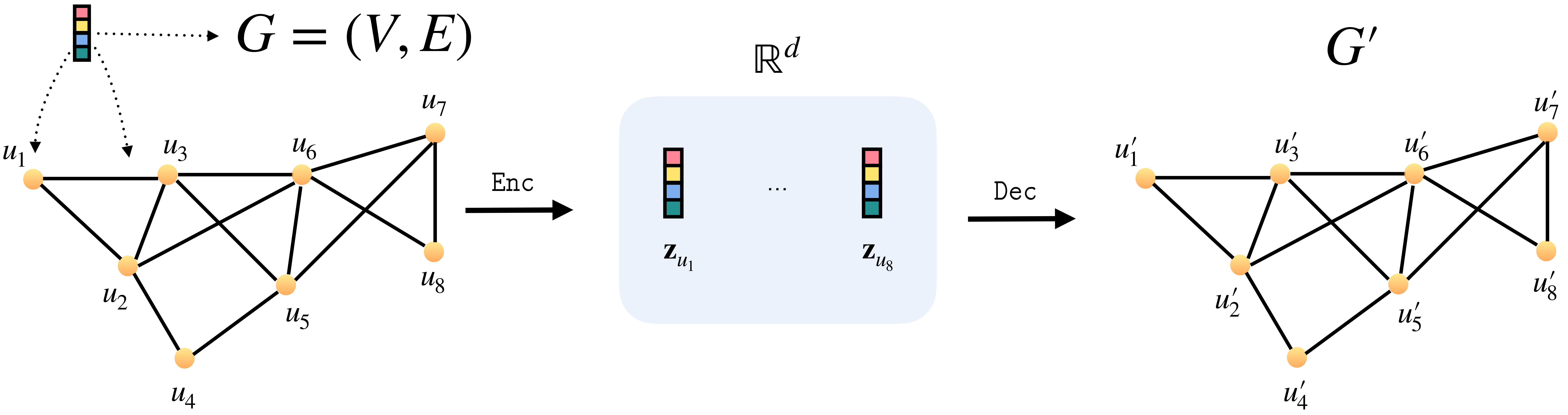
Lecture 4: Message Passing Neural Network Architectures

Relational Learning

İsmail İlkan Ceylan Advanced Topics in Machine Learning, University of Oxford 24.01.2022

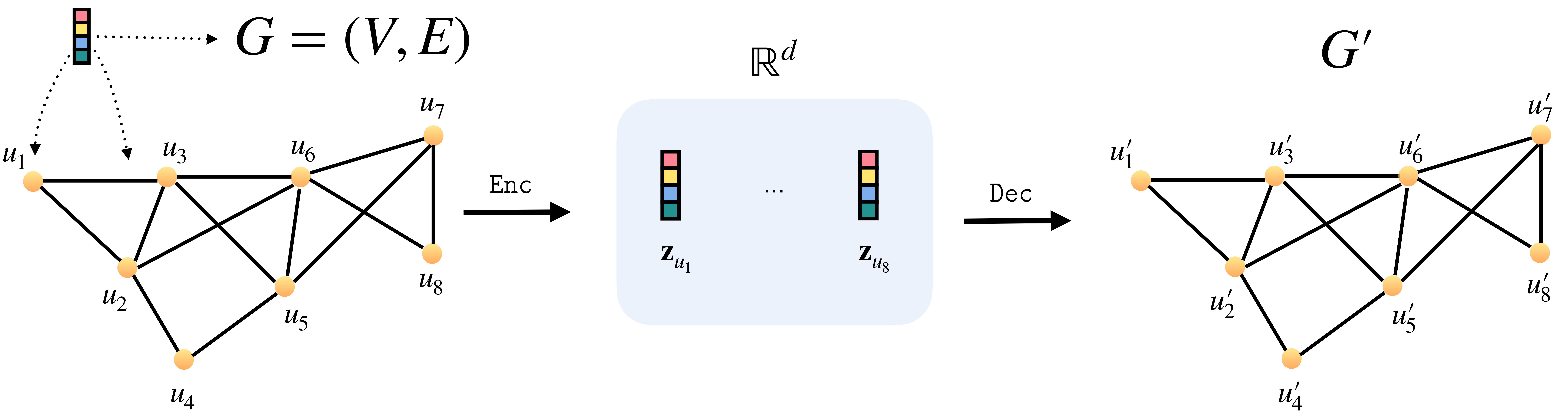
Encoder-Decoder



Knowledge Graph Embeddings

Lecture 1-2

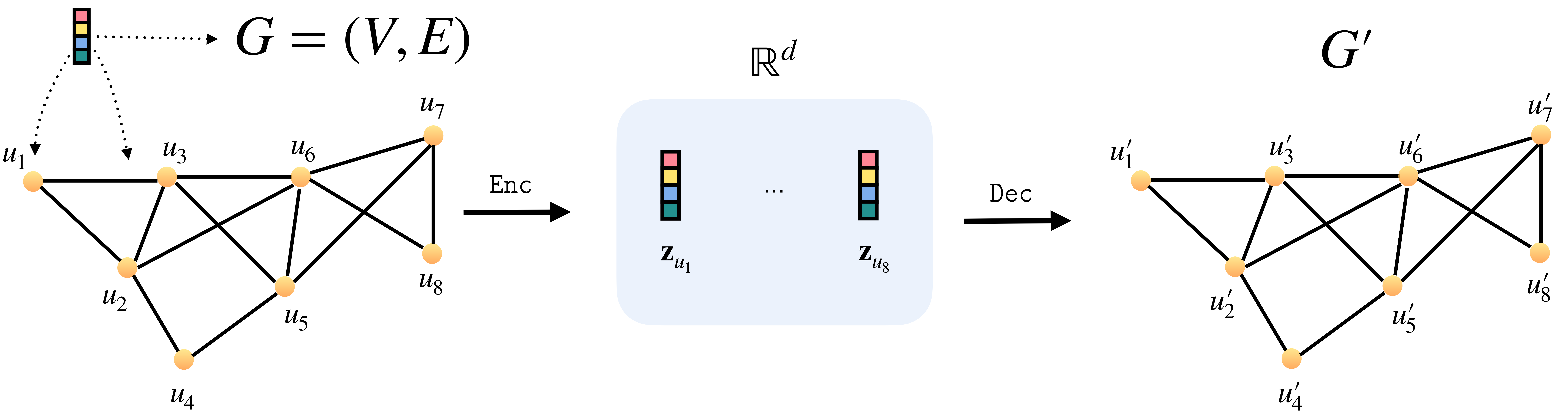
Encoder-Decoder



MPNNs (Lecture 3)

$$\mathbf{h}_u^{(t)} = \textit{combine}^{(t)}\left(\mathbf{h}_u^{(t-1)}, \textit{aggregate}^{(t)}\left(\left\{\mathbf{h}_v^{(t-1)} \mid v \in N(u)\right\}\right)\right)$$

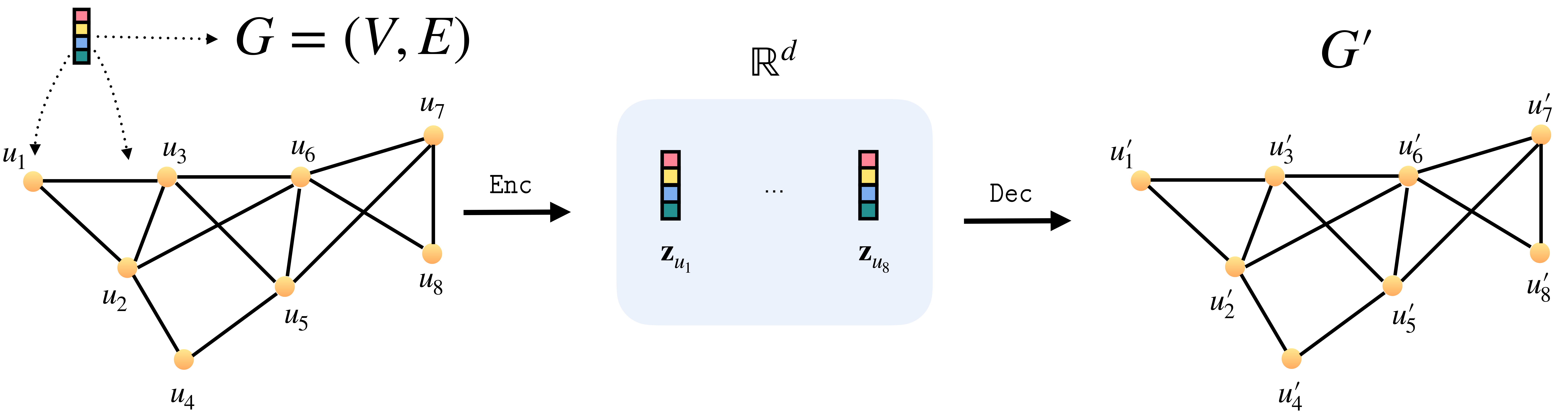
Encoder-Decoder



Base GNN Model (Lecture 3)

$$\mathbf{h}_u^{(t)} = \sigma\left(\mathbf{W}_{self}^{(t)}\mathbf{h}_u^{(t-1)} + \mathbf{W}_{neigh}^{(t)} \sum_{v \in N(u)} \mathbf{h}_v^{(t-1)}\right)$$

Encoder-Decoder



Today's Lecture

Popular GNN models

Overview

- Historical perspectives for graph neural network models
- Gated graph neural networks
- Graph convolutional networks
- Graph attention networks
- Graph isomorphism networks
- Relational message passing architectures
- Limitations of MPNNs: over-smoothing, over-squashing, inexpressiveness
- Summary

Historical Perspectives for Graph Neural Networks

From convolutions to graph convolutions:

Motivated by the success of convolutional neural networks: generalize Euclidean convolutions to the graph domain (Bruna et al., 2014) - Graph convolutional networks (Kipf and Welling, 2016).

From graph isomorphism testing to graph representation learning:

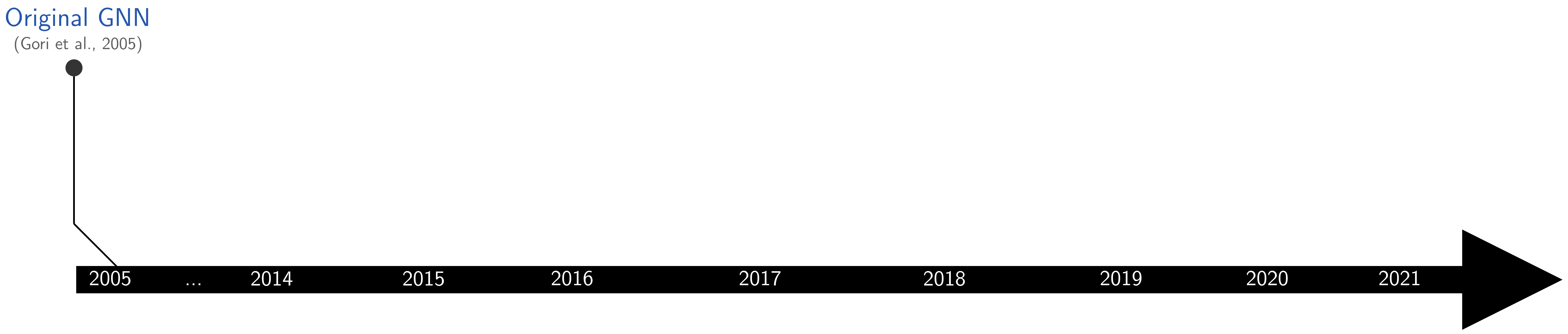
Learning over graphs requires to distinguish graphs: MPNNs cannot distinguish all graphs, and so they have limited expressive power. The connection to graph isomorphism testing offers many theoretical insights.

From belief propagation to MPNNs:

Message passing is used in the context of probabilistic graphical models (i.e., belief propagation (Pearl, 82)). Dai et al., (2016): Neural message passing algorithms are analogues of certain message passing algorithms common in variational inference to infer distributions over latent variables.

Graph Neural Networks

Graph Neural Networks



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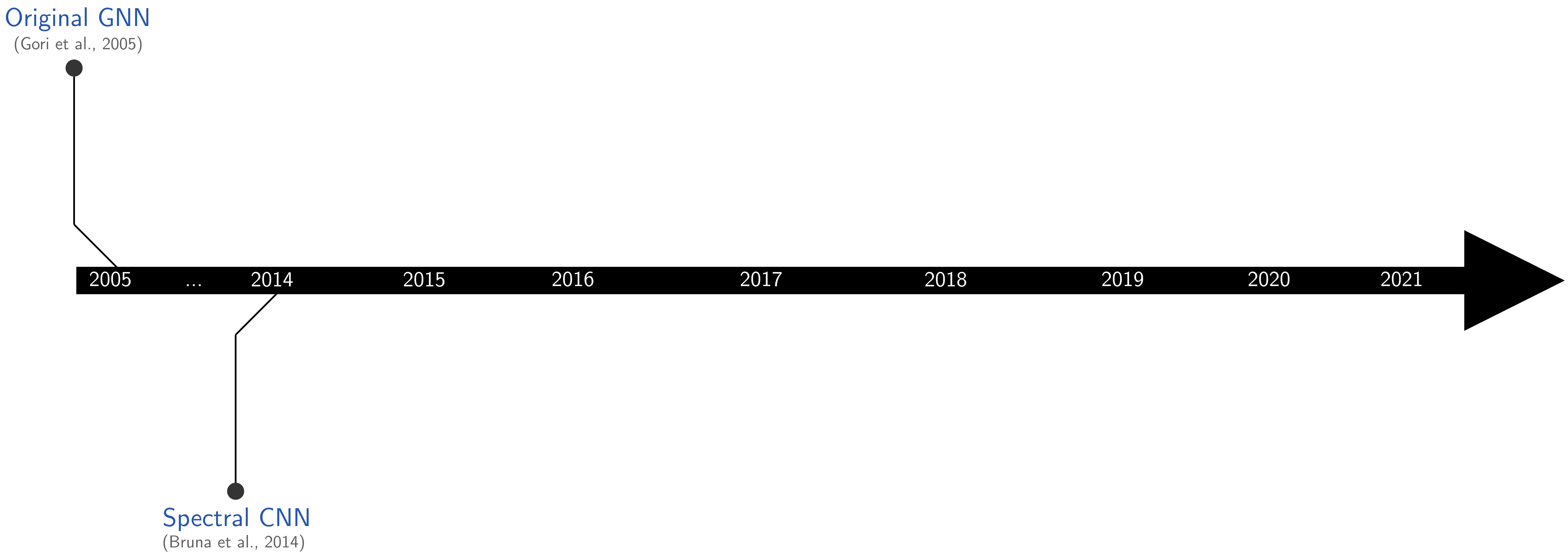

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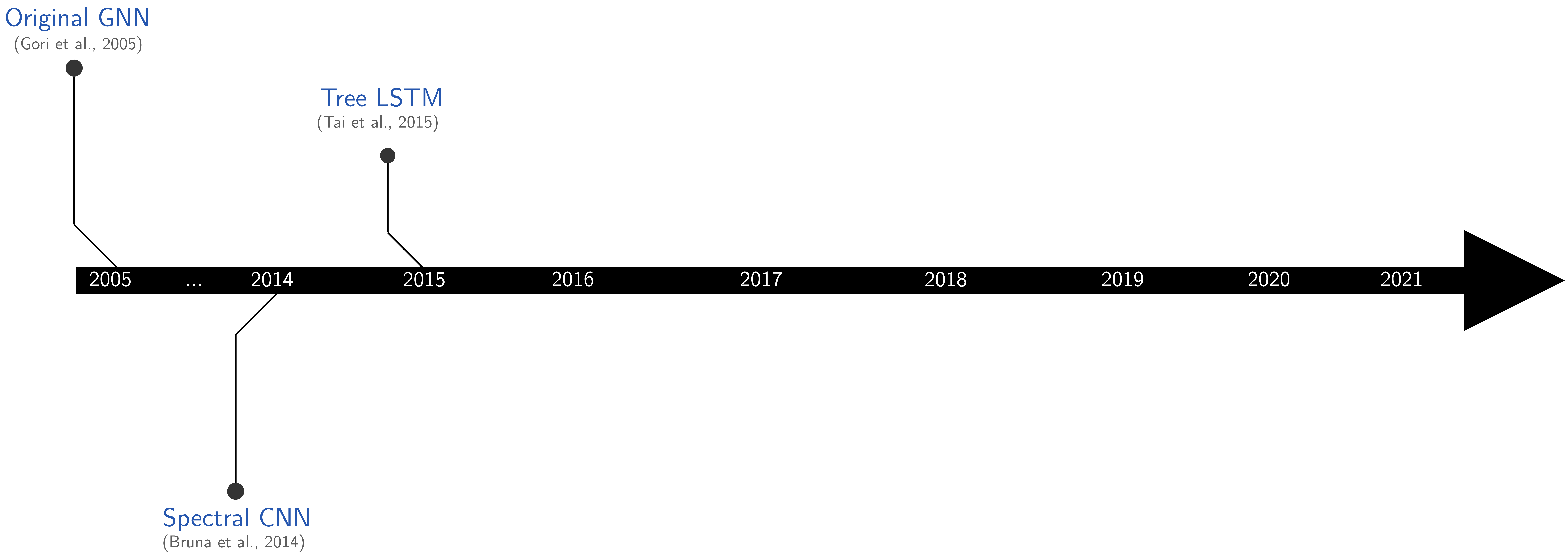

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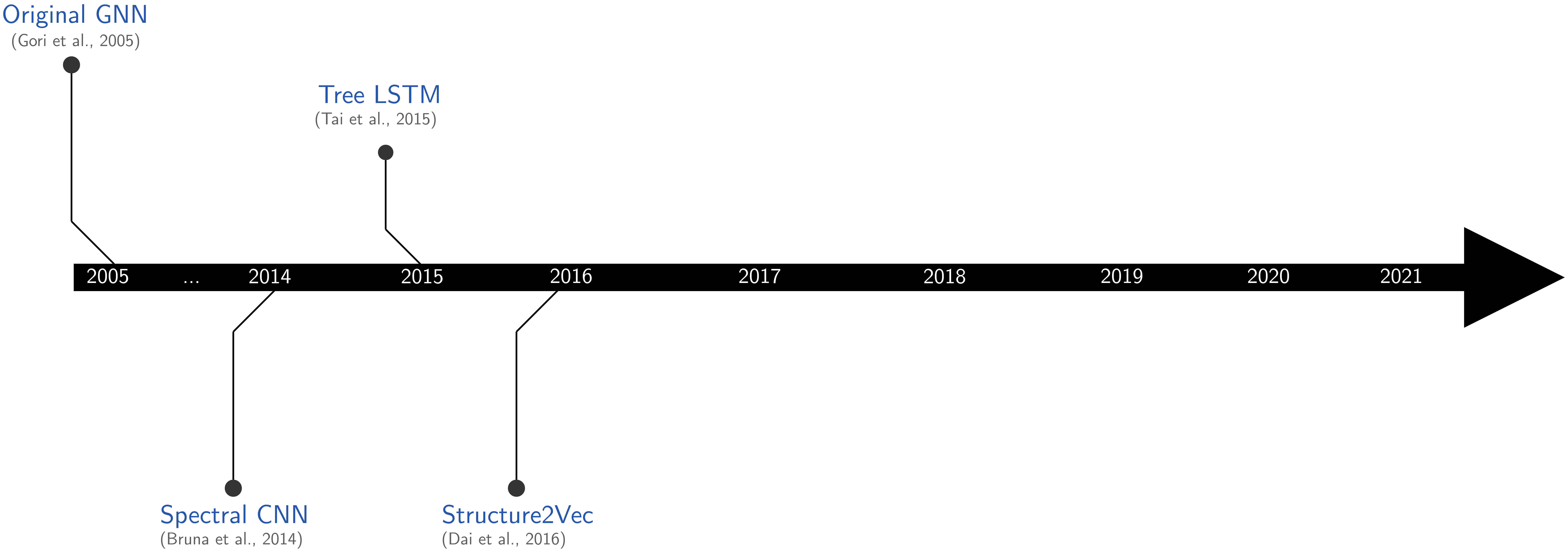

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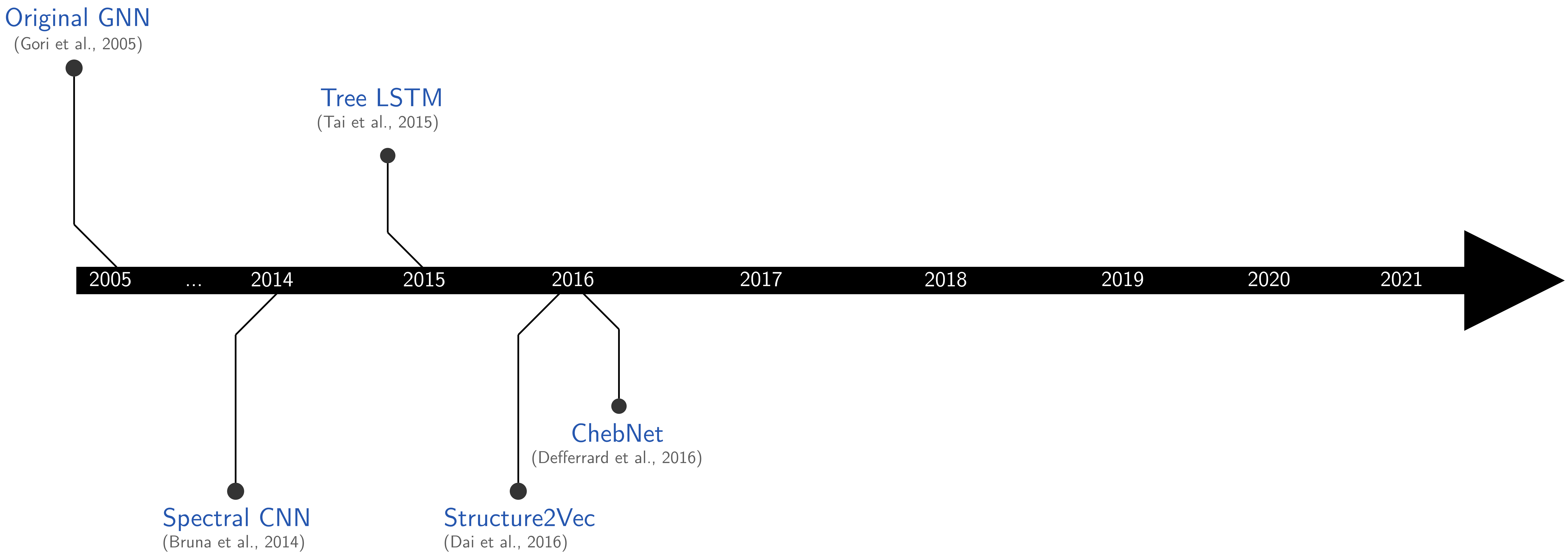

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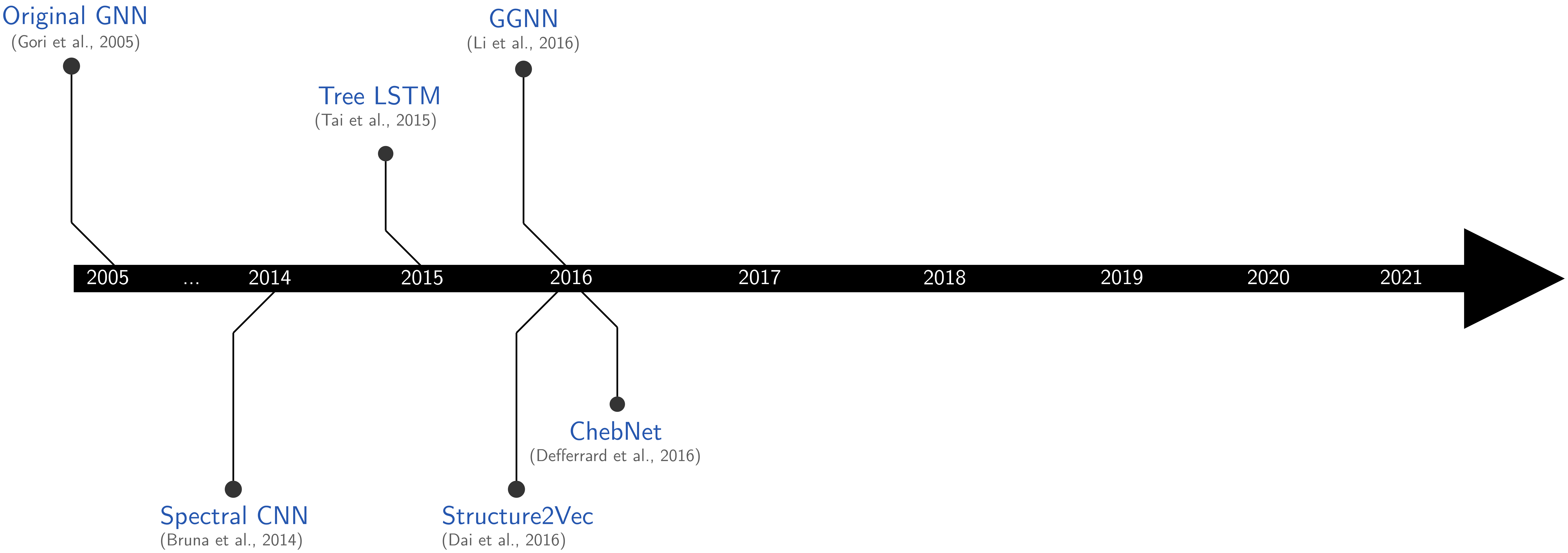

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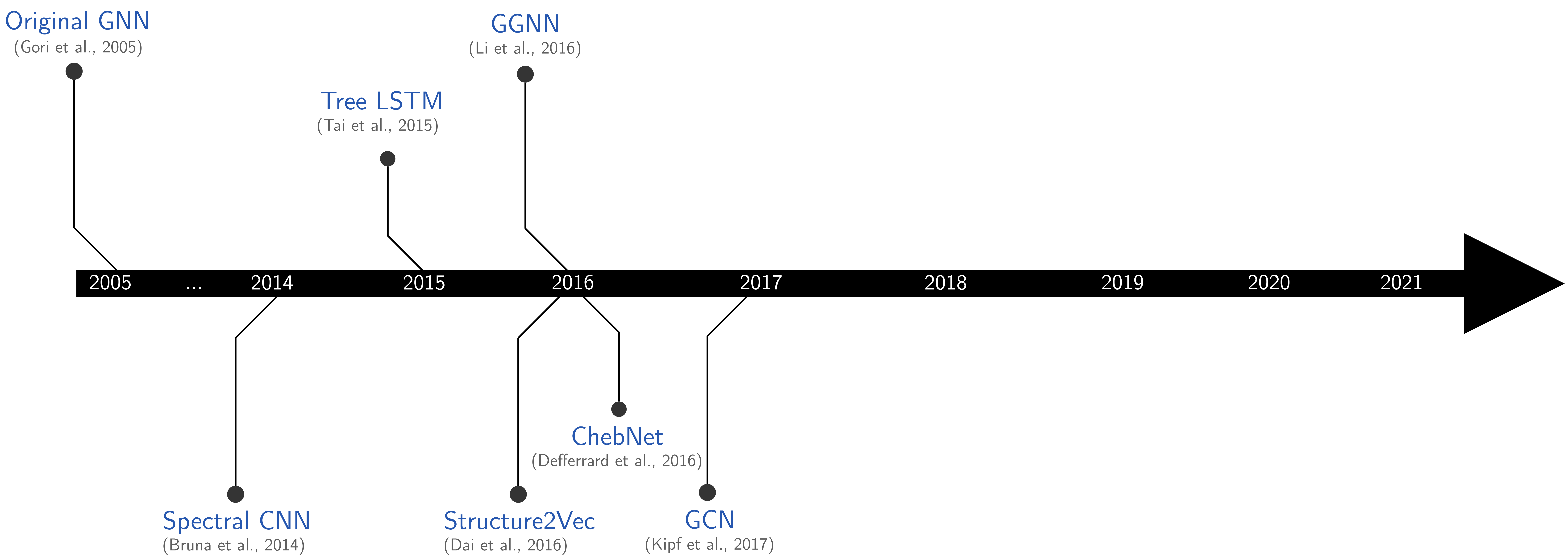

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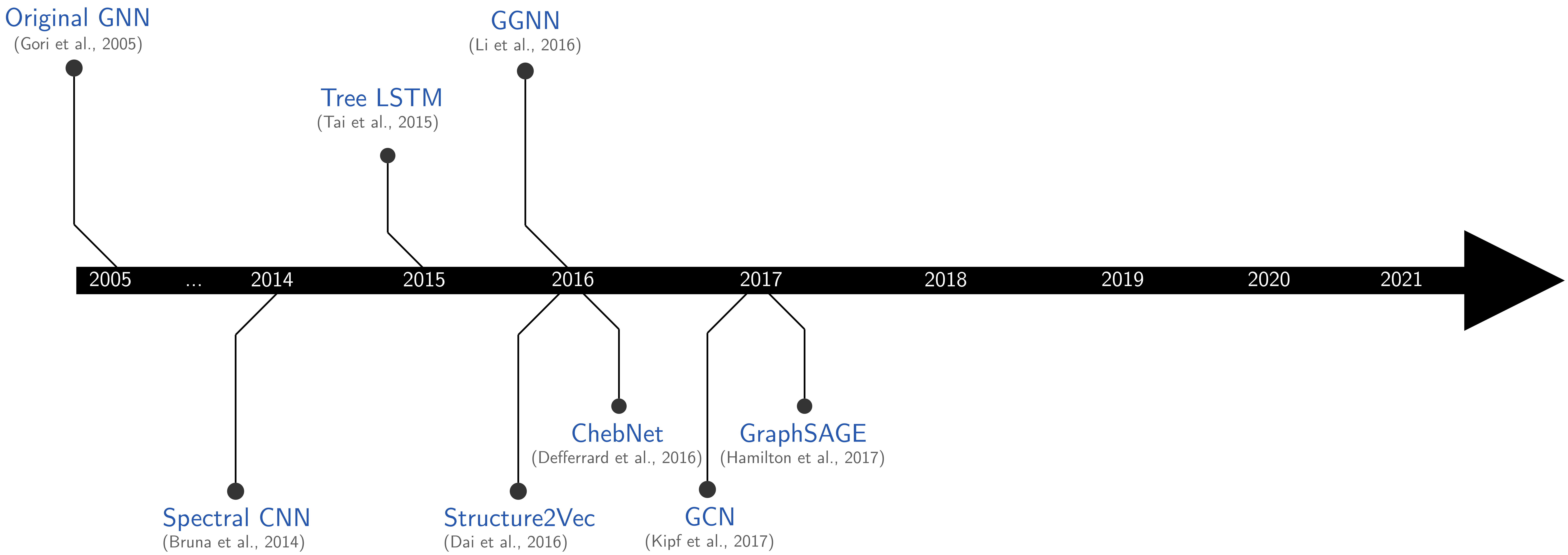

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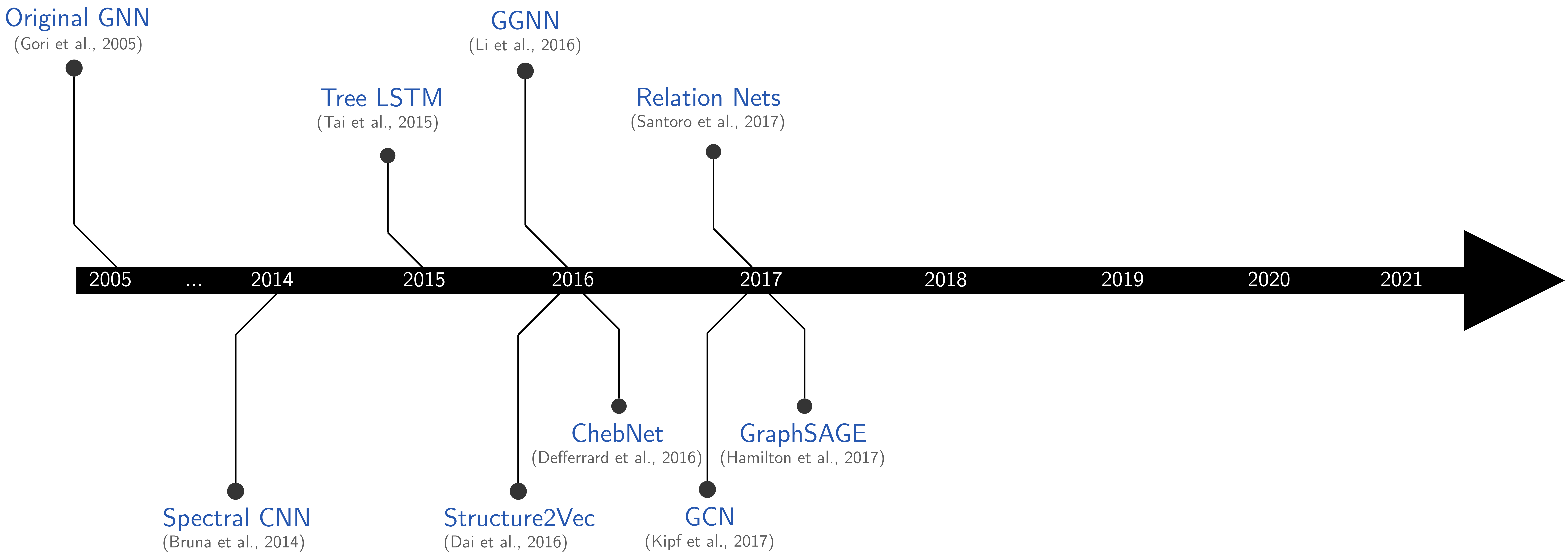

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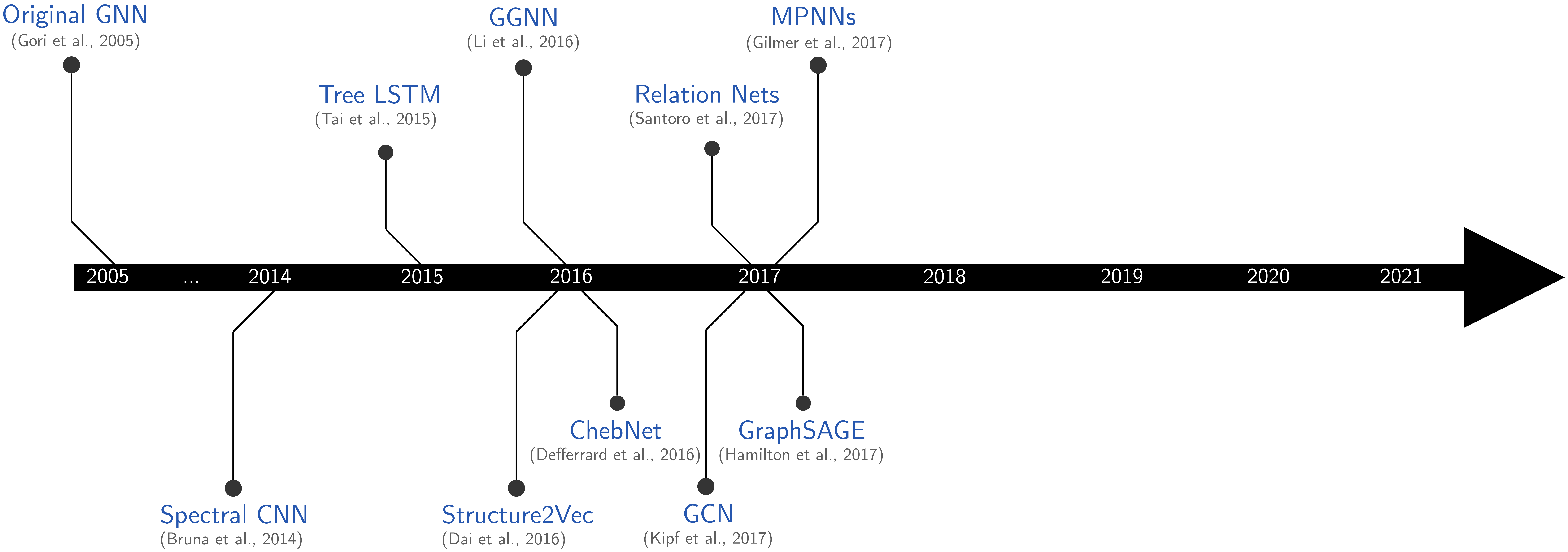

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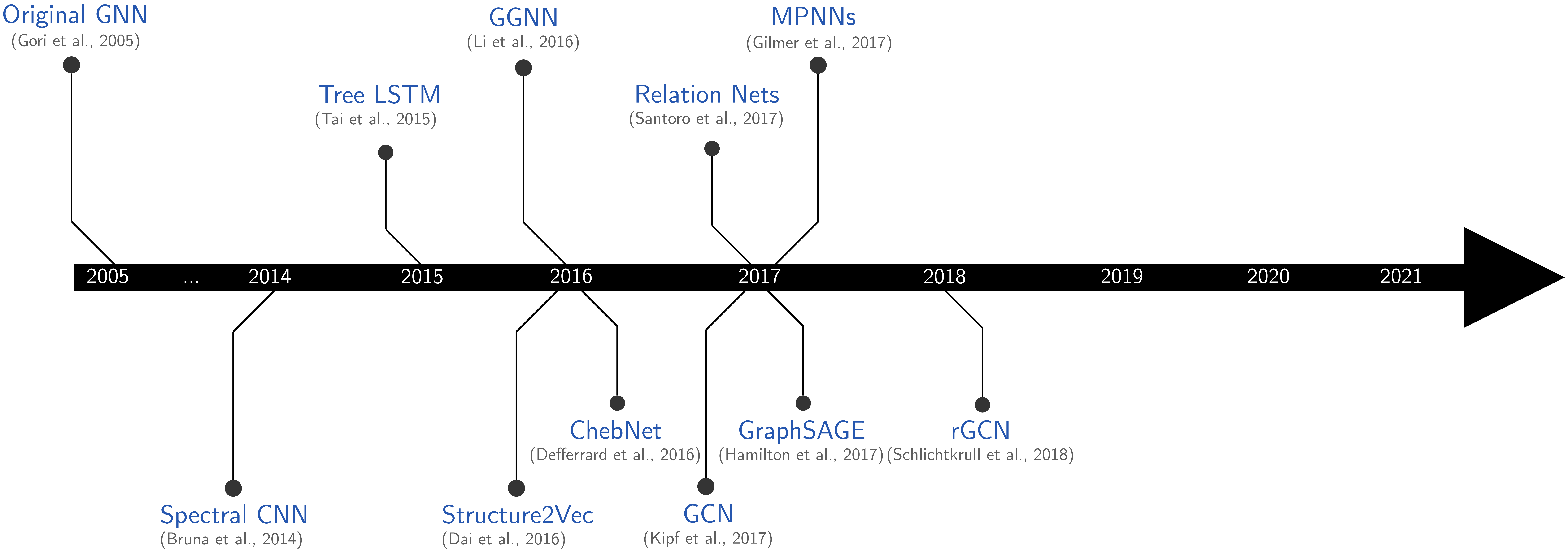

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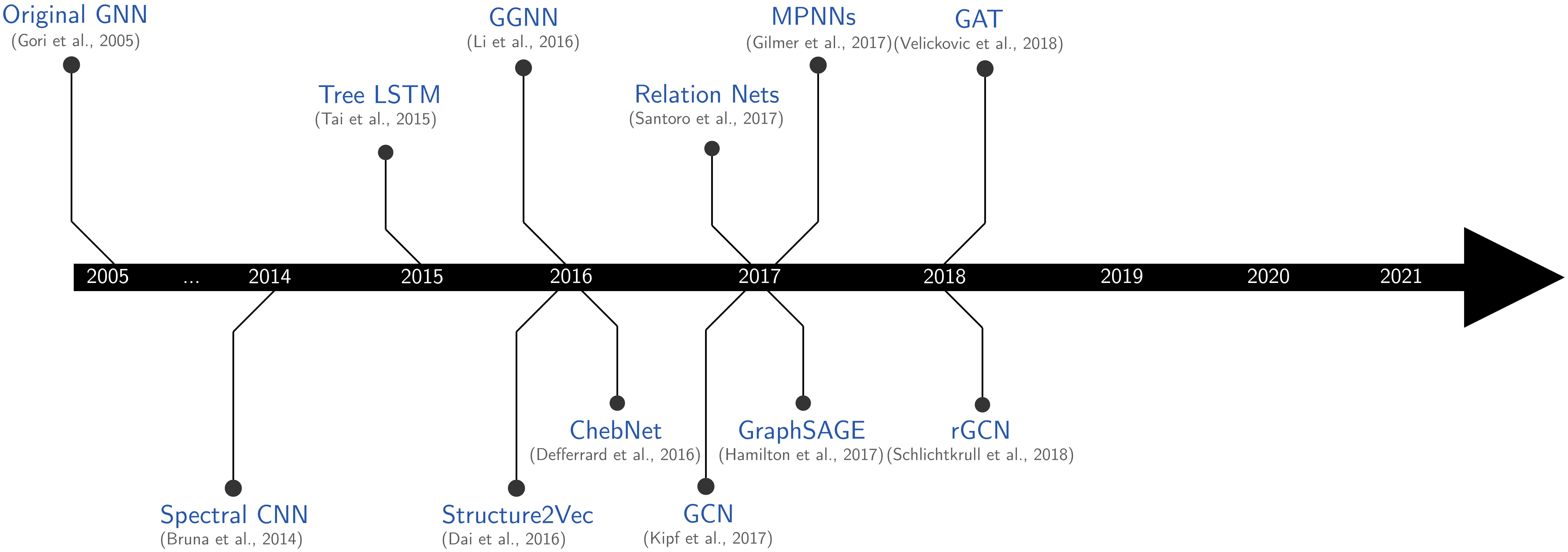

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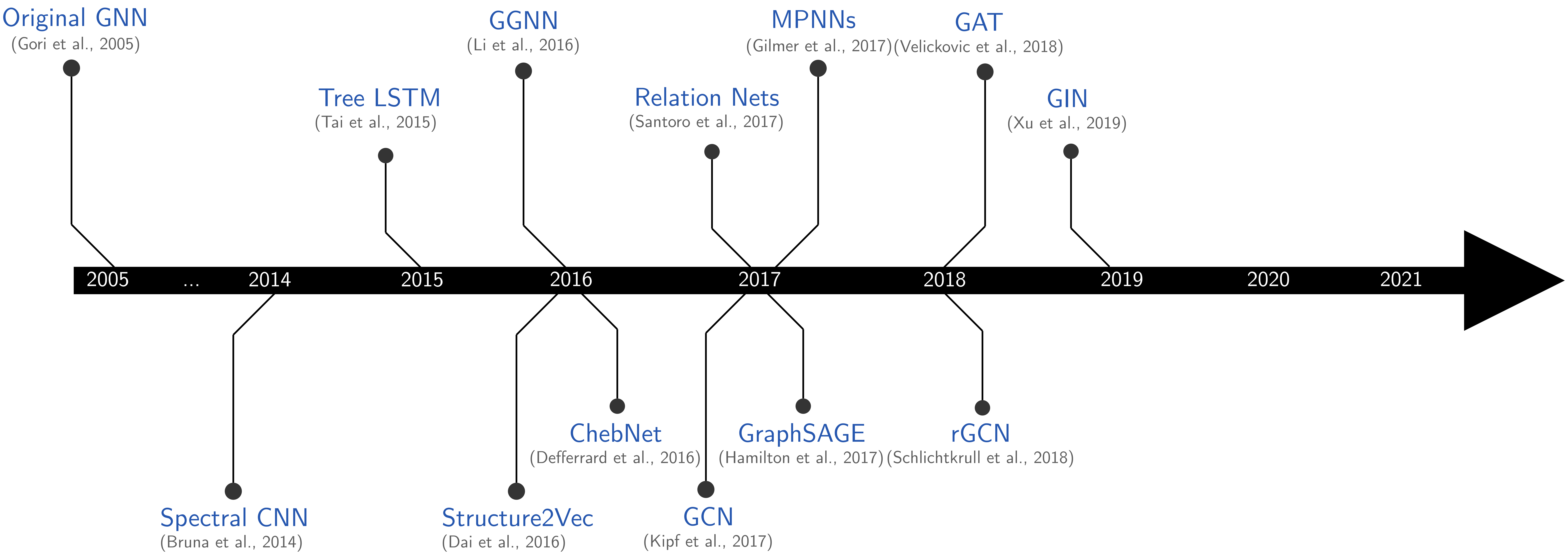

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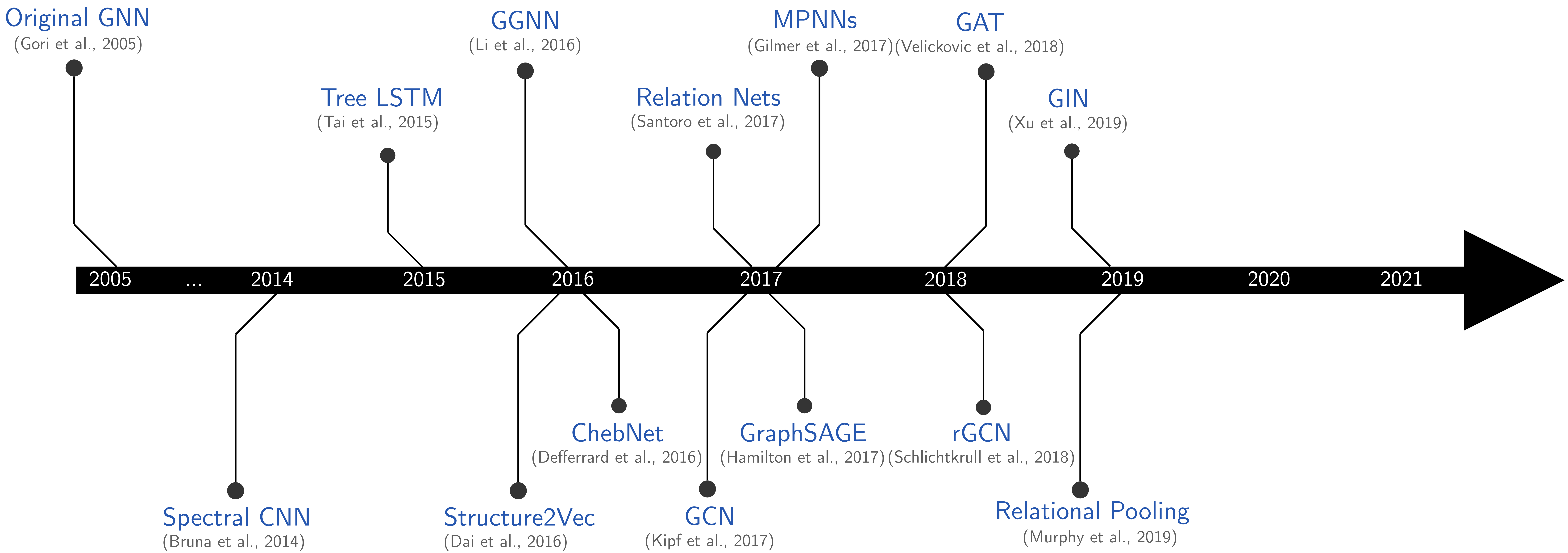

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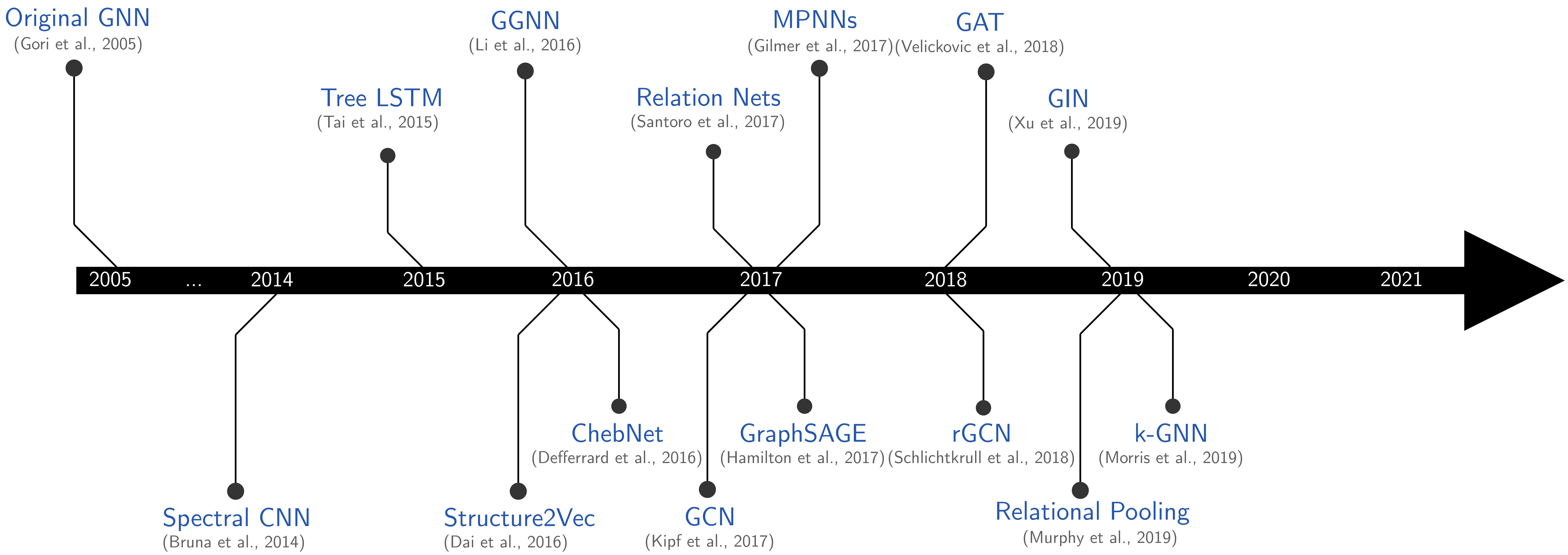

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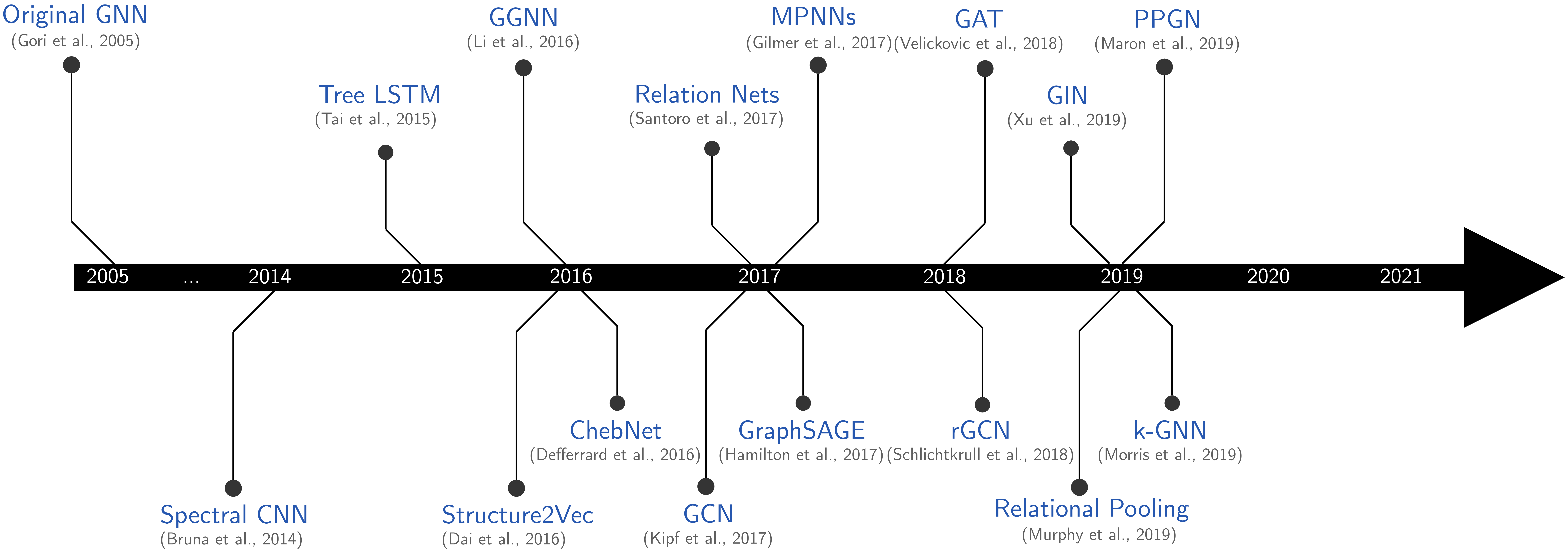

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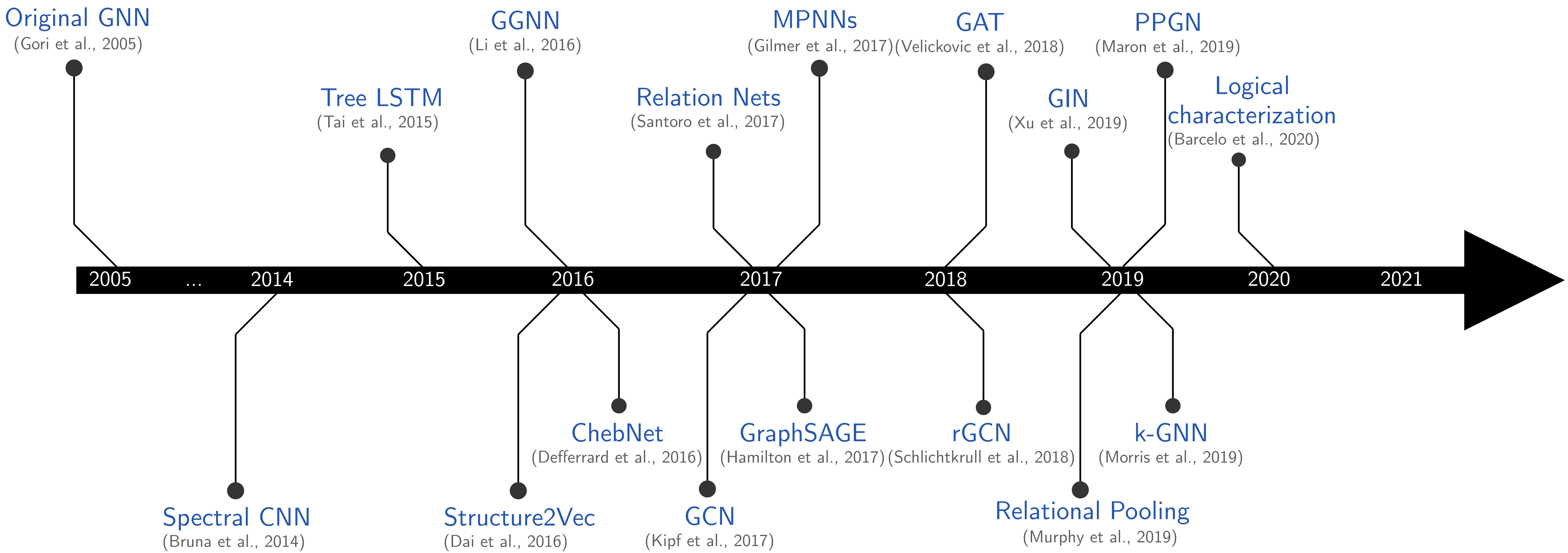

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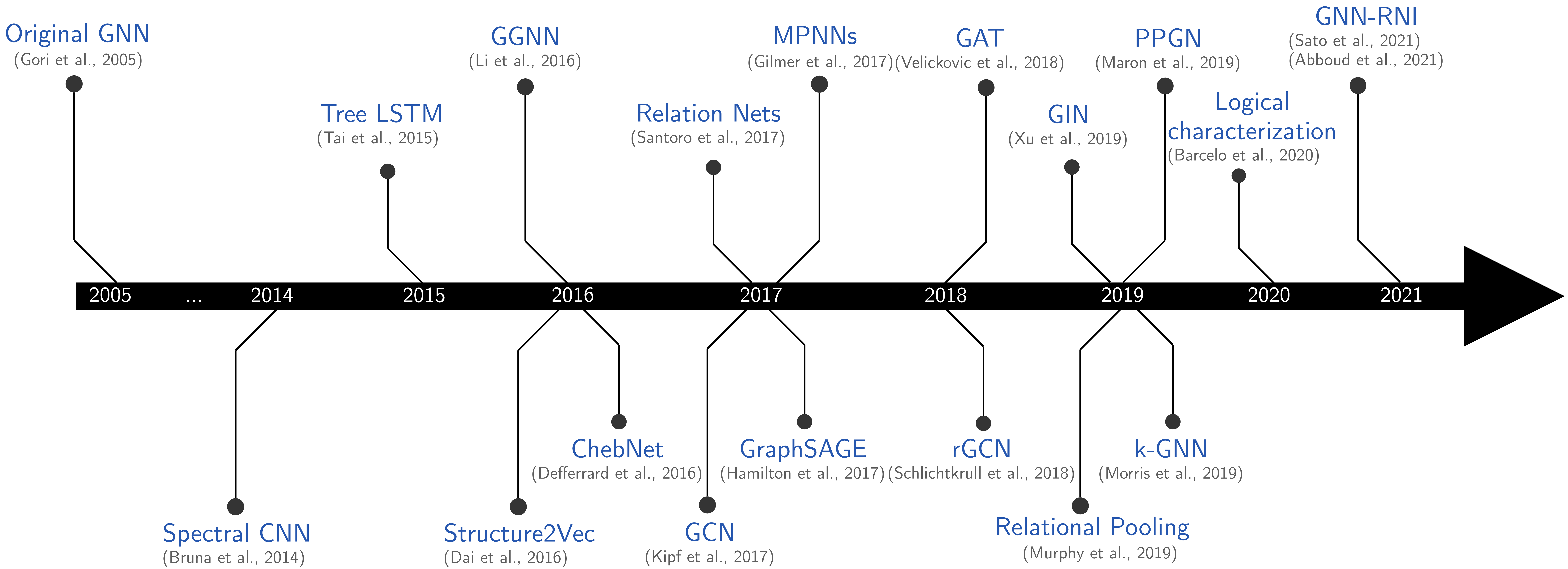

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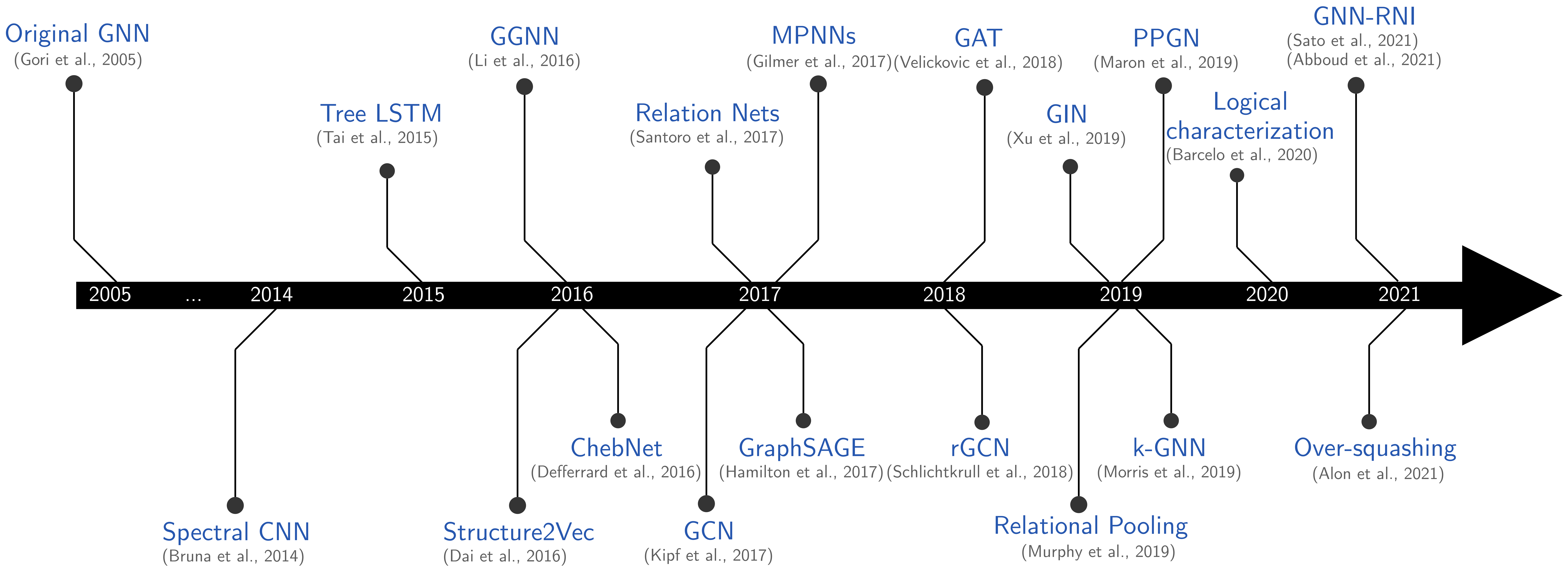

Gated Graph Neural Networks

Node Embeddings as a Sequence

MPNNs employ an iterative algorithm to learn node embeddings:

$$\mathbf{h}_u^{(t)} = \mathit{combine}^{(t)}\Big(\mathbf{h}_u^{(t-1)}, \mathit{aggregate}^{(t)}\big(\{\mathbf{h}_v^{(t-1)} \mid v \in N(u)\}\big)\Big)$$

Message passing can be seen as a sequential process:

- Every node has an initial state characterized by the node features $\mathbf{h}_u^{(0)} = \mathbf{x}_u$.
- Every node's state is updated after each message passing iteration based on:
  - Previous state of the node
  - States of the neighboring nodes
- This process terminates at the end of message passing, yielding final states.

Sequence Modeling: Refresher

Spam detection: Identify whether an email is spam or not.

- Sentences processed word by word by neural sequence models (e.g., GRU) and the state is updated based on
  - the most recent word,
  - a state which stores information about earlier words
- This process is repeated until we see each word, yields a final representation for the overall sentence.

Idea: Maintain a state in memory, and based on the new state and input, decide to retain or update your state:

$$\mathbf{R}^t = \sigma(\mathbf{X}^t\mathbf{W}_{xr} + \mathbf{H}^{(t-1)}\mathbf{W}_{hr} + \mathbf{b}_r) \qquad \mathbf{Z}^t = \sigma(\mathbf{X}^t\mathbf{W}_{xz} + \mathbf{H}^{(t-1)}\mathbf{W}_{hz} + \mathbf{b}_z)$$

$$\tilde{\mathbf{H}}^t = \tanh(\mathbf{X}^t\mathbf{W}_{xh} + \left(\mathbf{R}^t \odot \mathbf{H}^{(t-1)}\right)\mathbf{W}_{hh} + \mathbf{b}_h) \qquad \mathbf{H}^t = \mathbf{Z}^t \odot \mathbf{H}^{t-1} + (1 - \mathbf{Z}^t) \odot \tilde{\mathbf{H}}^t$$

Gated Graph Neural Networks

Using the state abstraction for nodes in a graph, MPNNs can employ three separate computations:

1. **Message computation**: Based on a node's current state
2. **Message aggregation**: Node-level aggregation
3. **State update**: A recurrent unit takes the current state, the aggregation of messages, and updates.

Gated graph neural networks (Li et al., 2016), update the representation $\mathbf{h}_u$ for each node $u \in V$ as:

$$\mathbf{h}_u^{(t)} = GRU\left(\mathbf{h}_u^{(t-1)}, \sum_{v \in N(u)} \mathbf{W}^{(t)} \mathbf{h}_v^{(t-1)}\right)$$

Message computation via multiplication by a weight matrix, aggregate by sum, and combine with a GRU.

Graph Convolutional Networks

Graph Convolutional Networks

The base GCN model is an instance of the MPNN framework and defined as:

$$\mathbf{h}_u^{(t)} = \sigma\left(\mathbf{W}^{(t)} \sum_{v \in N(u) \cup \{u\}} \frac{\mathbf{h}_v^{(t-1)}}{\sqrt{N(u) + N(v)}}\right)$$

The base MPNN model is very similar to the base MPNN with self-loops (modulo normalization):

$$\mathbf{h}_u^{(t)} = \sigma\left(\mathbf{W}^{(t)} \sum_{v \in N(u) \cup \{u\}} \mathbf{h}_v^{(t-1)}\right)$$

Question: Can we view this model as applying convolutions over graphs?

Idea: View each message as a signal and matrix transformations applying to the signals as convolutions.

Revisiting the Basic Model

The base MPNN model is defined as a node-level equation:

$$\mathbf{h}_u^{(t)} = \sigma\left(\mathbf{W}_{self}^{(t)}\mathbf{h}_u^{(t-1)} + \mathbf{W}_{neigh}^{(t)} \sum_{v \in N(u)} \mathbf{h}_v^{(t-1)}\right)$$

The base MPNN model can be written as a graph-level equation:

$$\mathbf{H}^{(t)} = \sigma\left(\mathbf{H}^{(t-1)}\mathbf{W}_{self}^{(t)} + \mathbf{A}\ \mathbf{H}^{(t-1)}\mathbf{W}_{neigh}\right),$$

...where the matrix $\mathbf{H}^{(t)} \in \mathbb{R}^{|V_G| \times d}$ has the node representations at layer t.

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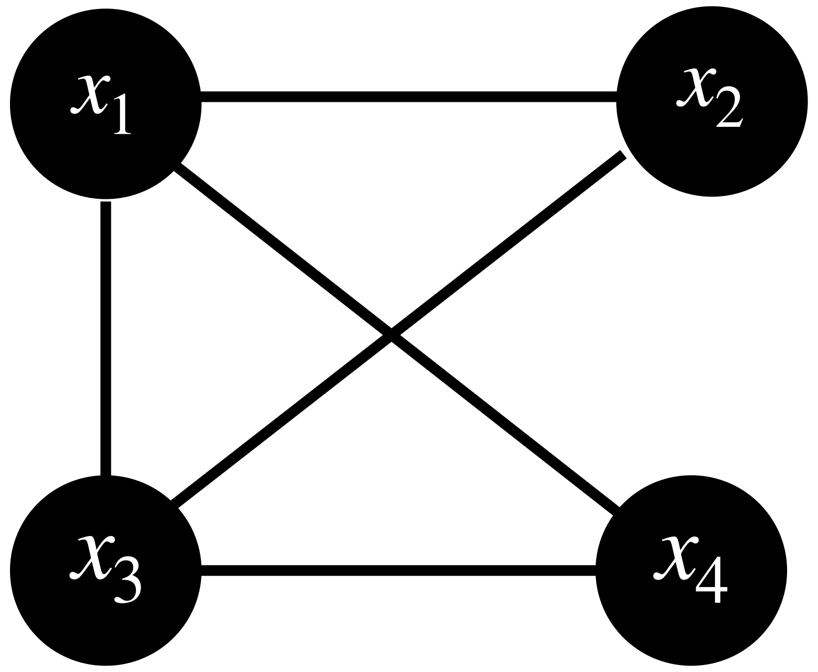
MPNN layers apply a filter $\mathbf{Q} = \mathbf{I} + \mathbf{A}$, combined with some weight matrices and a non-linearity.

Convolution based on spectral properties of the graph, e.g., via the adjacency matrix! Other matrices?

Graph Laplacian



$$\begin{bmatrix} 3 & 0 & 0 & 0 \\ 0 & 2 & 0 & 0 \\ 0 & 0 & 3 & 0 \\ 0 & 0 & 0 & 2 \end{bmatrix} \qquad \begin{bmatrix} 0 & 1 & 1 & 1 \\ 1 & 0 & 1 & 0 \\ 1 & 1 & 0 & 1 \\ 1 & 0 & 1 & 0 \end{bmatrix} \qquad \begin{bmatrix} 3 & -1 & -1 & -1 \\ -1 & 2 & -1 & 0 \\ -1 & -1 & 3 & -1 \\ -1 & 0 & -1 & 2 \end{bmatrix}$$

$$\mathbf{D} \qquad \mathbf{A} \qquad \mathbf{L} = \mathbf{D} - \mathbf{A}$$

Property: Commutativity of the filter with the adjacency matrix $\mathbf{AQ} = \mathbf{QA}$ or Laplacian $\mathbf{LQ} = \mathbf{QL}$.

Symmetric Normalized Filters

Filters are typically normalized to ensure that they have bounded spectra, and thus ensure numerical stability.

Symmetric normalized Laplacian $$\mathbf{L}_{sym} = \mathbf{D}^{-\frac{1}{2}}\mathbf{L}\mathbf{D}^{-\frac{1}{2}}$$

Symmetric normalized adjacency matrix $$\mathbf{A}_{sym} = \mathbf{D}^{-\frac{1}{2}}\mathbf{A}\mathbf{D}^{-\frac{1}{2}}$$

$$\mathbf{L}_{sym} = \mathbf{I} - \mathbf{A}_{sym}$$

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$$\mathbf{L}_{sym} = \mathbf{I} - \mathbf{A}_{sym}$$

These matrices share the set $\mathbf{U}$ of eigenvectors and are symmetrically diagonalizable:

$$\mathbf{L}_{sym} = \mathbf{U}\boldsymbol{\Lambda}\mathbf{U}^\top \qquad \mathbf{A}_{sym} = \mathbf{U}(\mathbf{I} - \boldsymbol{\Lambda})\mathbf{U}^\top$$

...where $\boldsymbol{\Lambda}$ is the diagonal matrix containing the Laplacian eigenvalues.

Observation: Filters based on one of these matrices implies commutativity with the other.

Graph Convolutional Networks

Symmetric normalized adjacency matrix with self-loop (and variants) widely adopted as filters in practice:

$$\hat{\mathbf{A}} = \left(\mathbf{D} + \mathbf{I}\right)^{-\frac{1}{2}}\left(\mathbf{I} + \mathbf{A}\right)\left(\mathbf{D} + \mathbf{I}\right)^{-\frac{1}{2}}$$

This is the convolutional filter underlying the basic graph convolutional network (GCN) model:

$$\mathbf{H}^{(t)} = \sigma\left(\hat{\mathbf{A}}\ \mathbf{H}^{(t-1)}\mathbf{W}^{(t)}\right) \qquad \mathbf{h}_u^{(t)} = \sigma\left(\mathbf{W}^{(t)} \sum_{v \in N(u) \cup \{u\}} \frac{\mathbf{h}_v^{(t-1)}}{\sqrt{N(u) + N(v)}}\right)$$

Intuitively, in the base GCN model:

- $\hat{\mathbf{A}}$ enables messaging between neighbors and with node's self representation through the identity.
- $\hat{\mathbf{A}}$ is a well-defined convolution over graphs: commutativity with the adjacency matrix.
- Node's own embedding is treated identically to messages from other nodes: self-loops. Variations exist.

Graph Attention Networks

Learning Aggregation

Pre-defined, fixed aggregation schemes based on, e.g., graph structure:

$$\sum_{v \in N(u) \cup \{u\}} \mathbf{h}_v^{(t-1)} \qquad \sum_{v \in N(u)} \mathbf{W}\mathbf{h}_v^{(t-1)} \qquad \sum_{v \in N(u) \cup \{u\}} \frac{\mathbf{h}_v^{(t-1)}}{\sqrt{N(u) + N(v)}}$$

Some learnable approaches to aggregation exist but uniform nevertheless.

Question: Can we learn to aggregate not necessarily uniformly across neighbors?

Idea: Use attention as a means to non-uniformly aggregate over the neighborhood.

Background: Attention models obtained strong results in, e.g., machine translation (Bahdanau et al., 2015).

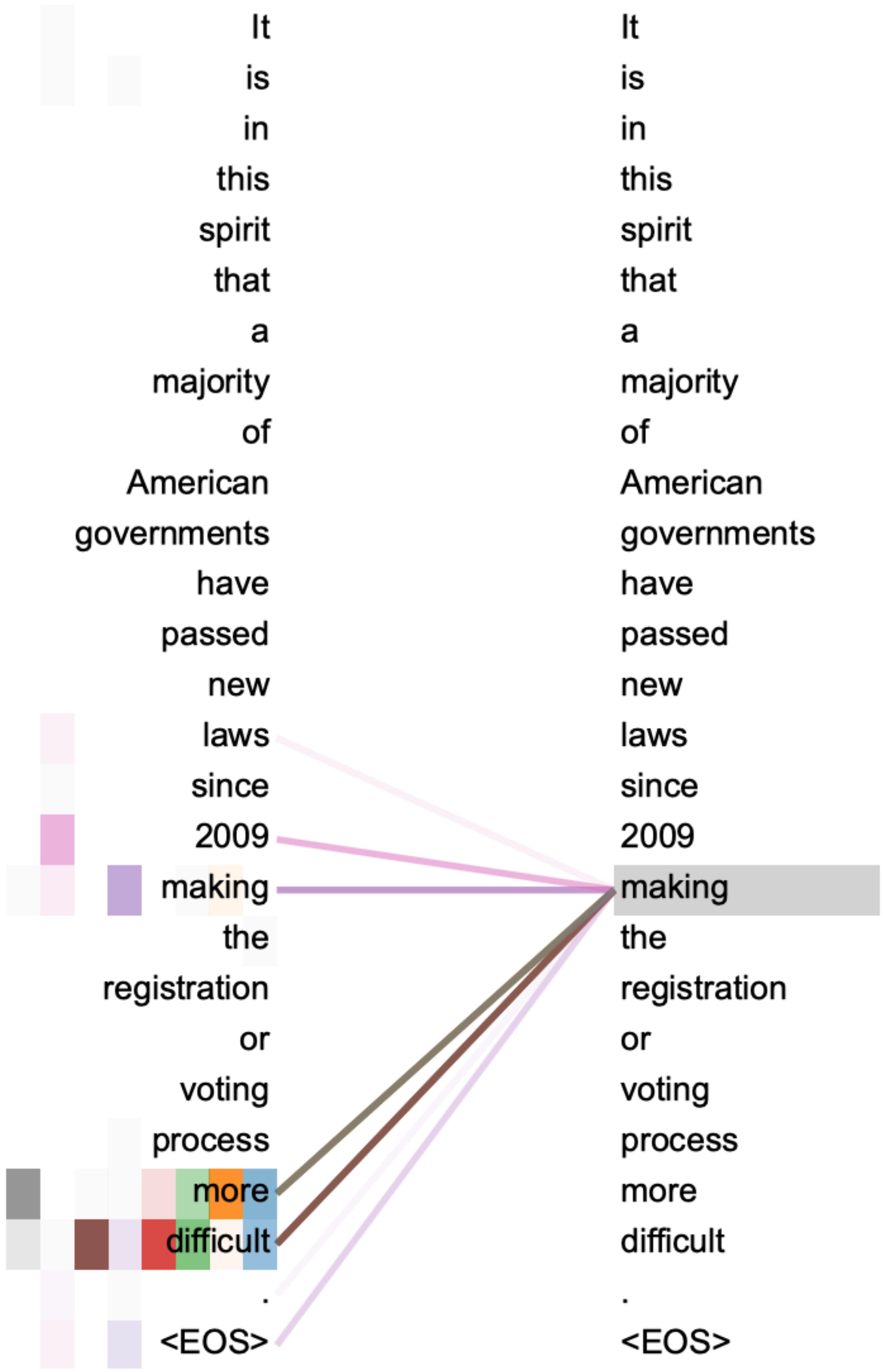
Attention

Attention: Allocate different weights to distinct inputs, based on their relevance to the learned task.

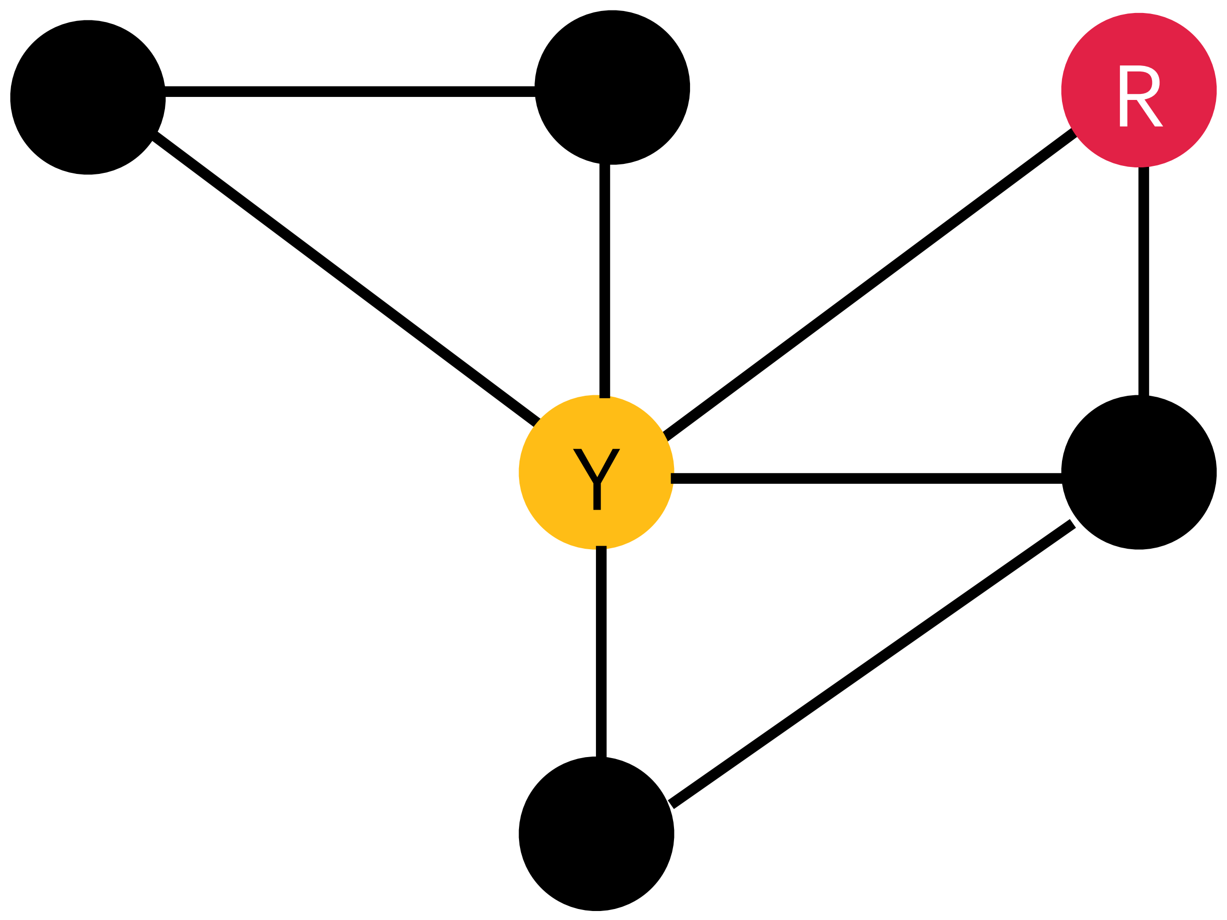
Transformer (Vaswani et al., 2017): Figure shows attention weights for the word 'making' encoding "making more difficult".

Breaking uniformity: Attend to more relevant tokens, rather than uniformly considering all possible tokens.

Graph attention: A node can benefit from weighing the relative importance of its neighbors.



Attention over Graphs



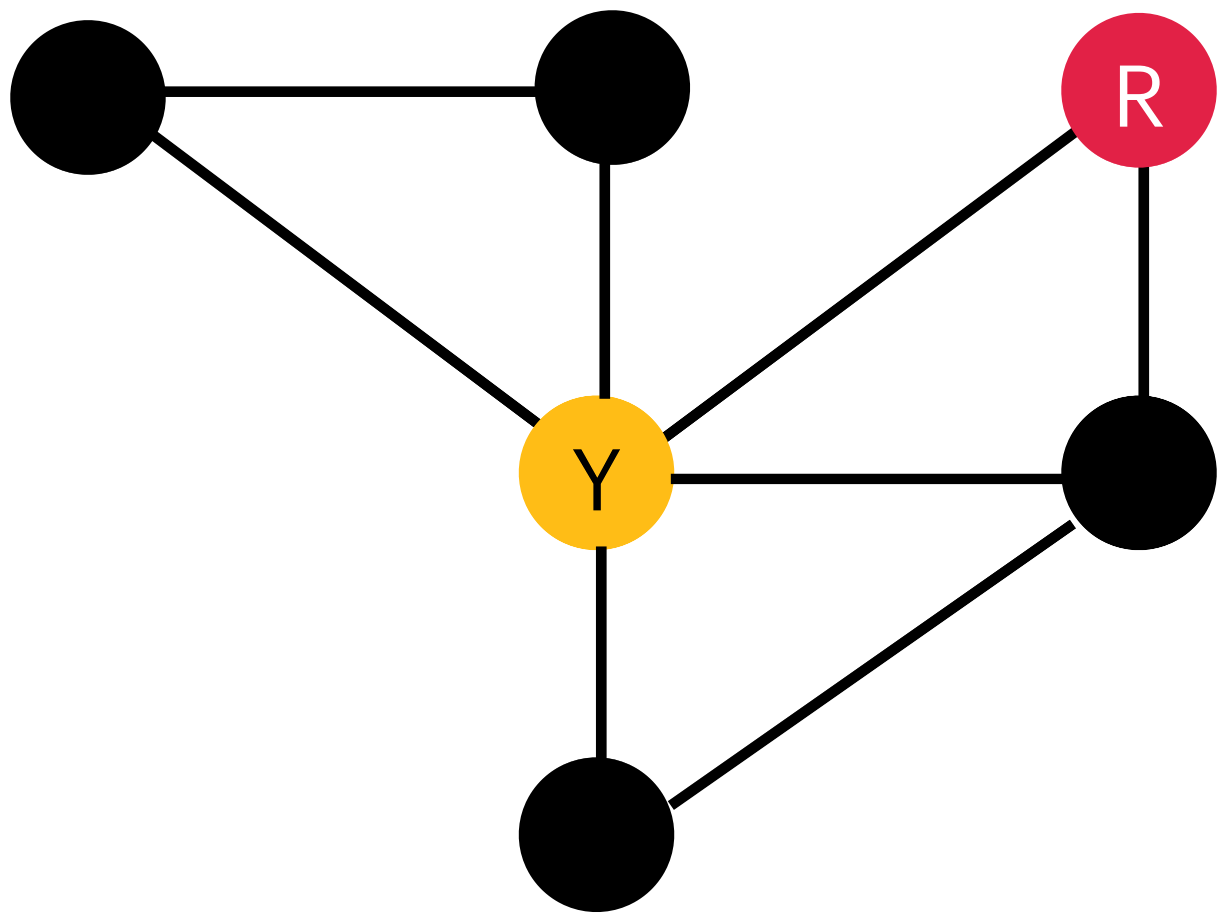
Example: Classify all nodes connected to a red node as true and every other node as false.

This task relies only to the fact that it is connected to a red node.

Neighborhood attention can produce a richer weighing of a node's neighbors, which results in potentially more descriptive and task-specific aggregation schemes.

Idea: Learn an attention weight for each neighbor: weighted aggregation functions.

Graph Attention Networks

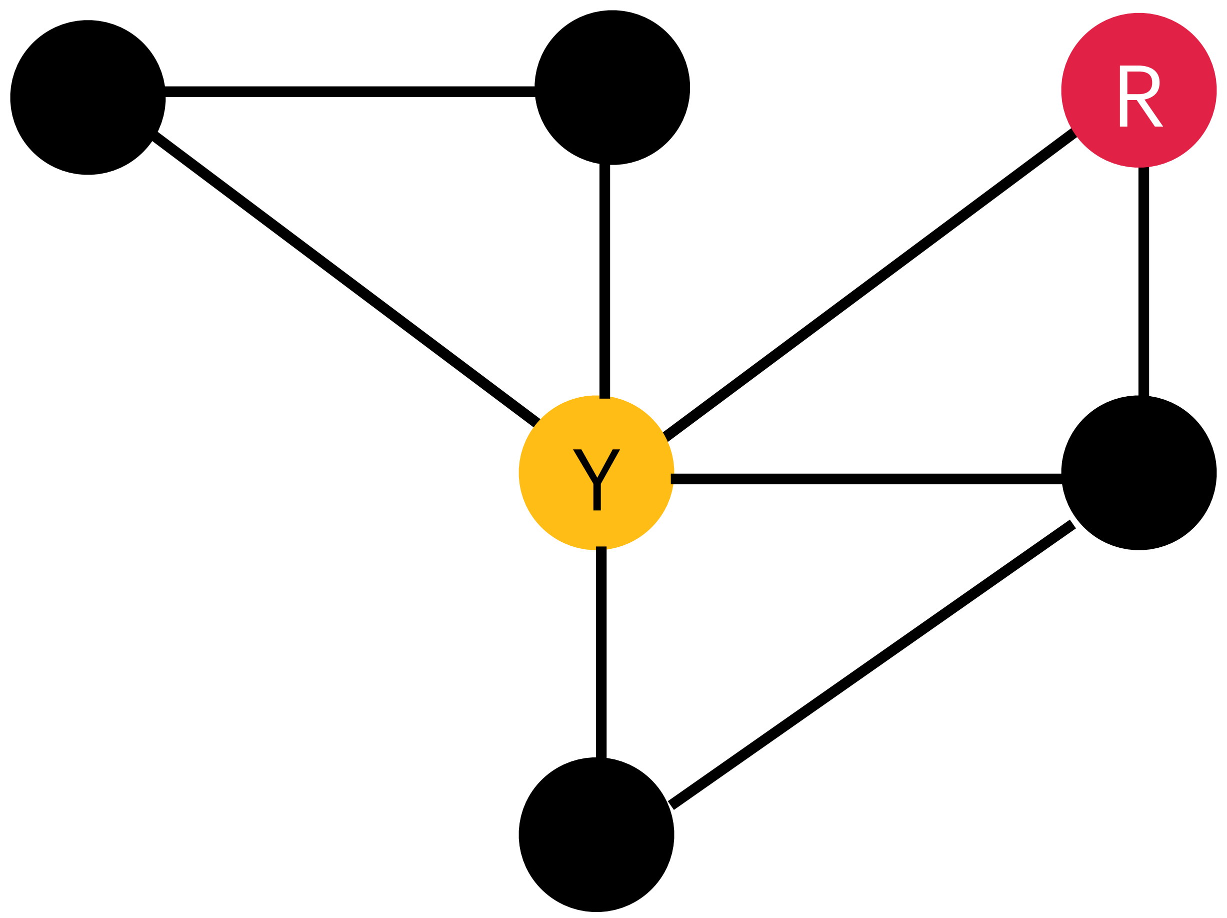


Graph attention networks (GAT) (Velickovic et al., 2018) apply weighted sum aggregation, and a pairwise node attention mechanism during message passing (using a self-loop approach):

$$\mathbf{h}_u^{(t)} = \sigma\left(\mathbf{W}^{(t)} \sum_{v \in N(u) \cup \{u\}} \alpha_{(u,v)}\, \mathbf{h}_v^{(t-1)}\right),$$

where $\alpha_{u,v}$ is the attention on a node $v \in N(u) \cup \{u\}$ when we aggregate information at node u.

What kind of Attention?

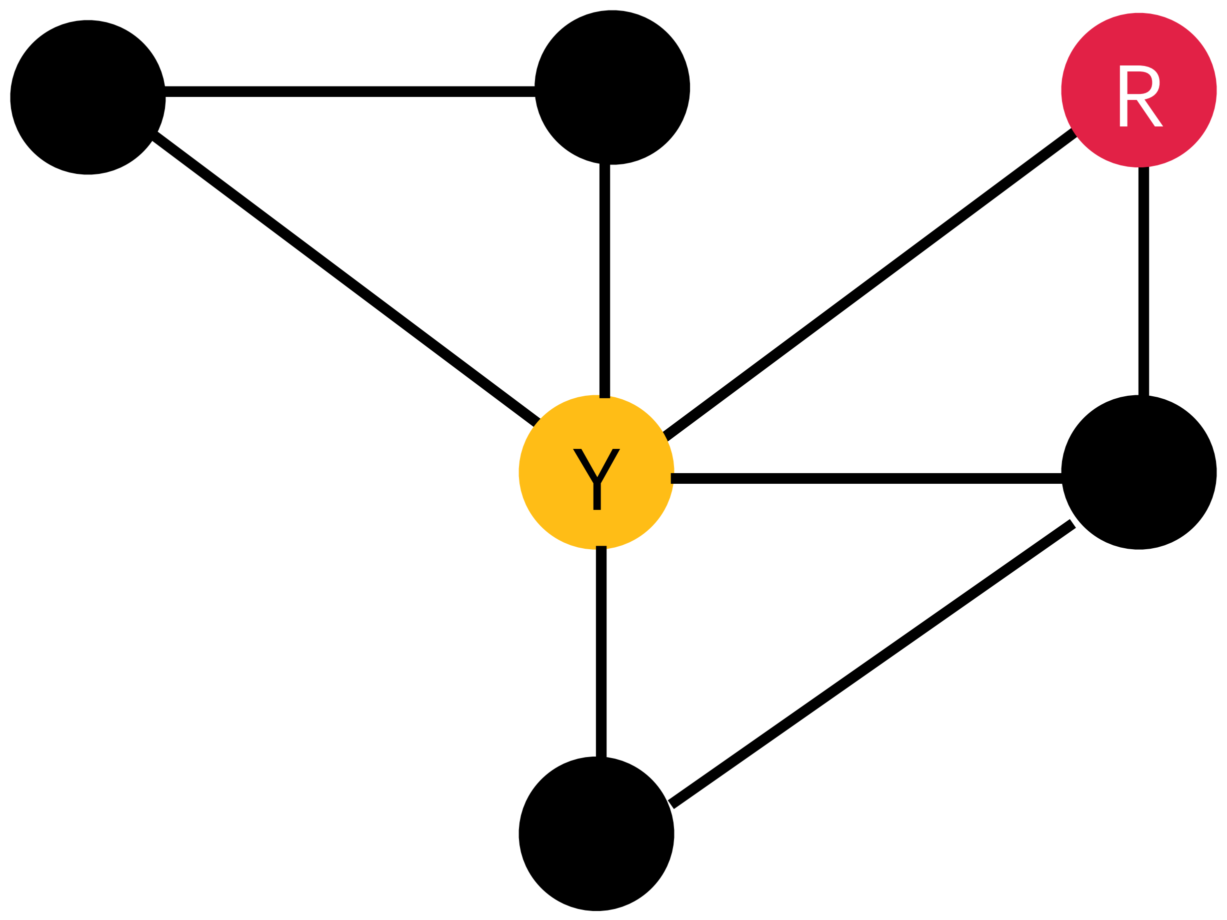


The attention weights $e_{u,v}$ between nodes u, v are normalized typically to yield final weights $\alpha_{u,v}$:

$$\alpha_{u,v} = \frac{\exp(e_{u,v})}{\sum_{v' \in N(u)} \exp(e_{u,v'})}$$

GAT: $e_{u,v} = \mathbf{a}^\top[\mathbf{W}\mathbf{h}_u \oplus \mathbf{W}\mathbf{h}_v]$ Bilinear: $e_{u,v} = \mathbf{h}_u^\top \mathbf{W}\mathbf{h}_v$

Multi-Head Attention?



Multi-head attention: Learn multiple, distinct, independently parametrized attention weights.

Multi-head attention over graphs: Learn k attention weights $\alpha_{u,v,1}, \ldots, \alpha_{u,v,k}$ for the nodes u, v.

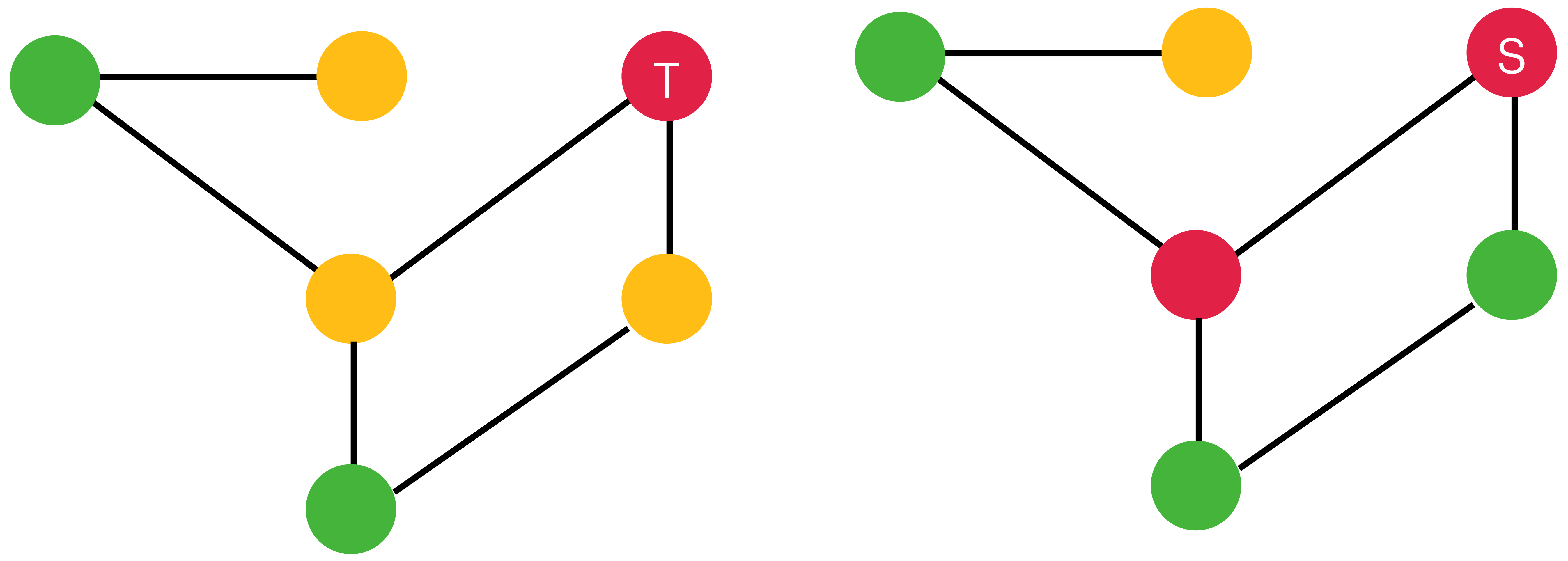
Node representations: This yields k node representations $\mathbf{h}_u[1], \ldots, \mathbf{h}_u[k]$ for each node u.

$$\mathbf{h}_u = \mathbf{h}_u[1] \oplus \ldots \oplus \mathbf{h}_u[k]$$

Transformer: Multiple attention heads to compute attention weights between all pairs of positions in the input. This coincides with GAT with multi-head attention on a fully connected graph as input.

Graph Isomorphism Networks

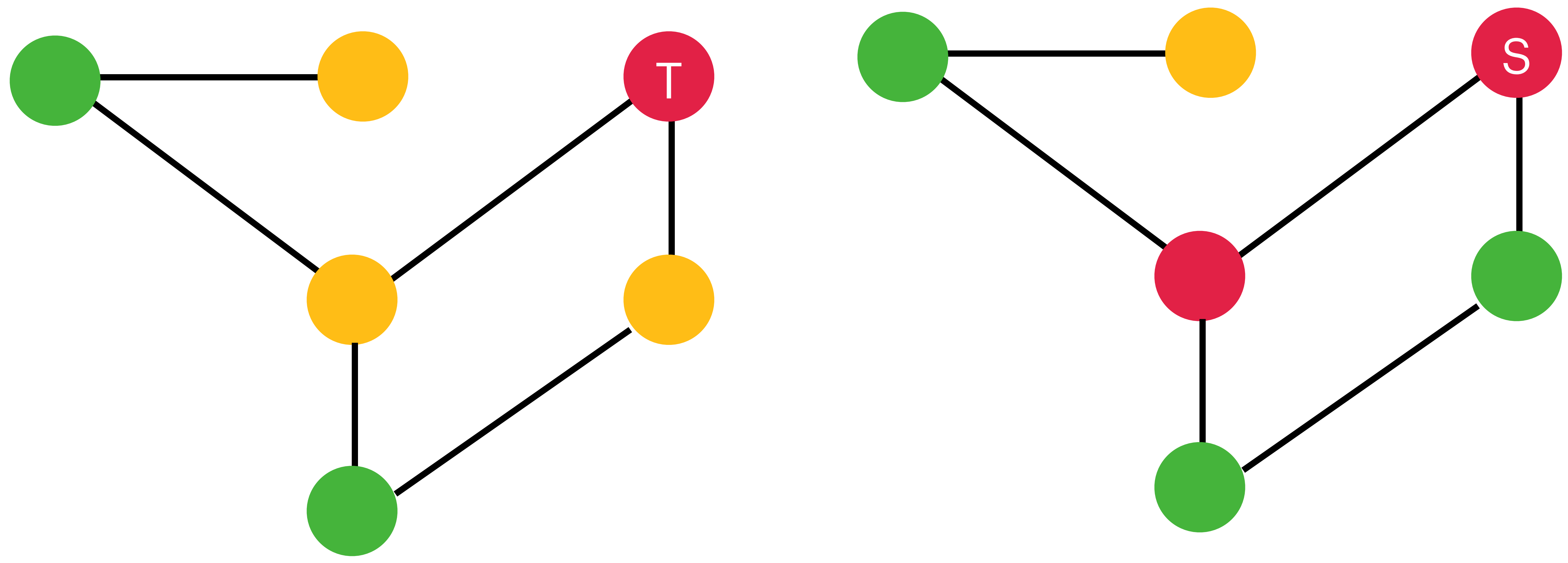
A Closer Look at Aggregation



Question: What is the impact of different choices of aggregation on the discrimination ability of GNNs?

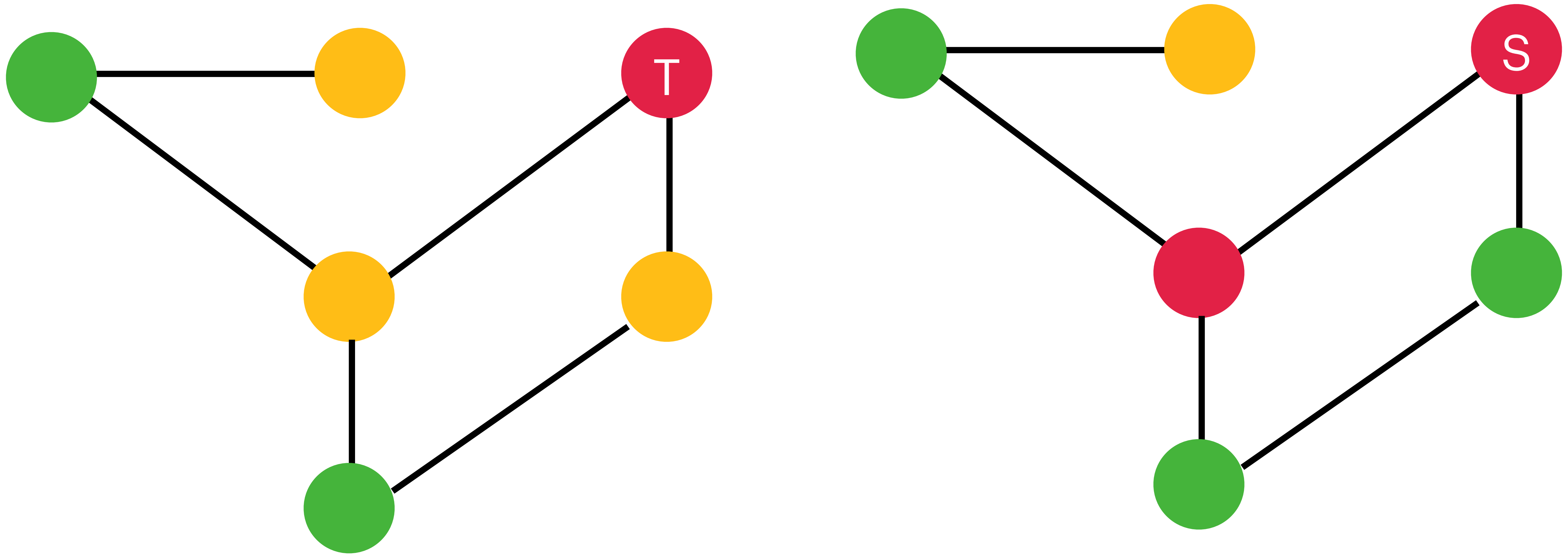
Task: Input graph with node types red, green and yellow, where the features are the RGB values. We consider a red node, and want to analyze how different functions aggregate neighbor messages.

A Closer Look at Aggregation



- **Sum**: Can discern between neighborhoods based on their sizes, but it can lead to false equality: In this example, sum cannot distinguish between a 2-yellow and a red-green neighborhood.
- **Mean**: Useful for bounding the range of aggregate messages, but cannot distinguish between neighbor sets such as 2-red and 3-red, as the mean operation eliminates cardinality.
- **Max**: Highlights a relevant element, but limited in discriminative ability. Considering red $<$ yellow $<$ green, then green is returned for any neighborhood involving at least 1 green node.

Aggregation and Expressiveness



Observation: An aggregation function must distinguish between distinct neighborhoods, and return different results given different neighborhood multisets.

Injective: The aggregation function must be injective relative to the neighborhood.

Expressive power: MPNNs are at their maximal expressiveness with injective functions (Xu et al.,2019).

Aggregation and Expressiveness

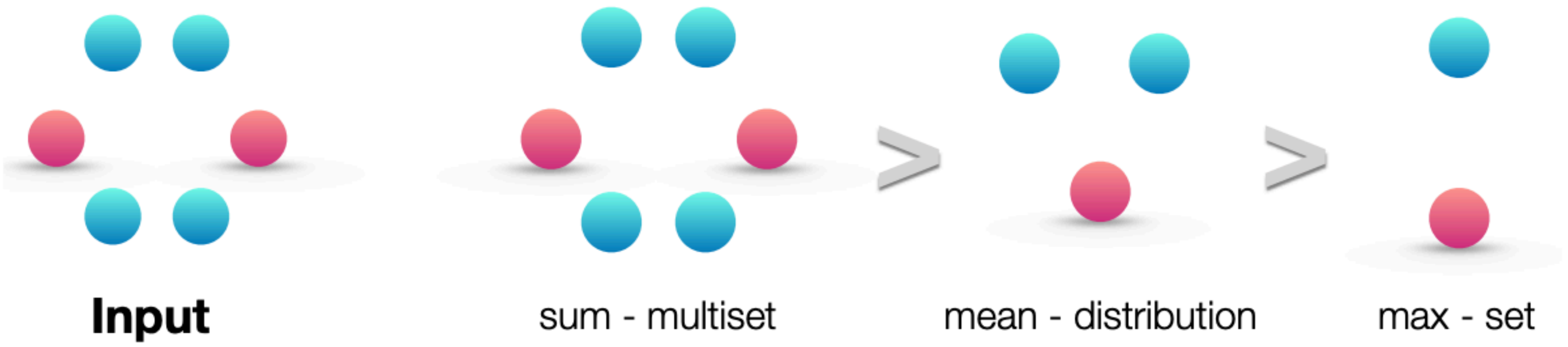
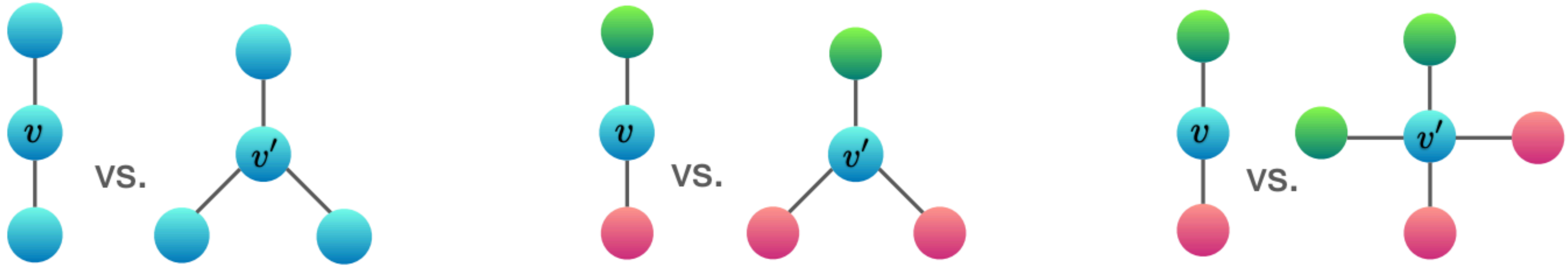


Figure 2: **Ranking by expressive power for sum, mean and max aggregators over a multiset.** Left panel shows the input multiset, *i.e.*, the network neighborhood to be aggregated. The next three panels illustrate the aspects of the multiset a given aggregator is able to capture: sum captures the full multiset, mean captures the proportion/distribution of elements of a given type, and the max aggregator ignores multiplicities (reduces the multiset to a simple set).

(Xu et al., 2019)

Aggregation and Expressiveness

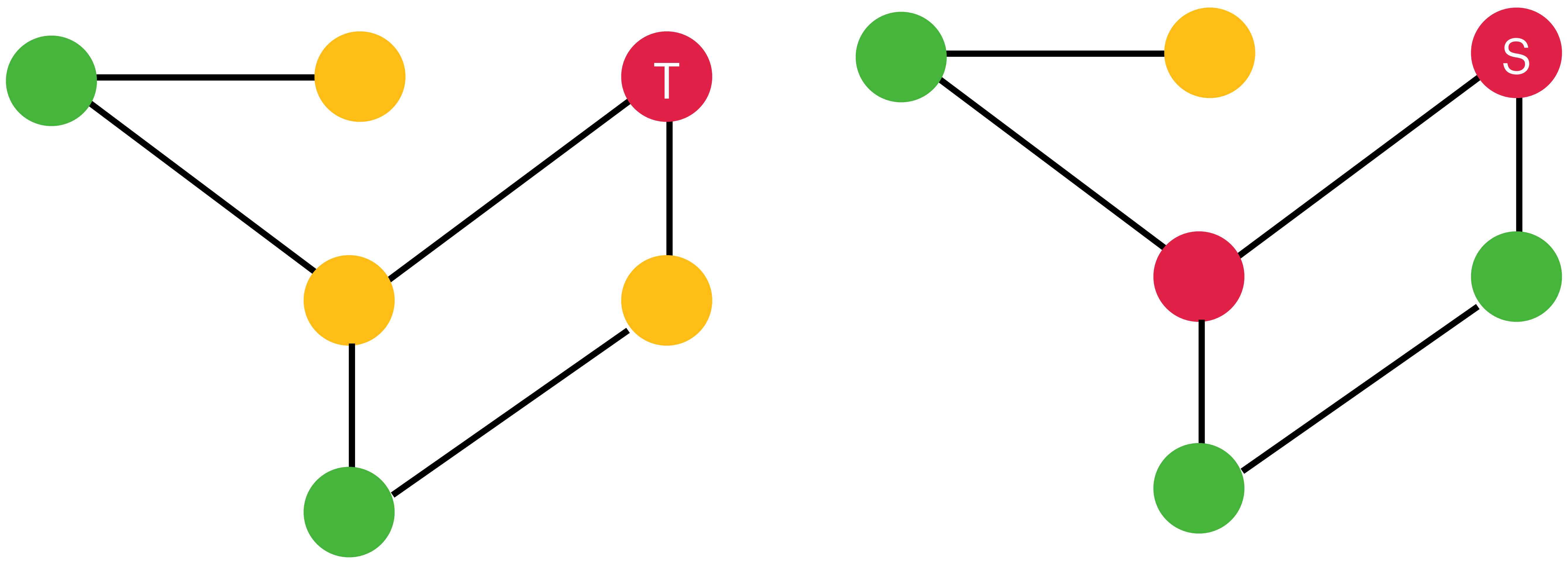


(a) Mean and Max both fail (b) Max fails (c) Mean and Max both fail

Figure 3: **Examples of graph structures that mean and max aggregators fail to distinguish.** Between the two graphs, nodes v and v' get the same embedding even though their corresponding graph structures differ. Figure 2 gives reasoning about how different aggregators "compress" different multisets and thus fail to distinguish them.

(Xu et al., 2019)

Graph Isomorphism Networks

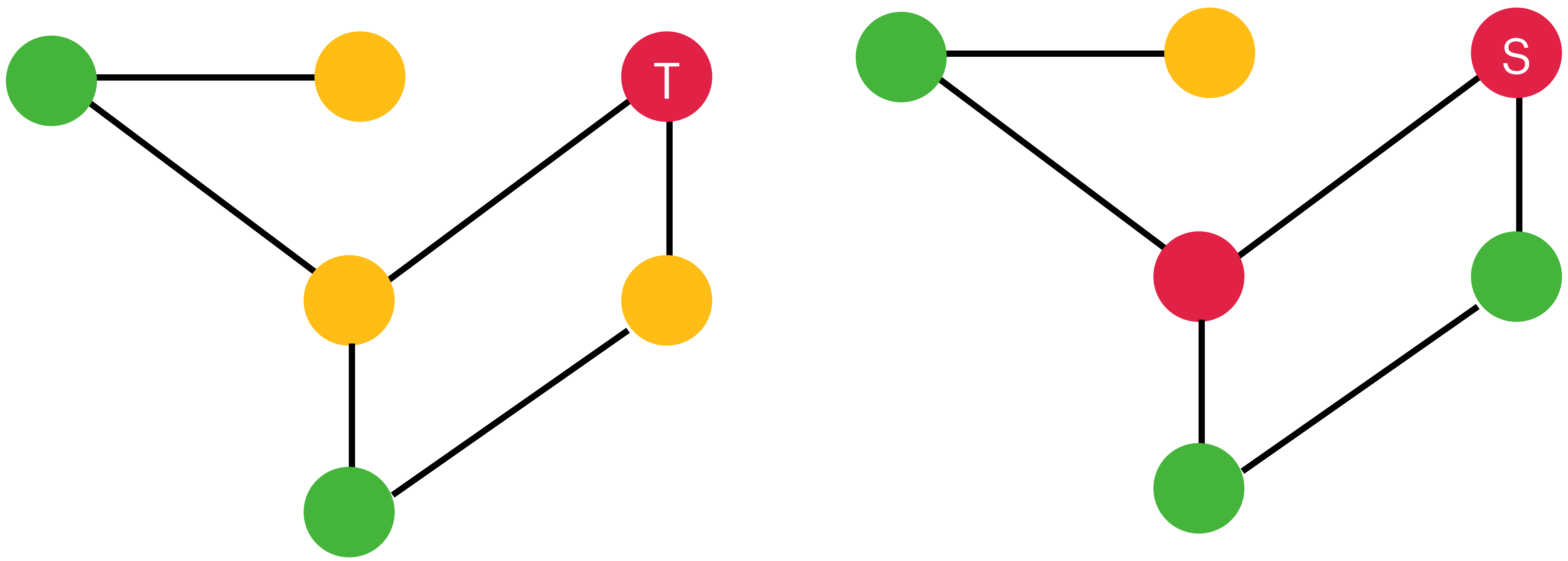


Idea: Let X be a bounded multi-set, ϕ and f some (expressive) non-linear functions, then the following

$$g = \psi\Big(\sum_{x \in X} f(x)\Big)$$

...defines an injective mapping.

Graph Isomorphism Networks

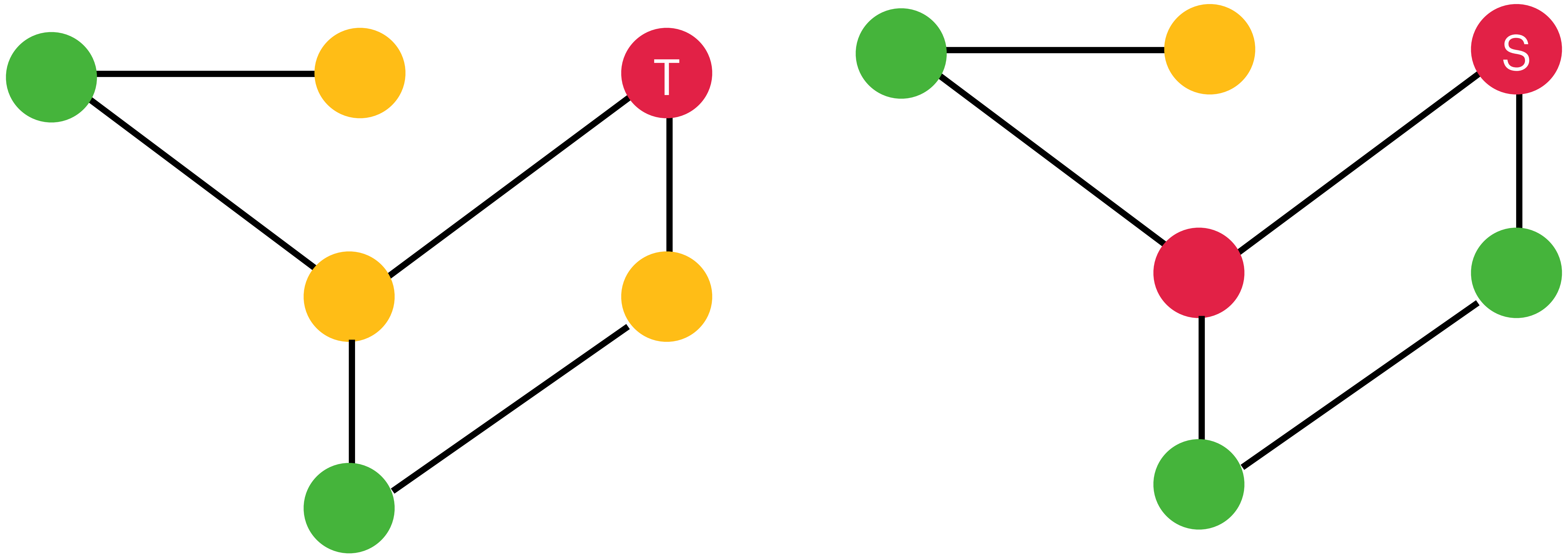


Example: Suppose we encode nodes states as $(R, G, Y)^T$

- $f(R) = (1,0,0)^T$, $f(G) = (0,1,0)^T$, $f(Y) = (0,0,1)^T$
- $g(\{\{Y, Y\}\}) = (0,0,2)^T$ and $g(\{\{R, G\}\}) = (1,1,0)^T$

$$g = \psi\Big(\sum_{x \in X} f(x)\Big)$$

Graph Isomorphism Networks

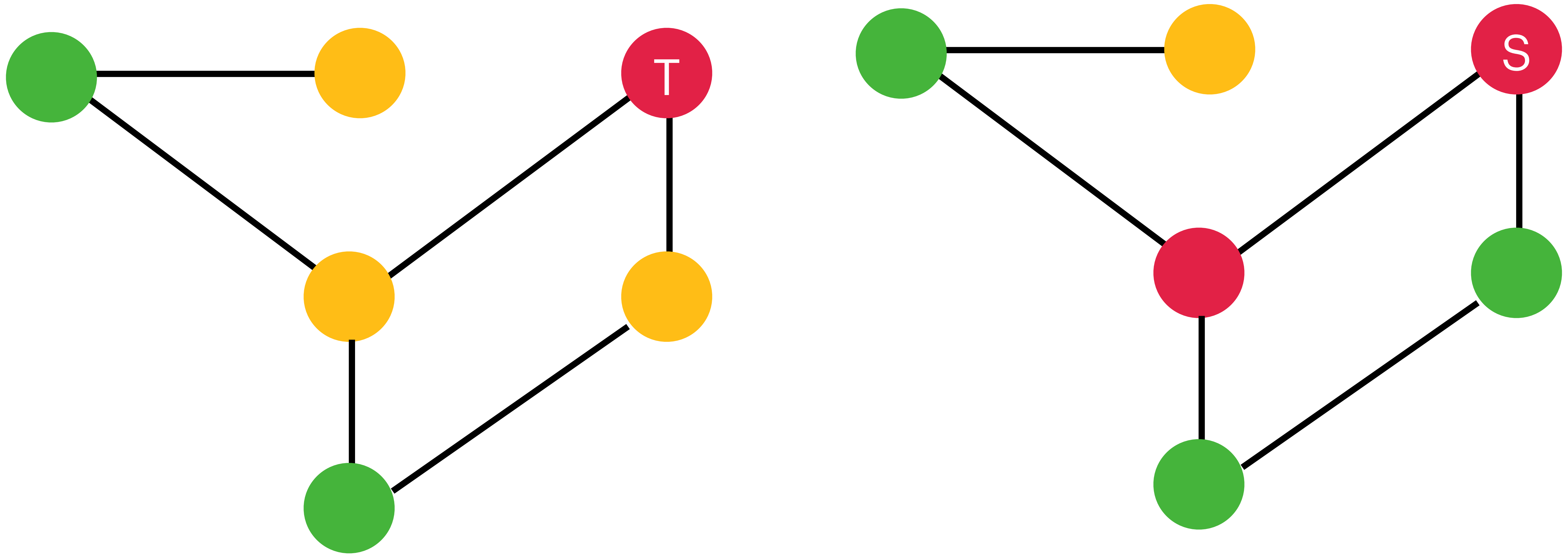


[**Lemma 5 & Corollary 6,** (Xu et al., 2019)] For a countable set $\mathscr{X}$, there exists a function $f : \mathscr{X} \to \mathbb{R}^n$ such that for any choice of ϵ, the function

$$g(c, X) = \psi\Big((1+\epsilon) \cdot f(c) + \sum_{x \in X} f(x)\Big)$$

is unique for each pair (c, X), where $X \subset \mathscr{X}$ is a multiset of bounded size and $c \in X$.

Graph Isomorphism Networks

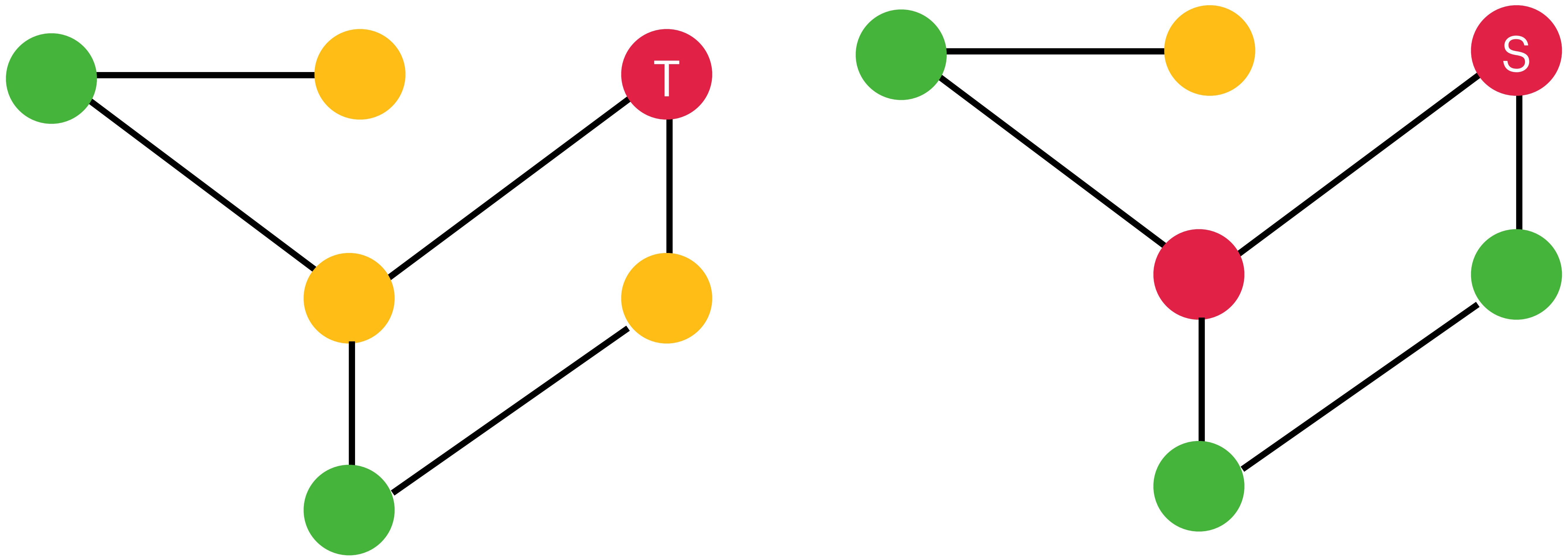


We can use MLPs to learn these functions, as MLPs are universal approximators (Hornik et al., 1989):

$$\mathbf{h}_u^{(t)} = MLP_\psi\Big((1+\epsilon)\cdot MLP_f\big(\mathbf{h}_u^{(t-1)}\big), \sum_{v\in N(u)} MLP_f\big(\mathbf{h}_v^{(t-1)}\big)\Big)$$

...which yields another instance of MPNNs.

Graph Isomorphism Networks



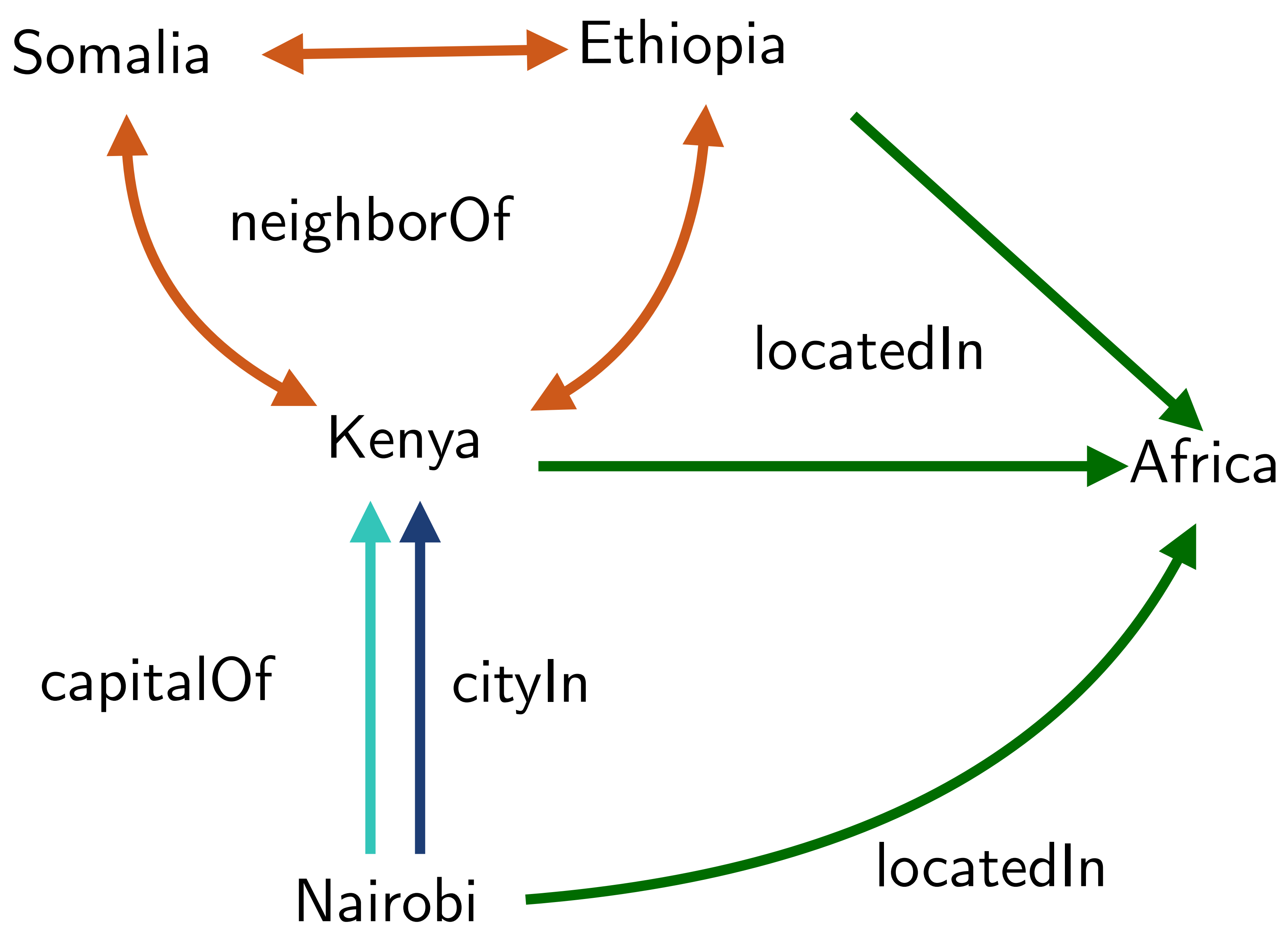
Graph isomorphism networks (GINs) update the representation $\mathbf{h}_u$ for each node $u \in V$ is iteratively as:

$$\mathbf{h}_u^{(t)} = MLP\left((1+\epsilon) \cdot \mathbf{h}_u^{(t-1)}, \sum_{v \in N(u)} \mathbf{h}_v^{(t-1)} \right)$$

...by setting $MLP = f^{(t+1)} \circ \psi^{(t)}$ and assuming the features are encoded as one-hot initially.

Relational Message Passing

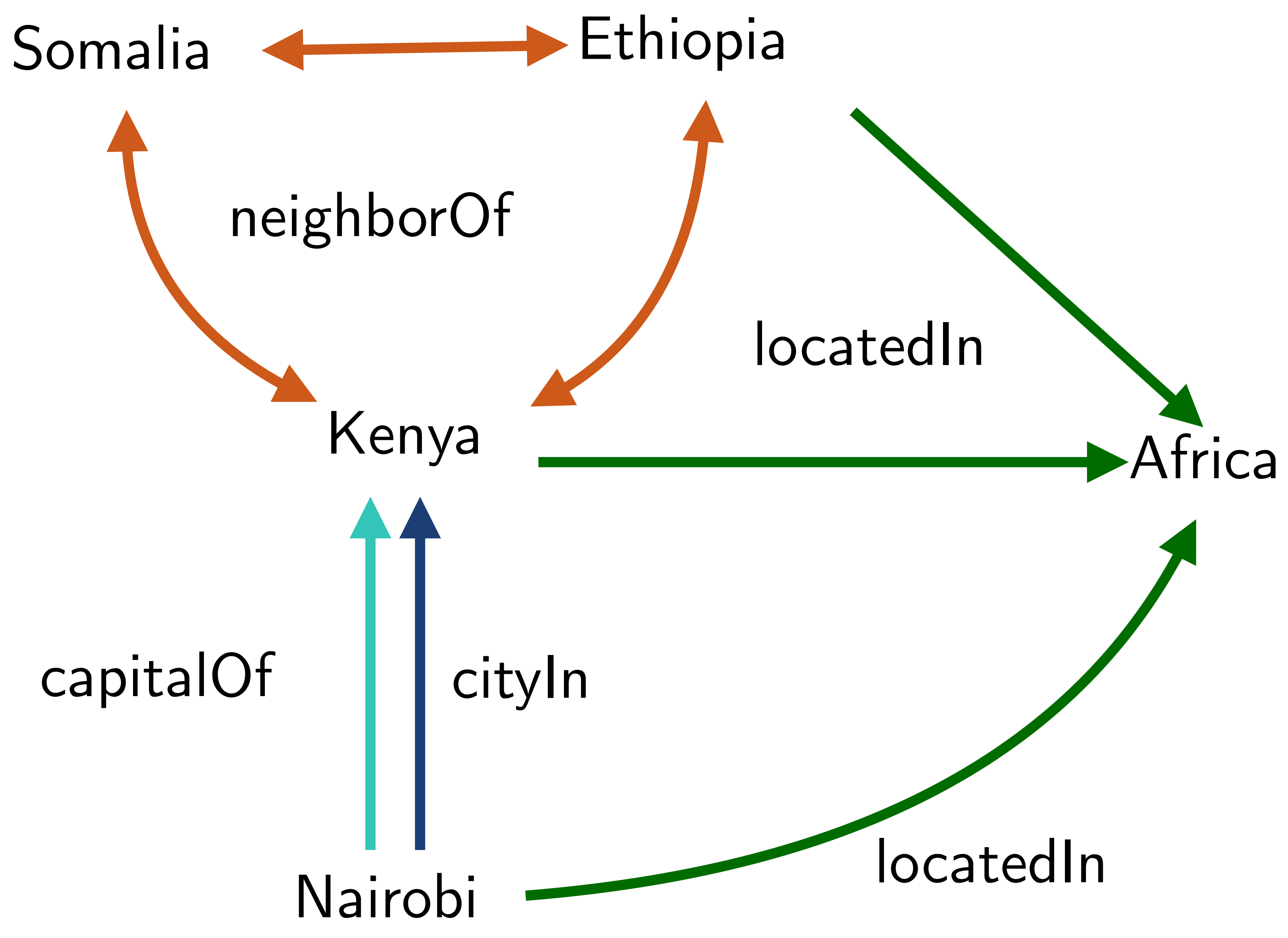
Relational Graphs



Relational graphs: Relevant for a variety of tasks, e.g., entity/node classification, KG completion.

GNNs are extended to the multi-relational setting to deal with multi-relational graphs.

Relational Graphs

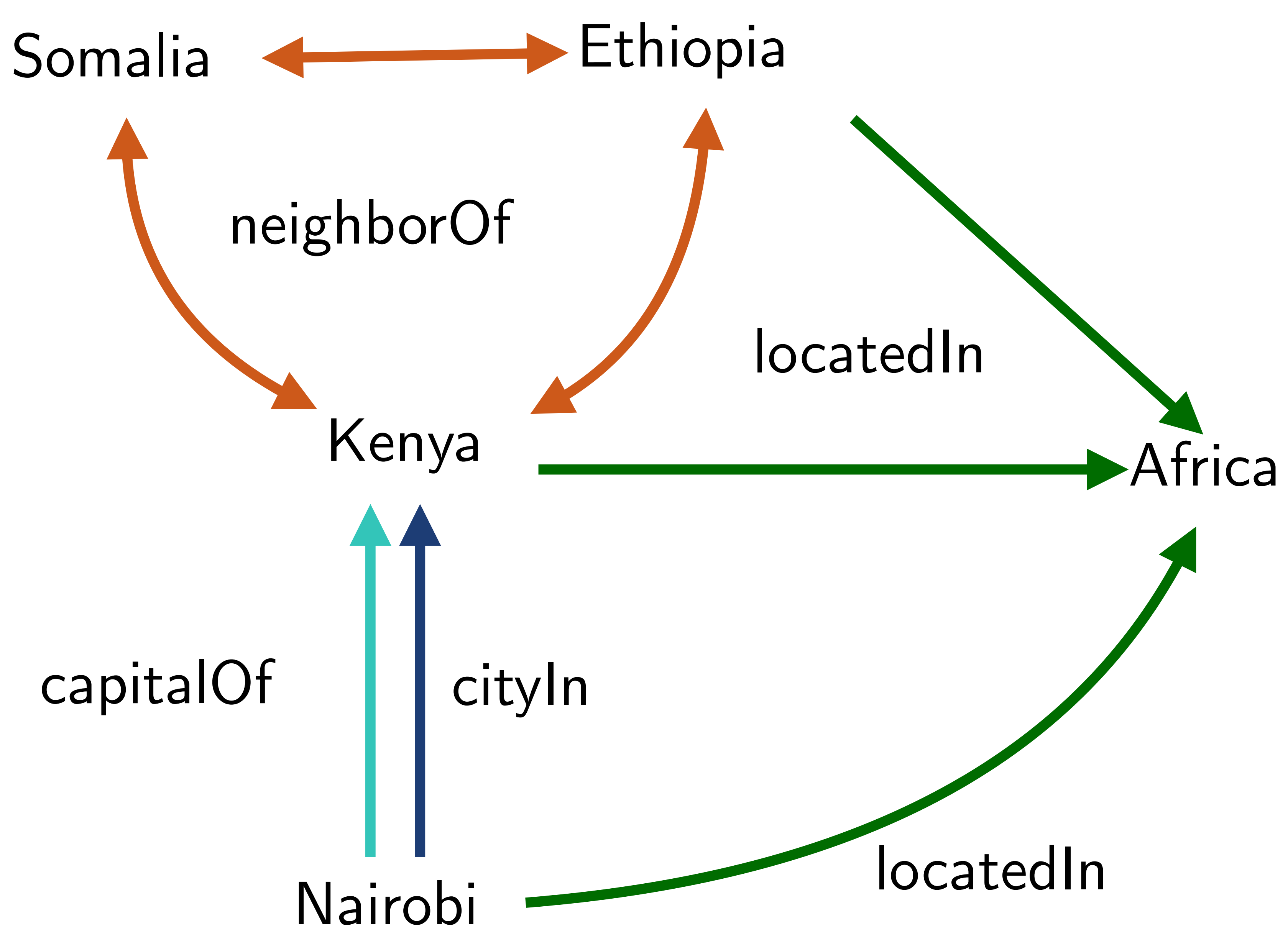


The model rGCNs (Schlichtkrull et al., 2018) defines a relation-specific message passing:

$$\mathbf{h}_u^{(t)} = \sigma\Big(\sum_{r \in \mathbf{R}} \sum_{v \in N^r(u)} \big(\frac{1}{c_{u,r}}\big) \mathbf{W}_r^{(t)} \mathbf{h}_v^{(t-1)} + \mathbf{W}_{self}^{(t)} \mathbf{h}_u^{(t-1)}\Big)$$

where $r \in \mathbf{R}$ is a relation, and $c_{u,r}$ is a normalization constant.

Relational Graphs



The rGCN model applies to both for node/graph classification but also KG completion.

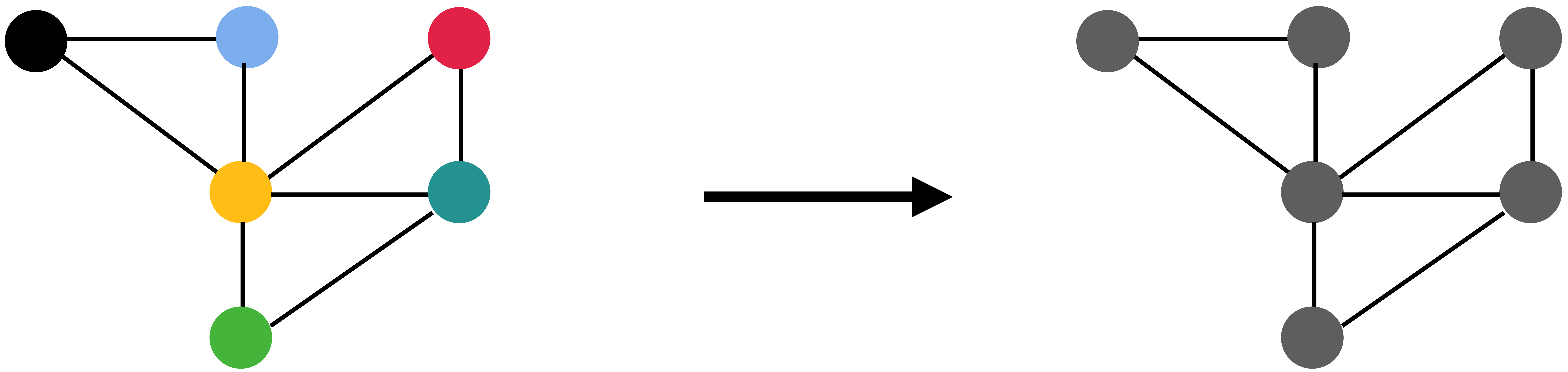
The learned embeddings are used as the entity embeddings and fed to a decoder, e.g., DistMult.

Note that rGCNs combine many aspects of this course: shallow KGC models and GNNs!

rGCN performs usually worse than shallow tools which motivated a line of work, e.g., GrAIL...

Limitations of Message Passing Neural Networks

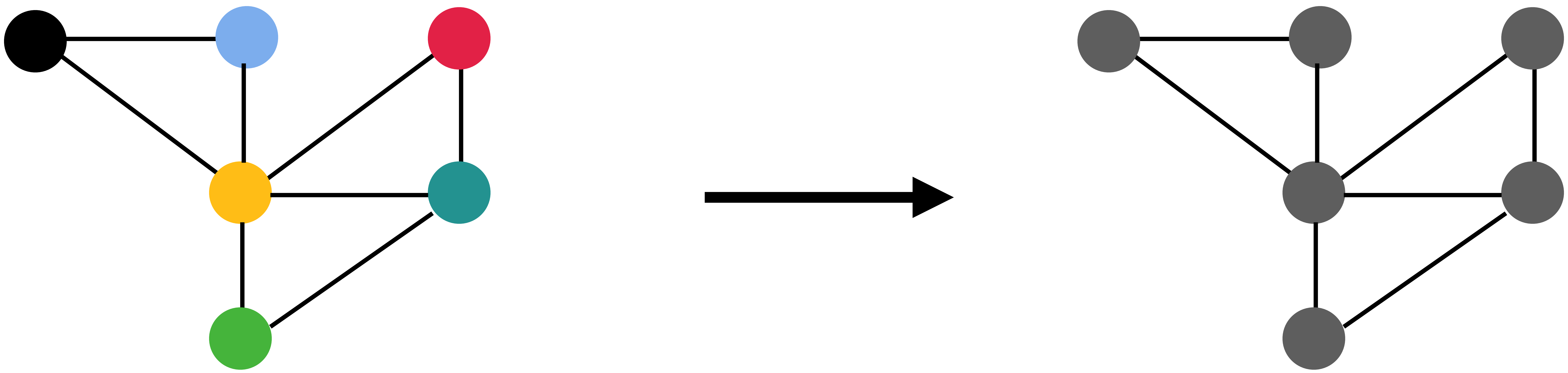
Over-smoothing



Over-smoothing: The representations of the nodes in the graph become indistinguishable after several message passing iterations (Li et al., 2018).

Long-range dependencies: Hard to make meaningful predictions — especially for deep GNN models, where the goal is to pass information across many layers so as to capture long-range dependencies.

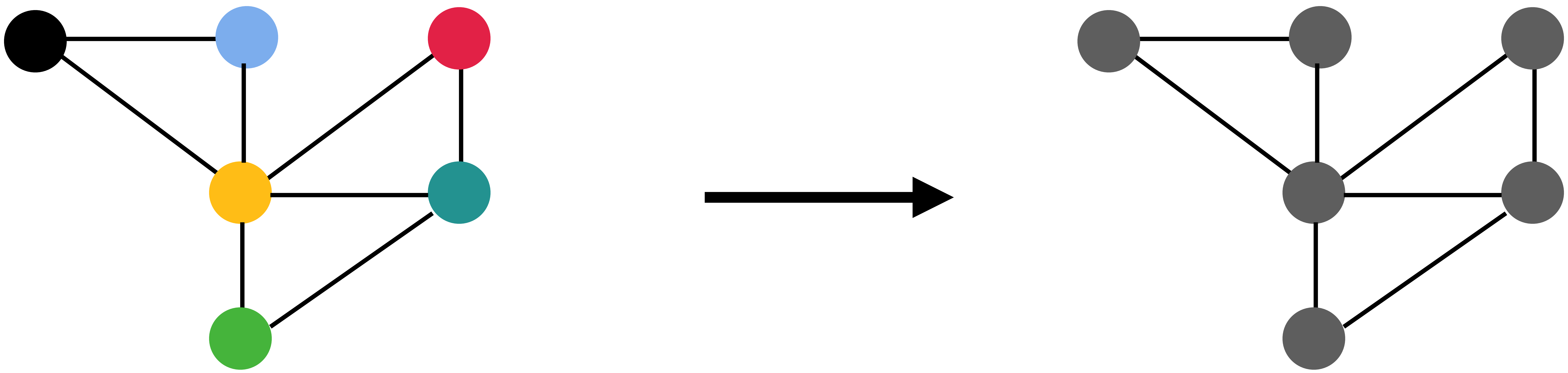
Over-smoothing



Intuition: Messages aggregated from the neighbors become too prominent, rendering the effect of the embeddings from the previous layers less and less important.

Practice: Significant performance degradation has been observed when stacking many layers on GNNs (Kipf & Welling, 2017); especially for GCNs (Li et al., 2018). Models such as GGNNs are somewhat better...

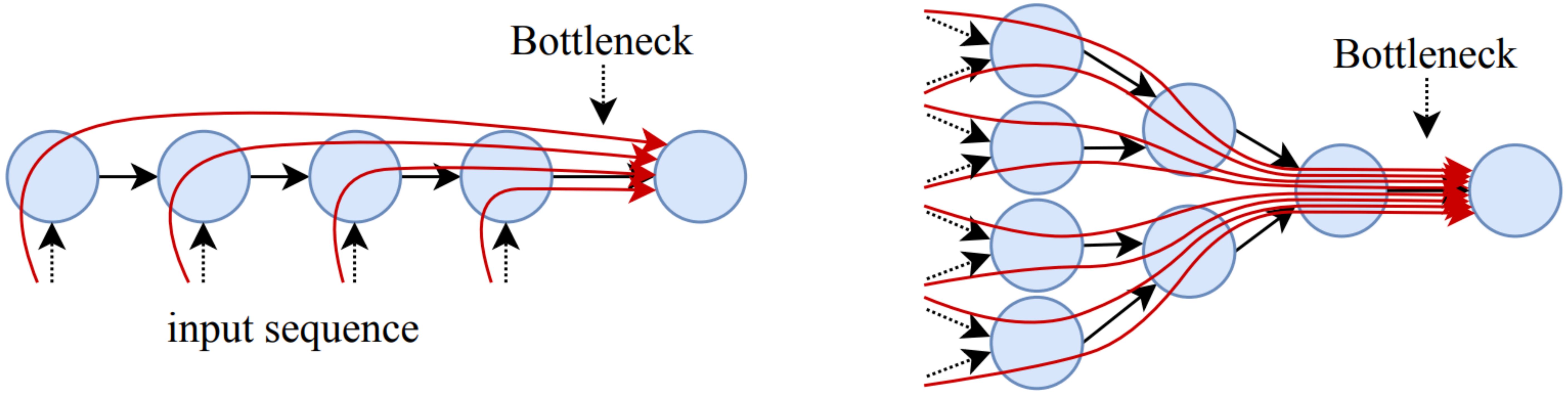
Over-smoothing



(**Theorem 3**, (Xu et al., 2018)) Informally, with a k-layer GCN, the influence of a node u on node v is proportional the probability of reaching node v on a k-step random walk starting from node u.

To partially alleviate over-smoothing: Concatenate each node's previous representation with the output of the combine function to preserve information from previous rounds.

Over-squashing



(a) The bottleneck of RNN seq2seq models

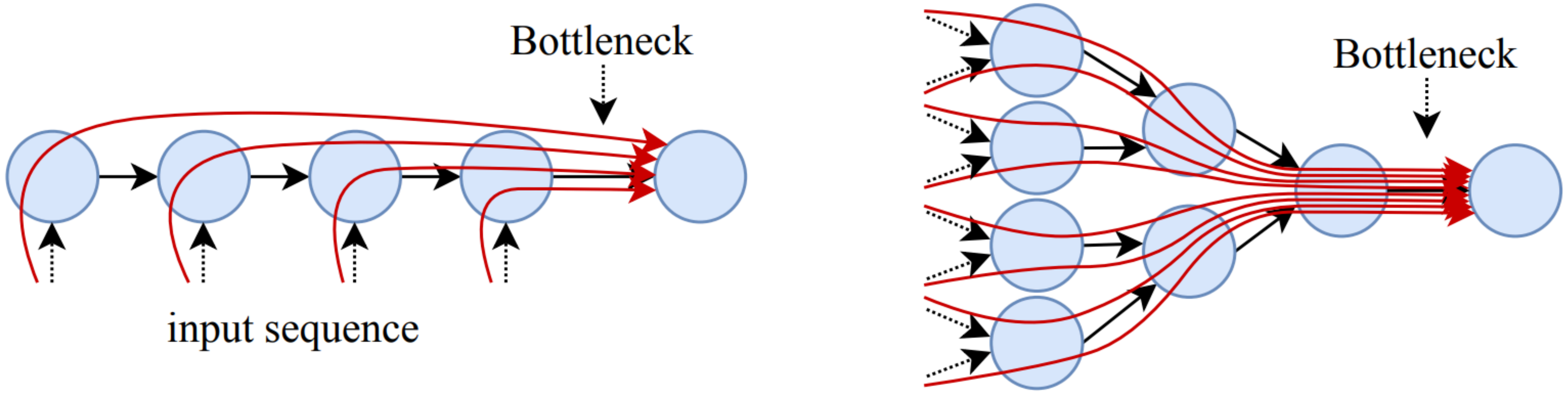
(b) The bottleneck of graph neural networks

Figure 1: The bottleneck that existed in RNN seq2seq models (before attention) is strictly more harmful in GNNs: information from a node's exponentially-growing receptive field is compressed into a fixed-size vector. Black arrows are graph edges; red curved arrows illustrate information flow.

Over-squashing (Alon and Yahav, 2021): The number of nodes in each node's receptive field grows exponentially, which is eventually compressed into fixed-length node state vectors, hence over-squashing information.

Long-range: Failure in propagating messages flowing from distant nodes - learning only from short-range signals.

Over-squashing



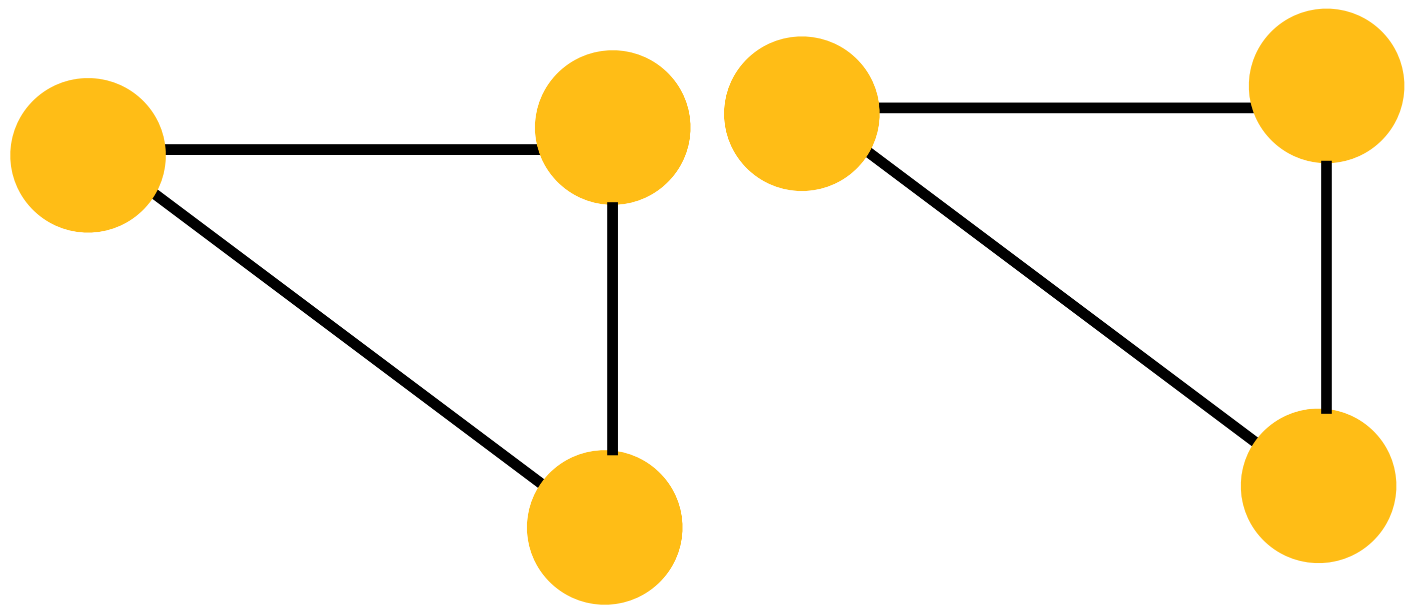
(a) The bottleneck of RNN seq2seq models (b) The bottleneck of graph neural networks

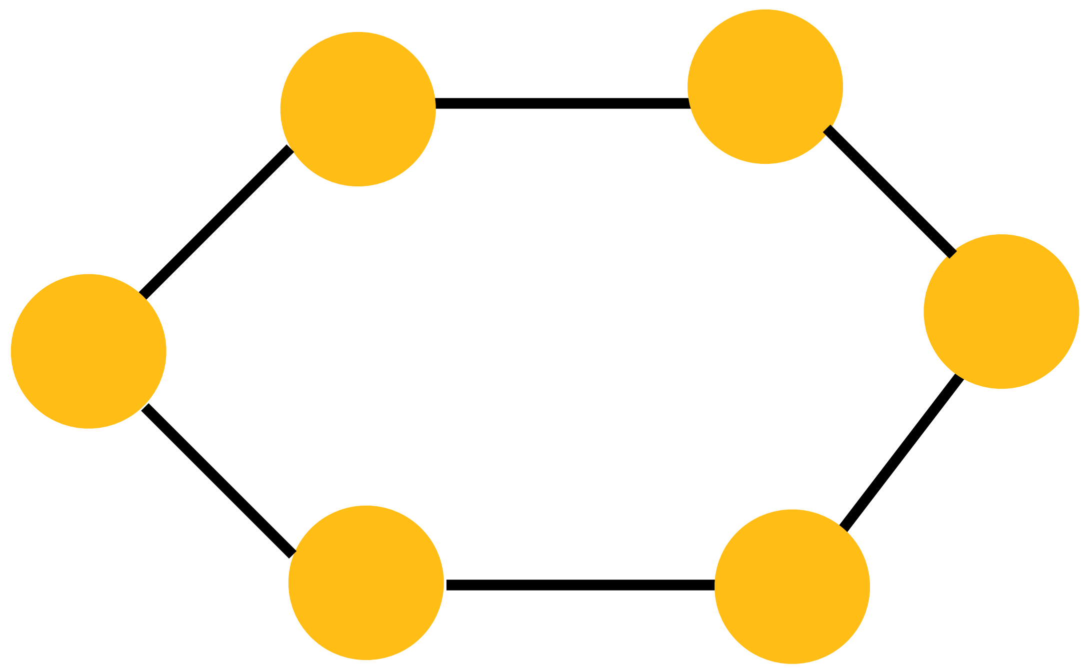
Figure 1: The bottleneck that existed in RNN seq2seq models (before attention) is strictly more harmful in GNNs: information from a node's exponentially-growing receptive field is compressed into a fixed-size vector. Black arrows are graph edges; red curved arrows illustrate information flow.

Practice: Poor performance when the task depends on long-range interactions, e.g., reachability task on graphs require as many iterations as the diameter of the graph, as otherwise it will suffer from under-reaching.

Global Information: Global feature computation can alleviate the issue to some extent. Alon and Yahav (2021) report improvements by using an additional fully connected layer.

Expressive Power





Expressive power: MPNNs is limited by the 1-WL graph isomorphism test

Example: Any MPNN learns the same embeddings for the graphs shown

This is the topic of the next lecture.

Summary

- An historical overview of graph neural networks:
  - **Gated graph neural networks**: graphs as sequences — gated units as the combine function.
  - **Graph convolutional networks**: each iteration of message passing is a convolution.
  - **Graph attention networks**: distinguish messages from neighbors via attention
  - **Graph isomorphism network**: injective aggregation
- Each of these models fall into the MPNN framework of Gilmer et al, (2017).
- Additional reading material: This lecture is partially based on Chapters 5 - 7 of Hamilton, (2020).
- We have not identified the expressive power of MPNNs: Lecture 5.
- There are a plethora of other GNN models, beyond MPNNs: Lecture 6.

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