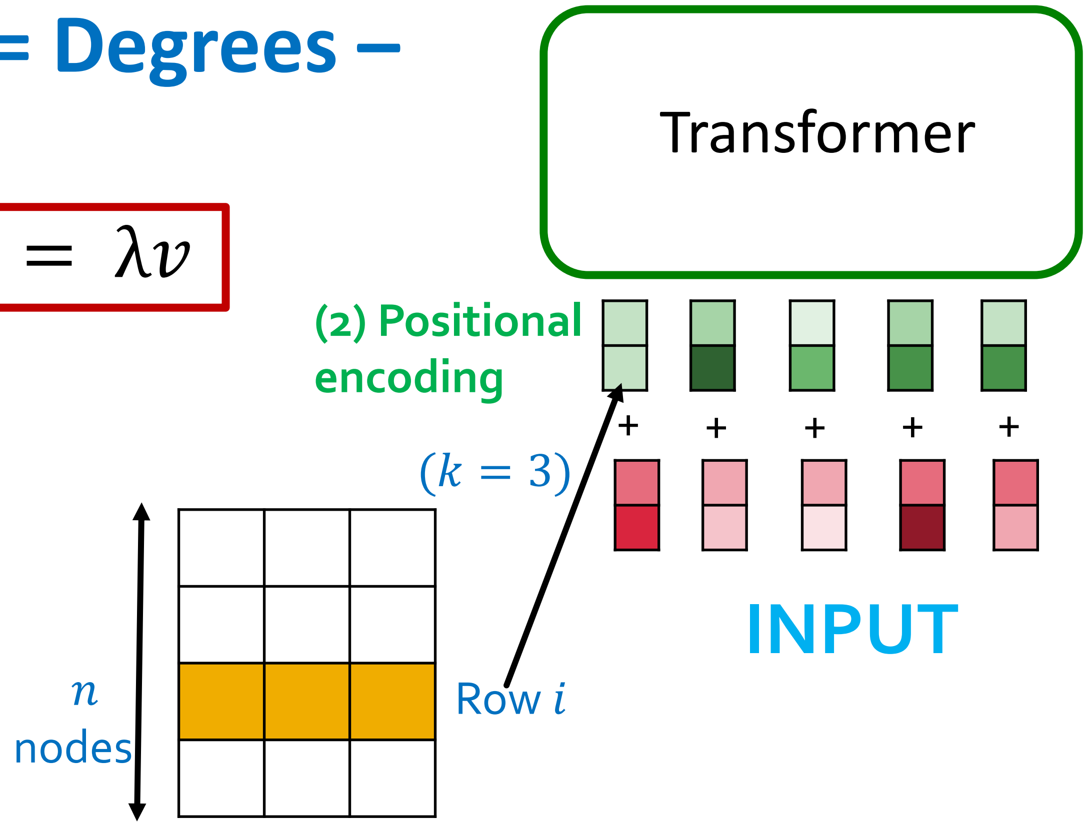
Stanford … ful Positional Encodings for Graph Transformers

CS224W: Machine Learning with Graphs
Jure Leskovec, Stanford University

http://cs224w.stanford.edu

Recall: Laplacian Eigenvector Positional Encodings

- Laplacian Matrix **L = Degrees – Adjacency**
- Eigenvector: v such that $Lv = \lambda v$

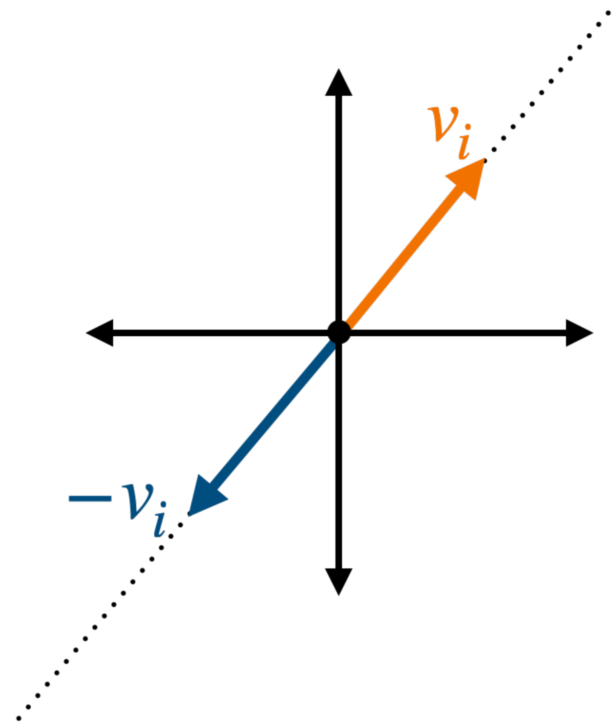


Laplacian Eigenvector Positional Encodings

- 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

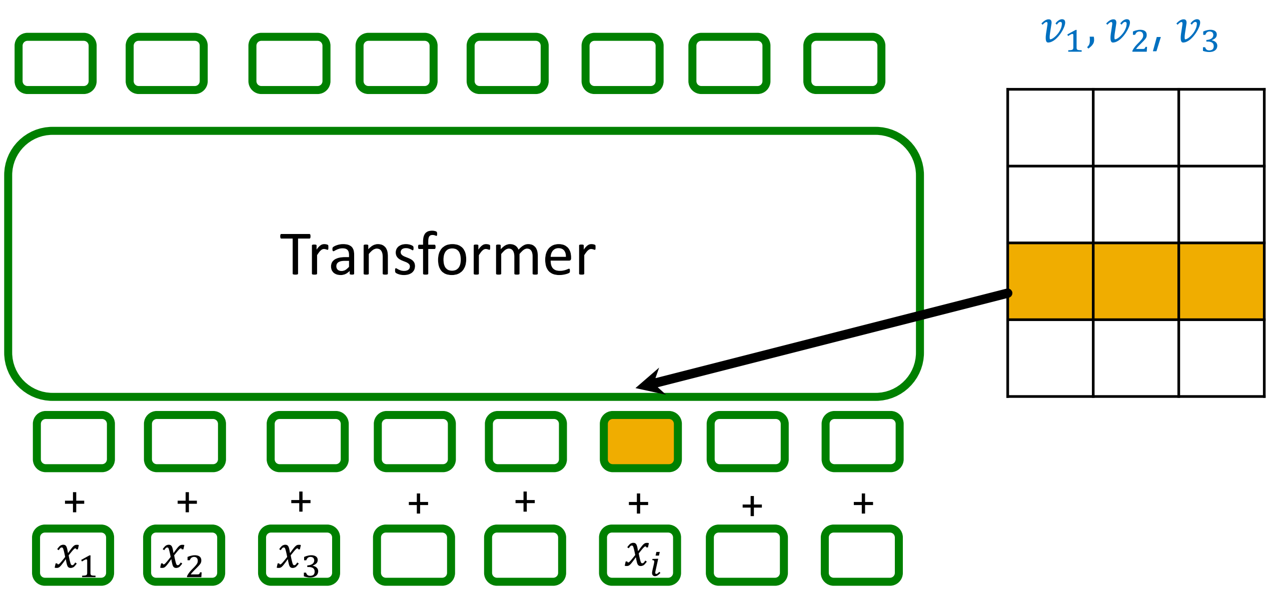
- Suppose v is a Laplacian eigenvector
  - So $Lv = \lambda v$
- But this means:
  - Also $L(-v) = \lambda(-v)$
- So $-v$ is also a Laplacian eigenvector



The choice of sign is arbitrary!

Sign Ambiguity is a Problem

- Both v and $-v$ are eigenvectors
- But when we use them as positional encodings we **pick one arbitrarily**
- **Why does this matter for positional encodings?**



Sign Ambiguity is a Problem

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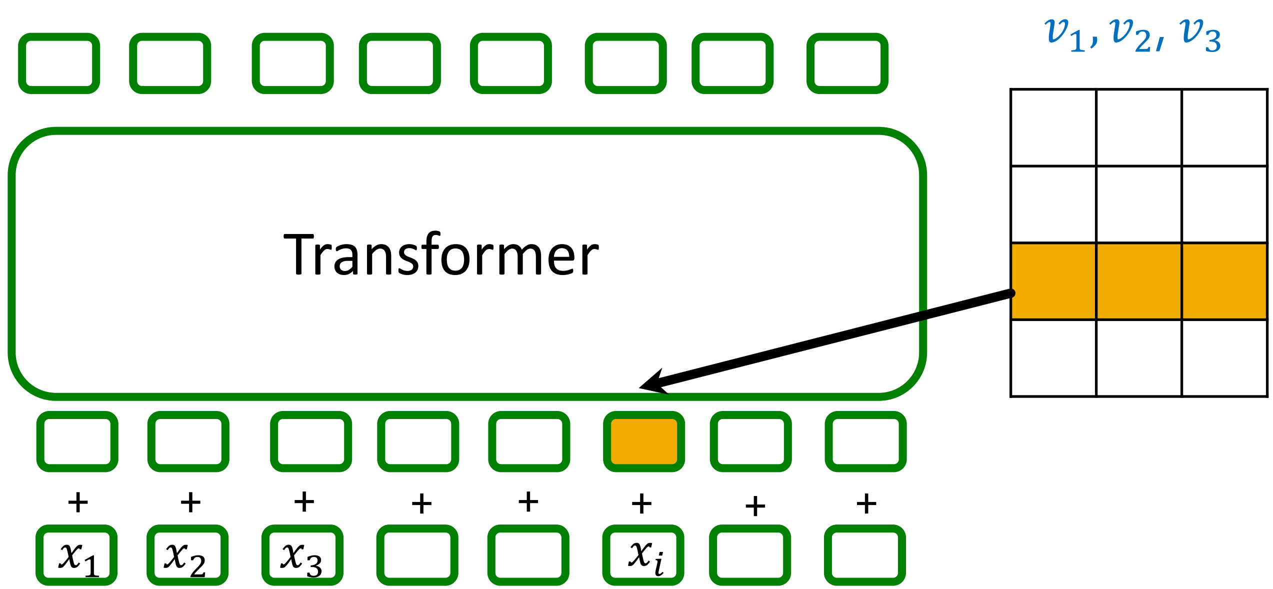
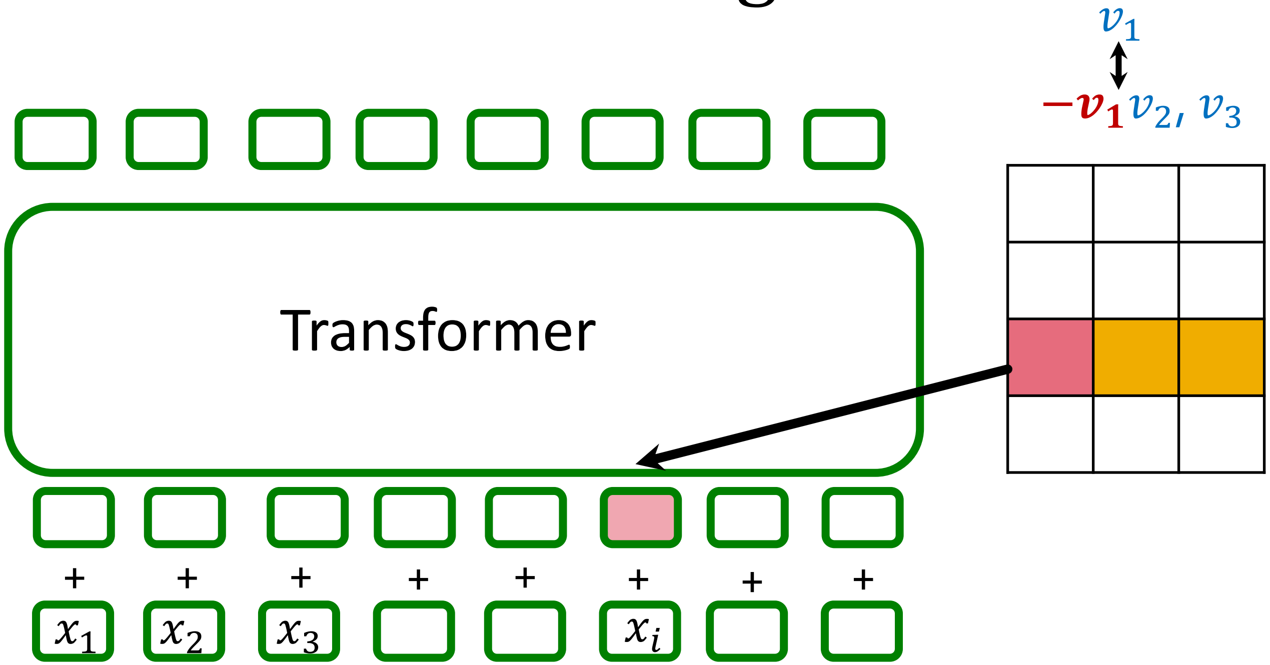
- **What if we picked the other sign?**



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!

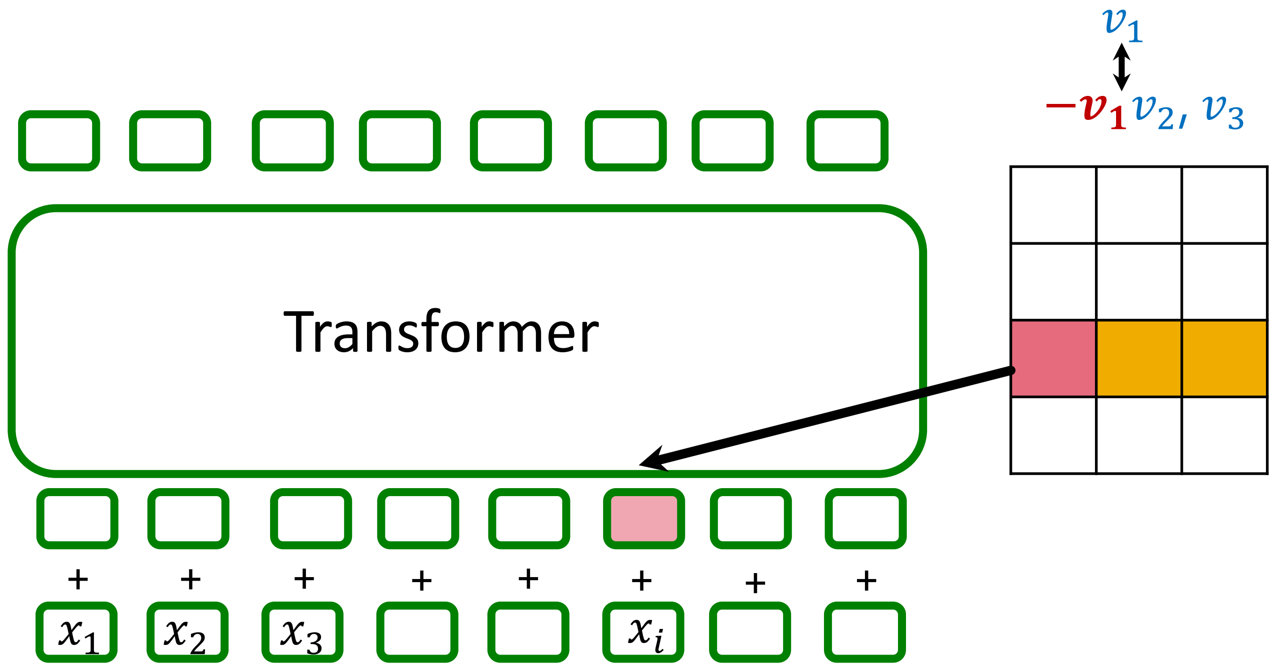


How to fix sign ambiguity

- **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



Sign Invariant Neural Networks

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

Sign Invariant Neural Networks

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Sign Invariant Neural Networks

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- **Goal:** design a neural network $f(v_1)$ such that

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- **Proposition:** f satisfies $f(v_1) = f(-v_1)$ if and only if there is a ϕ such that

$$f(v_1) = \phi(v_1) + \phi(-v_1)$$

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Proof:

<=: If $f(v_1) = \phi(v_1) + \phi(-v_1)$, then $f(-v_1) = \phi(-v_1) + \phi(v_1) = f(v_1)$,

=>: If $f(v_1) = f(-v_1)$, define $\phi(v_1) = f(v_1)/2$.

Then $\phi(v_1) + \phi(-v_1) = f(v_1)/2 + f(-v_1)/2 = f(v_1)$

Sign Invariant Neural Networks

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

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

Sign Invariant Neural Networks

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Use model for one eigenvector

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

Combine using another neural net $AGG = \rho$

Sign Invariant Neural Networks

- **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:**

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

$\rho, \phi =$ any neural network (MLP, GNN etc.)

SignNet

Sign Invariant Neural Networks

- **Recall Goal:** design a neural network $f(v_1, v_2, \dots v_k)$ such that:
  - $f(v_1, v_2, \dots v_k) = f(\pm v_1, \pm v_2, \dots \pm v_k)$ for all $\pm$ choices
    - **SignNet is sign invariant.**
  - f is "expressive"
    - **Is SignNet expressive?**

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

$\rho, \phi =$ any neural network (MLP, GNN etc.)

SignNet

Sign Invariant Neural Networks

- **Recall Goal:** design a neural network $f(v_1, v_2, \dots v_k)$ such that:
  - $f(v_1, v_2, \dots v_k)$ = $f(\pm v_1, \pm v_2, \dots \pm v_k)$ for all $\pm$ choices
    - **SignNet is sign invariant.**
  - f is "expressive"
    - **Is SignNet expressive?**

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

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

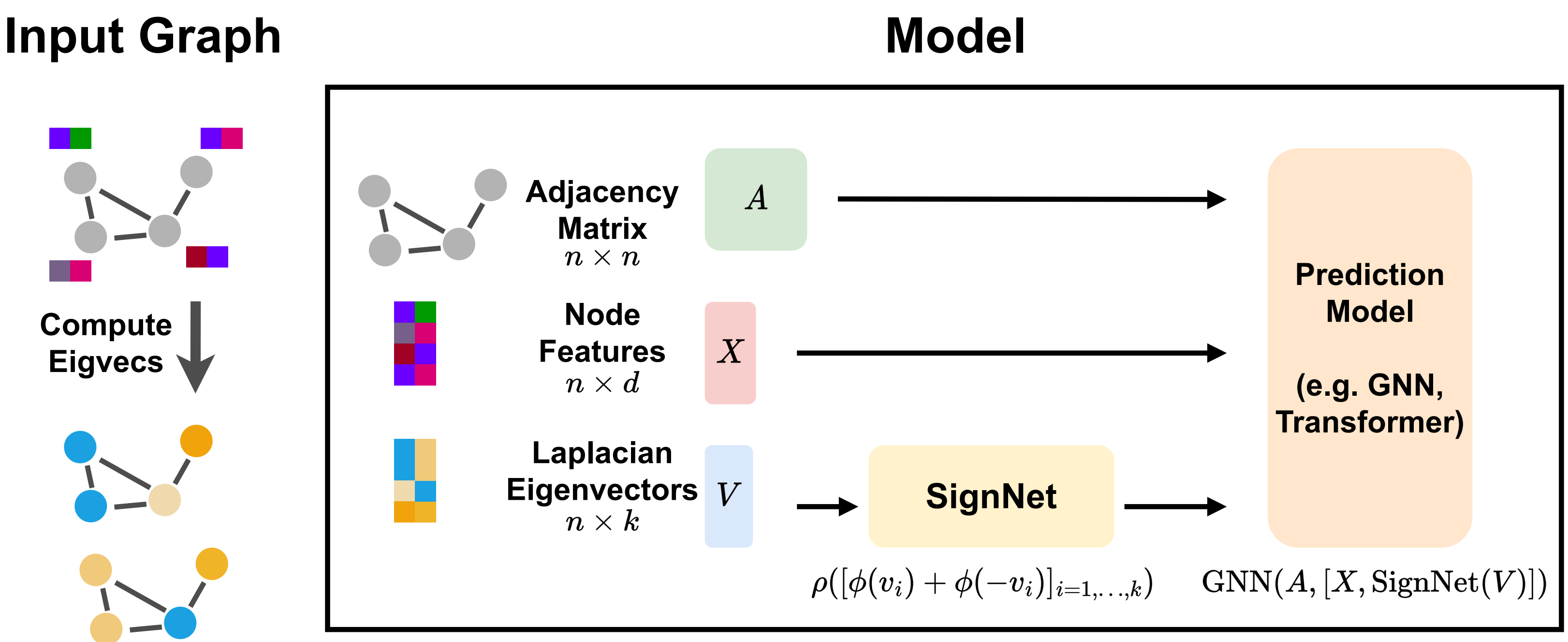
SignNet can express all sign invariant functions!!

Sign Invariant Neural Networks

- **Many eigenvector case**
- **Strategy:** 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
$$f(v_1) = \phi(v_1) + \phi(-v_1)$$

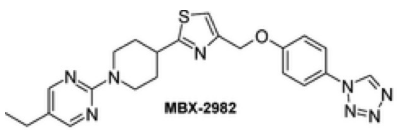
SignNet in practice

- **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.

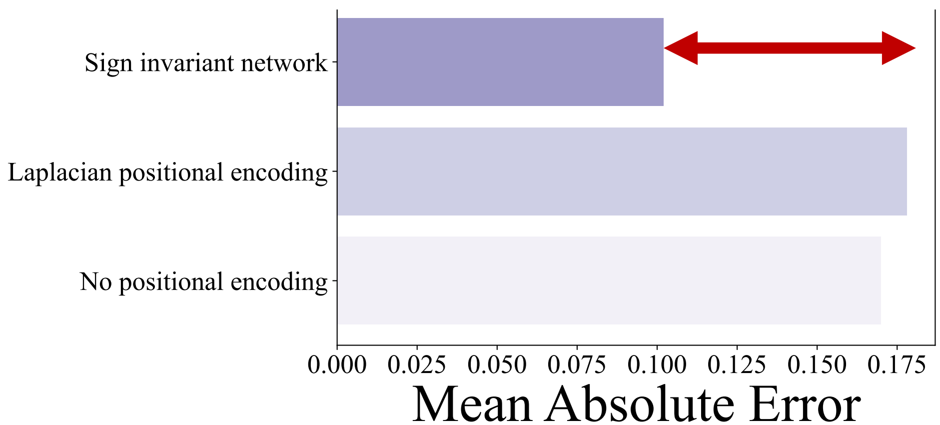


Small molecule property prediction with SignNet

- **Task:** given a small molecule, predict its **solubility**

$f($  $) =$ solubulity

50% reduction in test error



Plan for Today

- **Part 1:**
  - Transformers to message passing on fully connected graph
- **Part 2:**
  - New design landscape for graph Transformers
    - Tokenization
    - Positional encoding
    - Modified self-attention
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Summary: Graph Transformer Design Space

- New design space for graph Transformers