Lecture 4: Message Passing Neural Network Architectures

Relational Learning

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Advanced Topics in Machine Learning, University of Oxford

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Overview

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- A glimpse at graph neural network models

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- Graph convolutional networks

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- Gated graph neural networks

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- Summary

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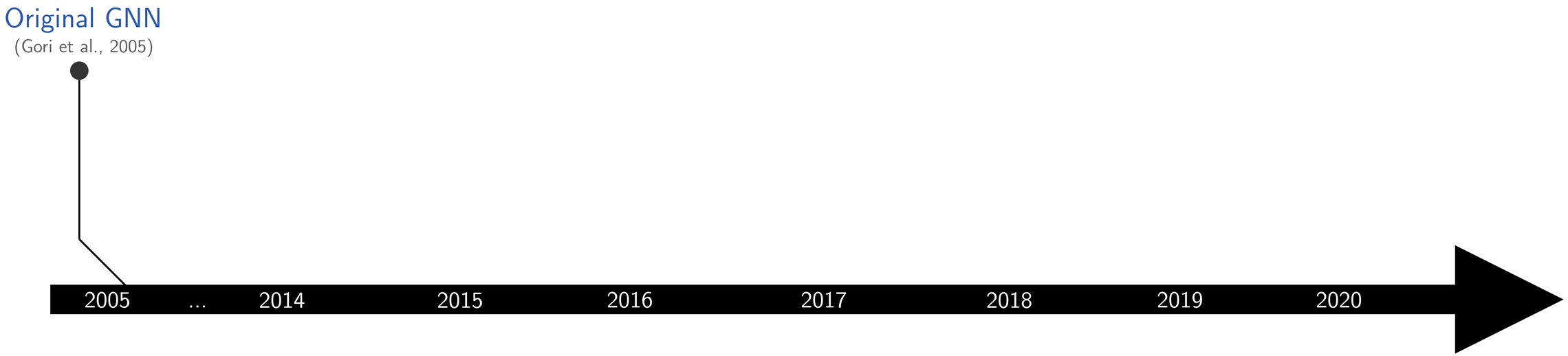

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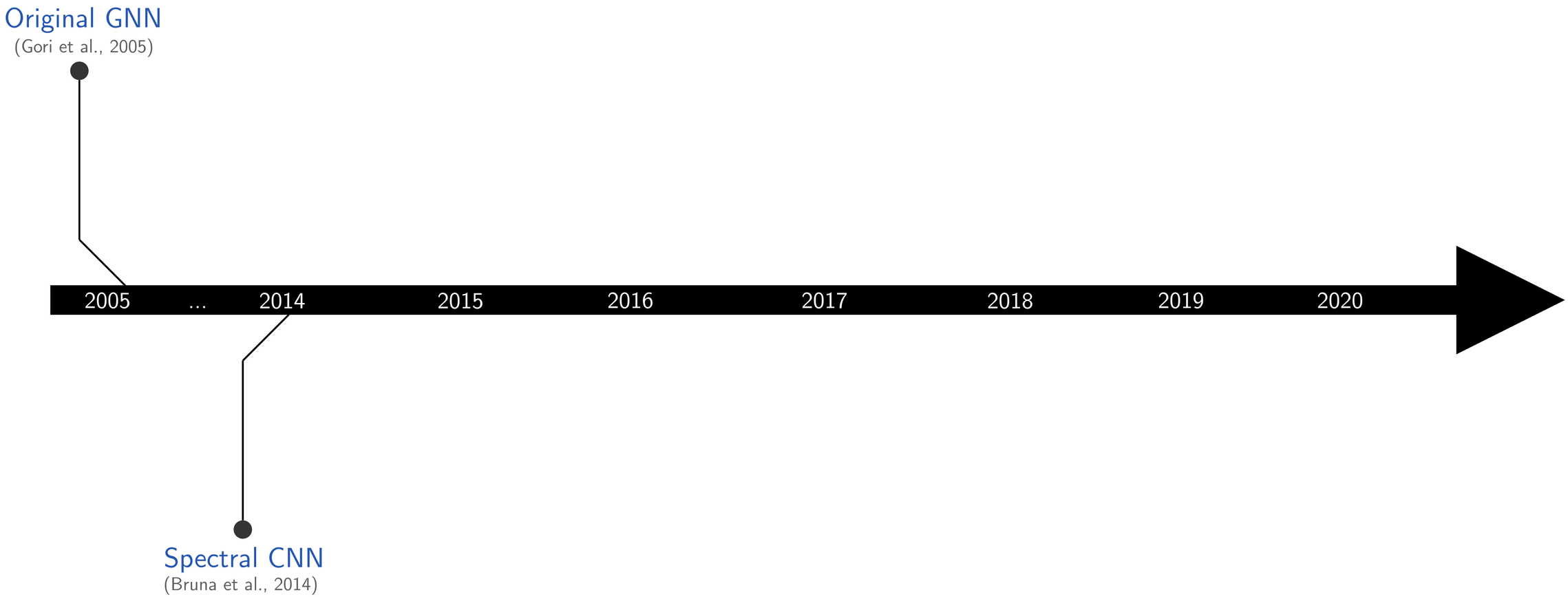

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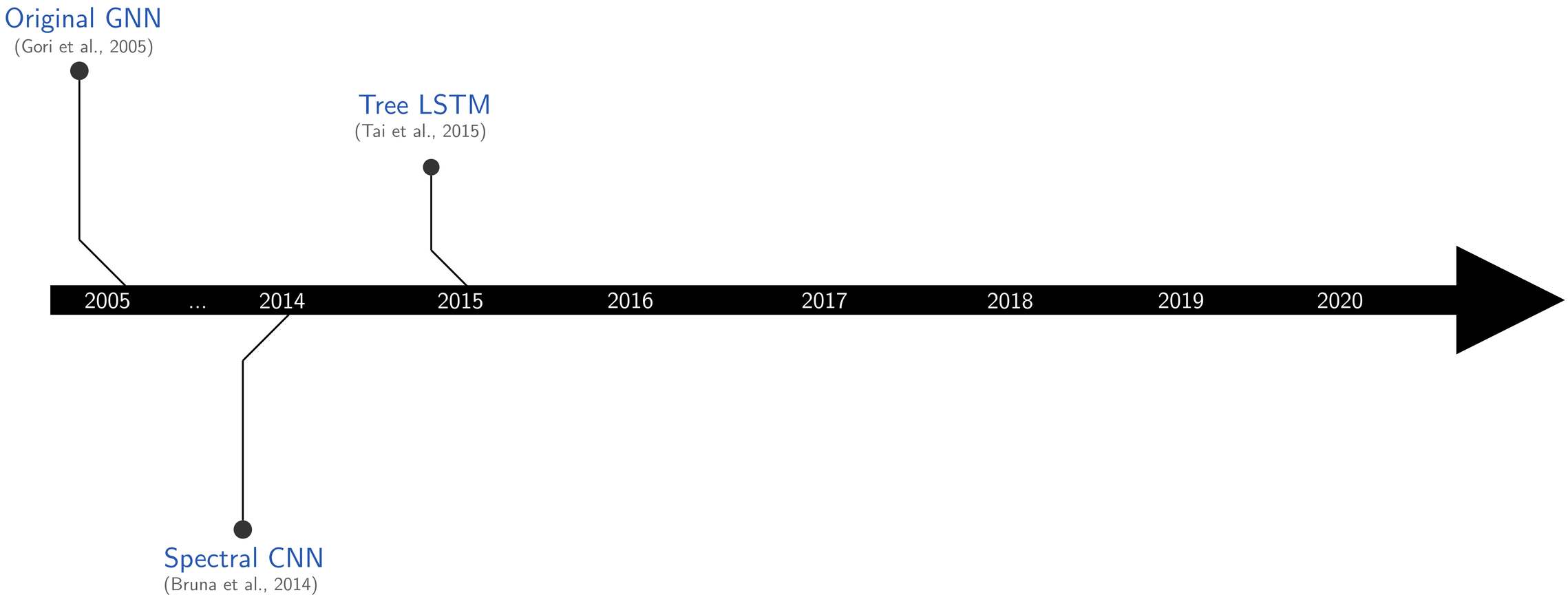

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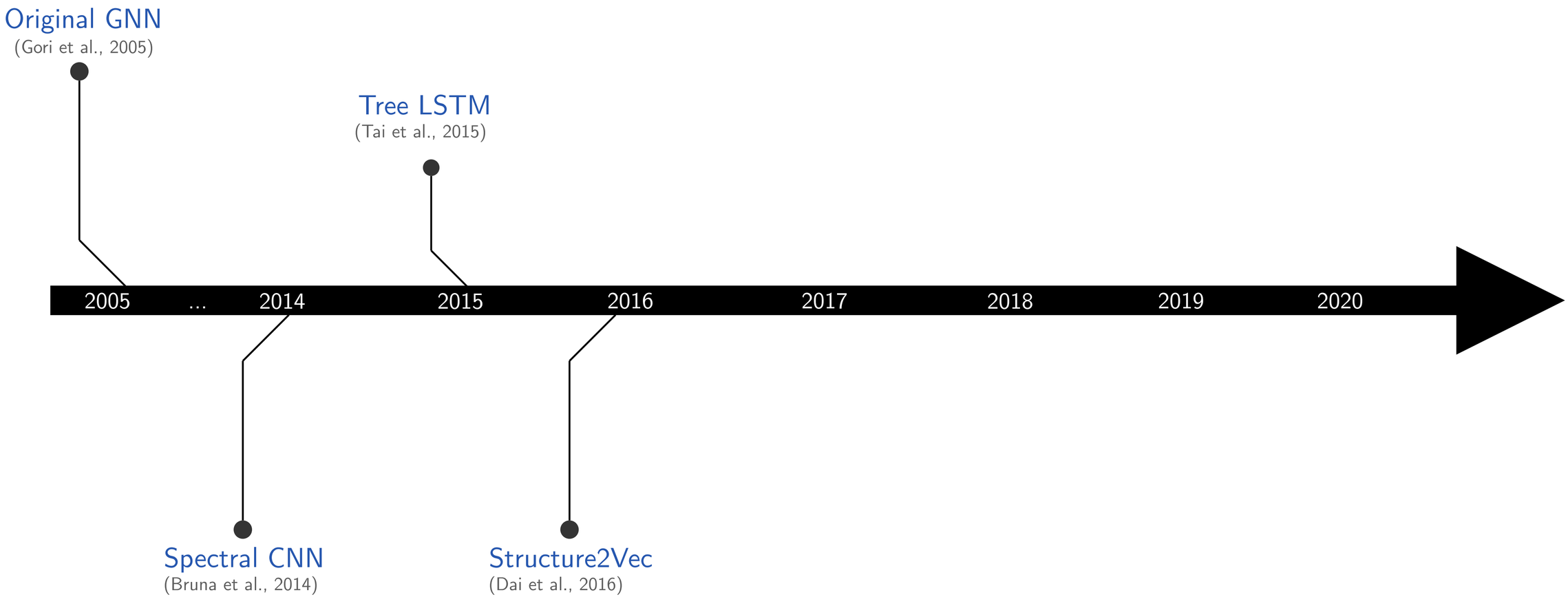

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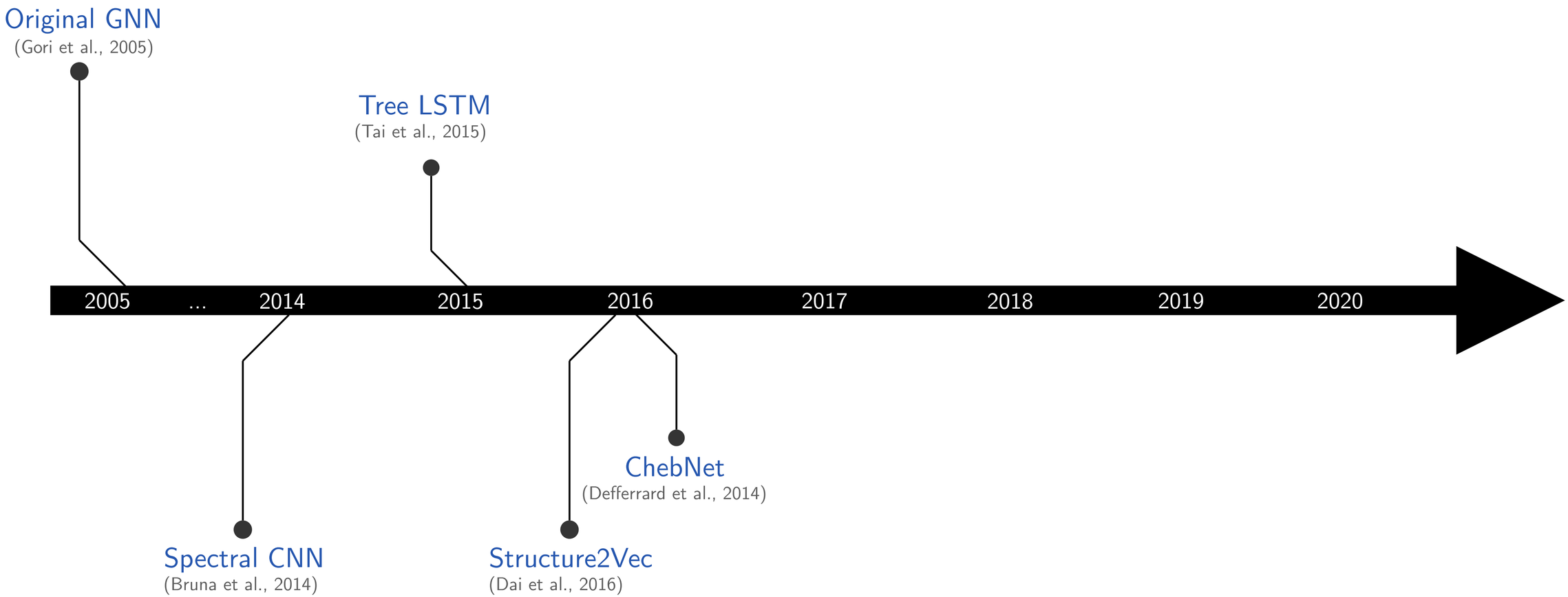

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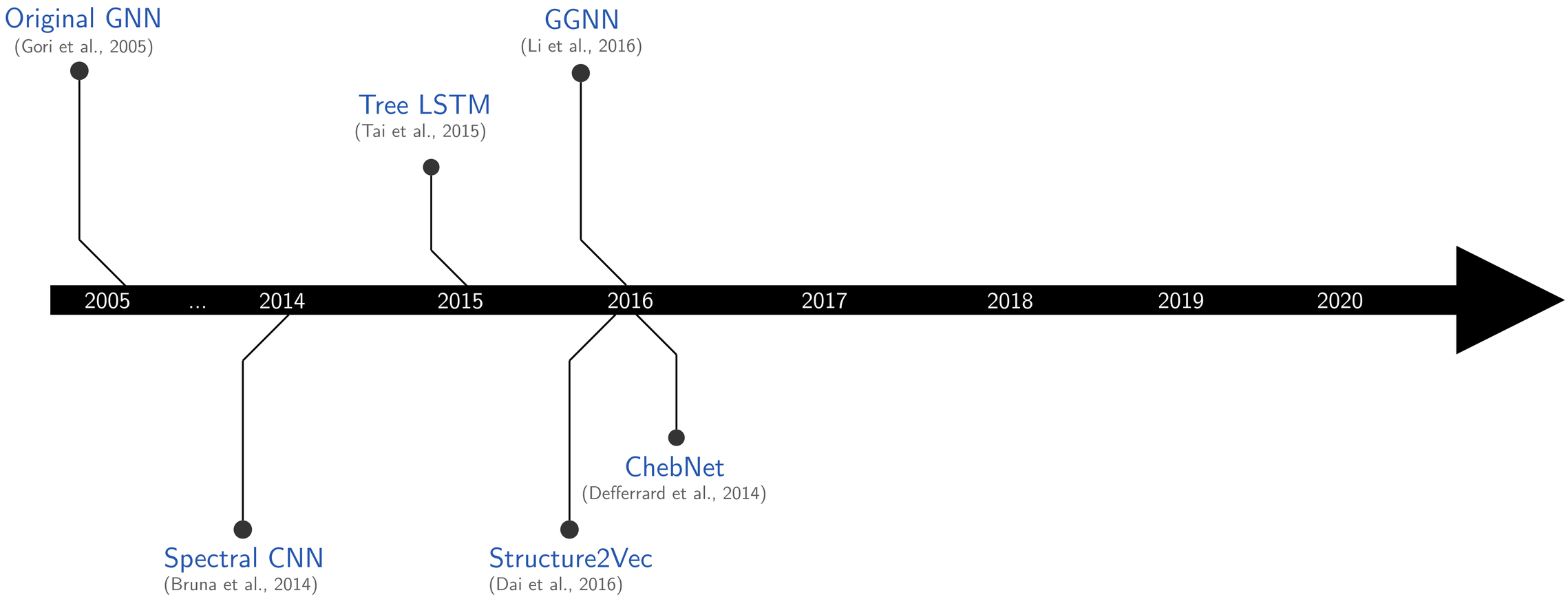

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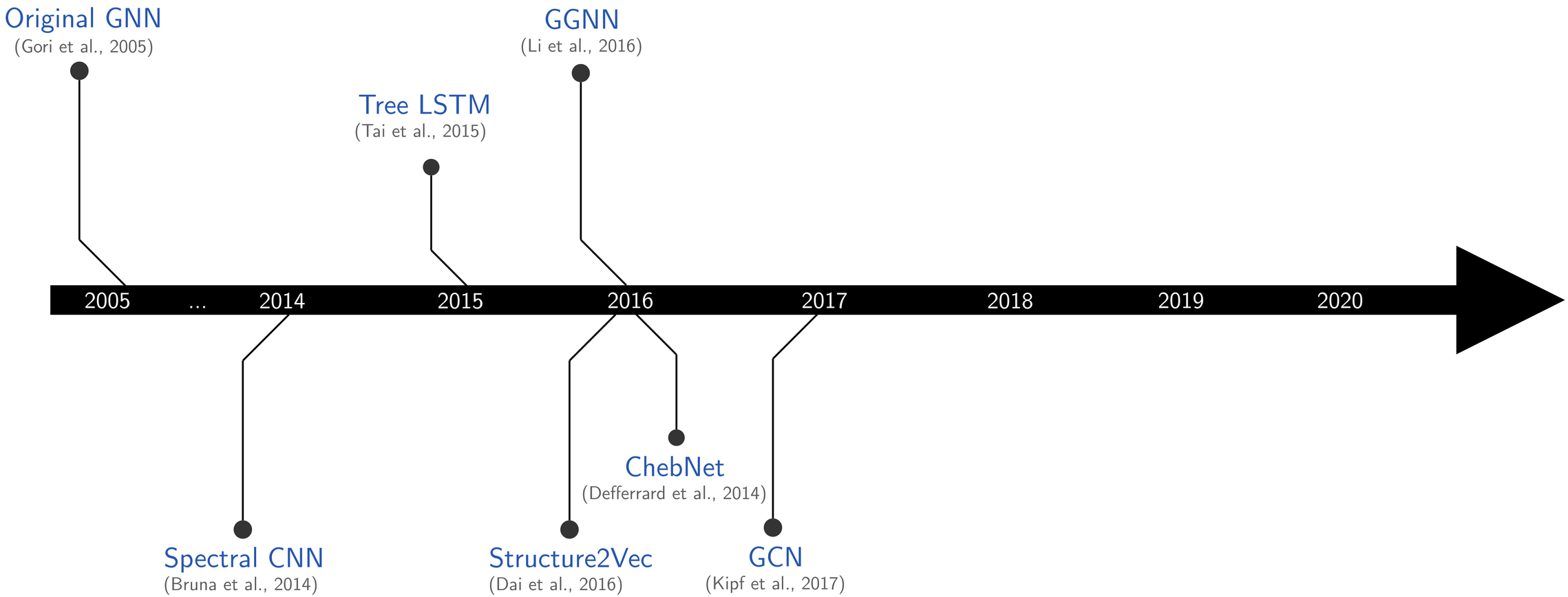

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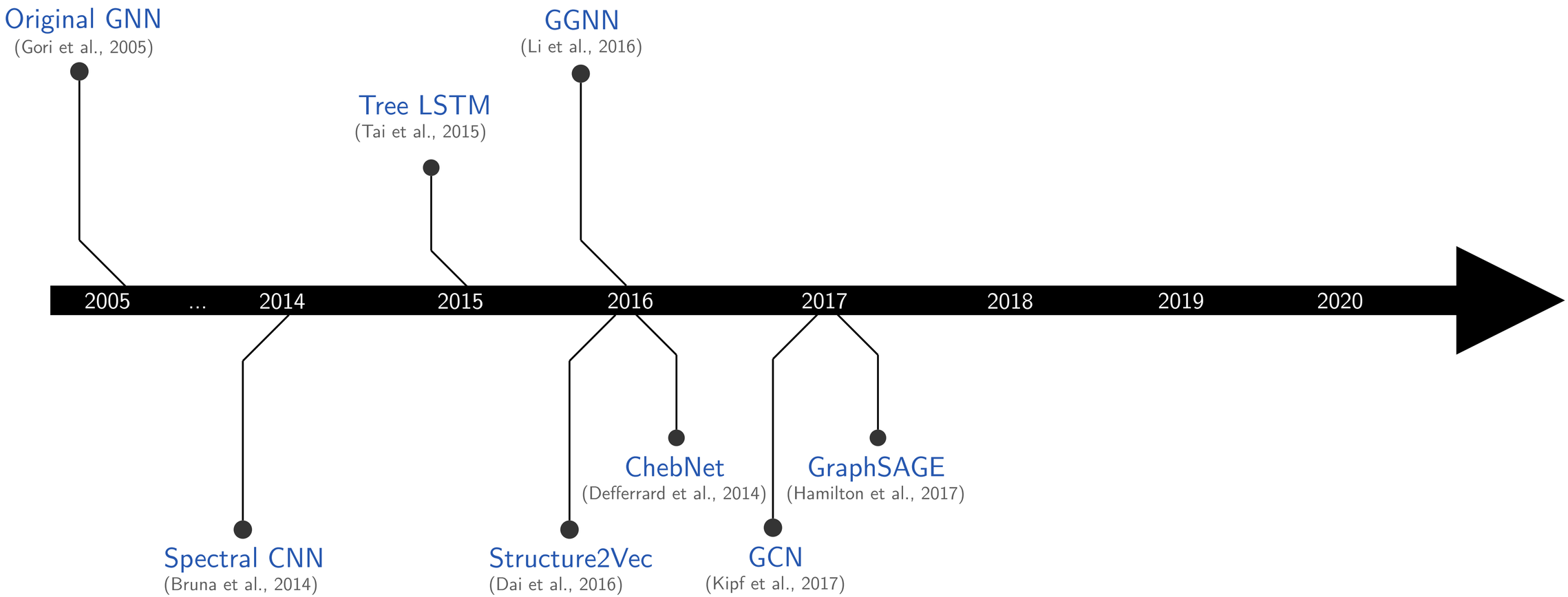

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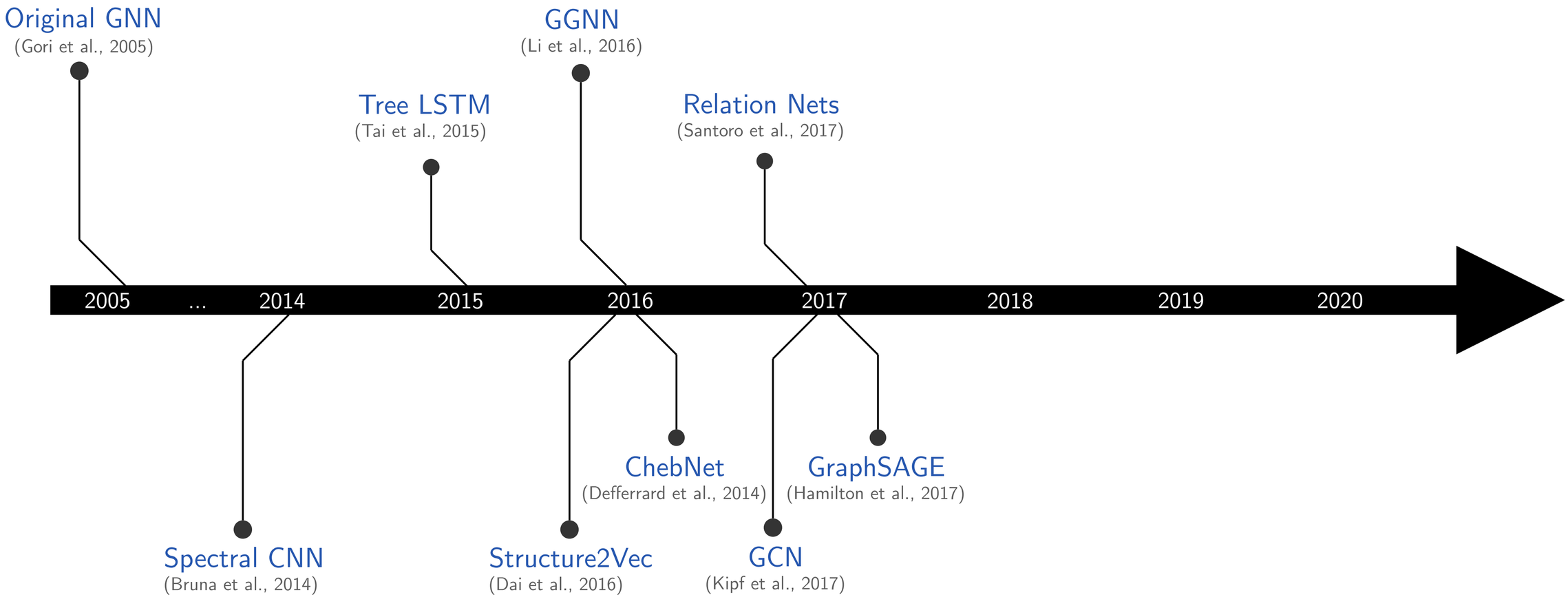

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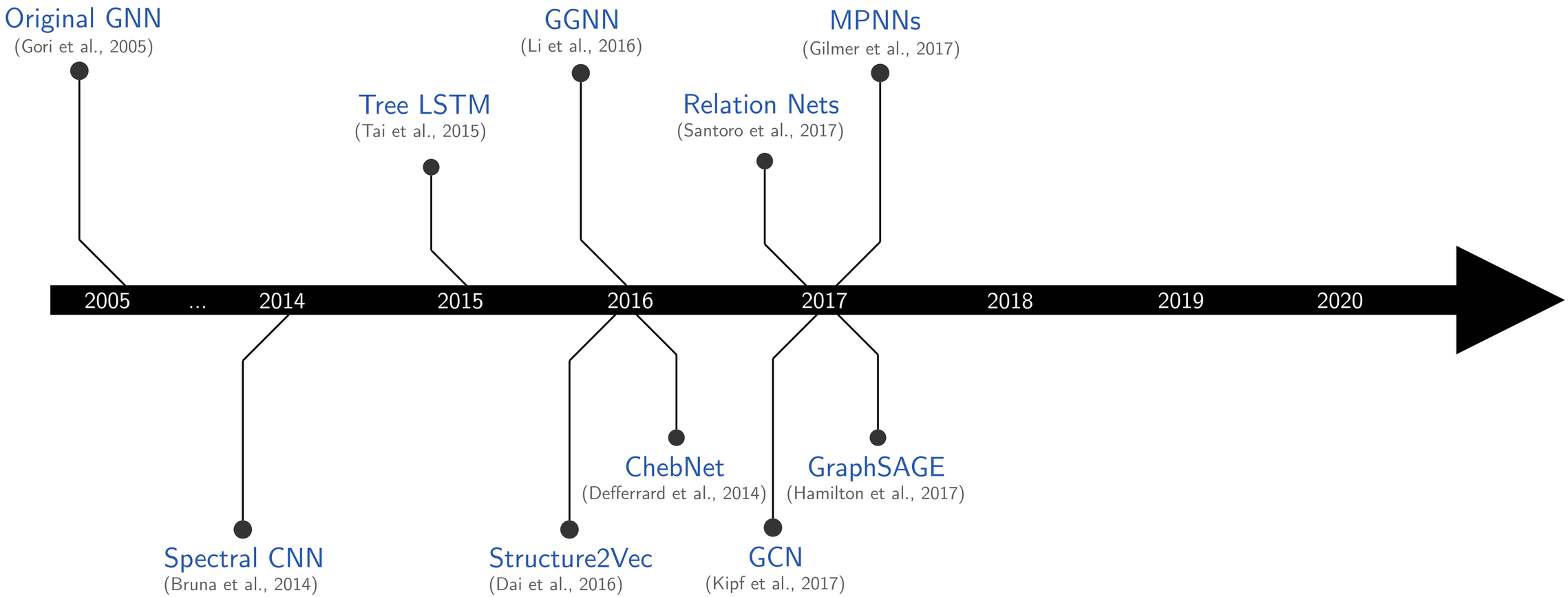

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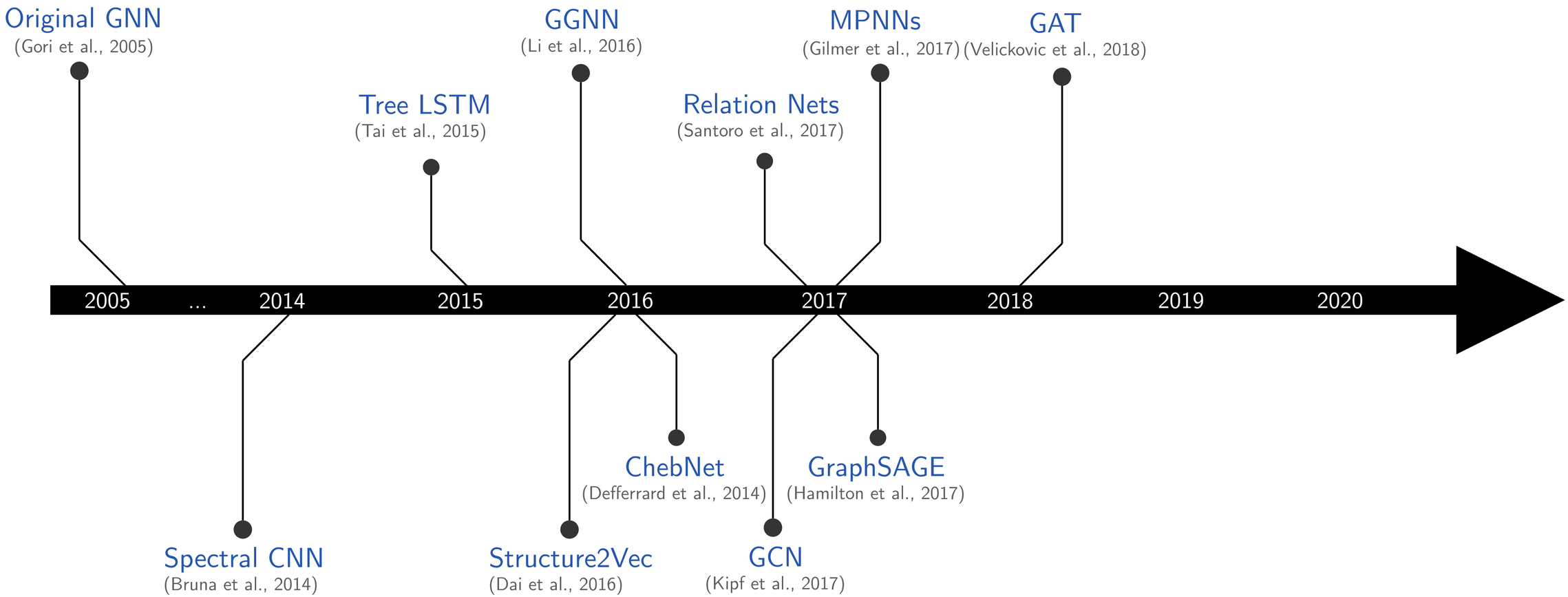

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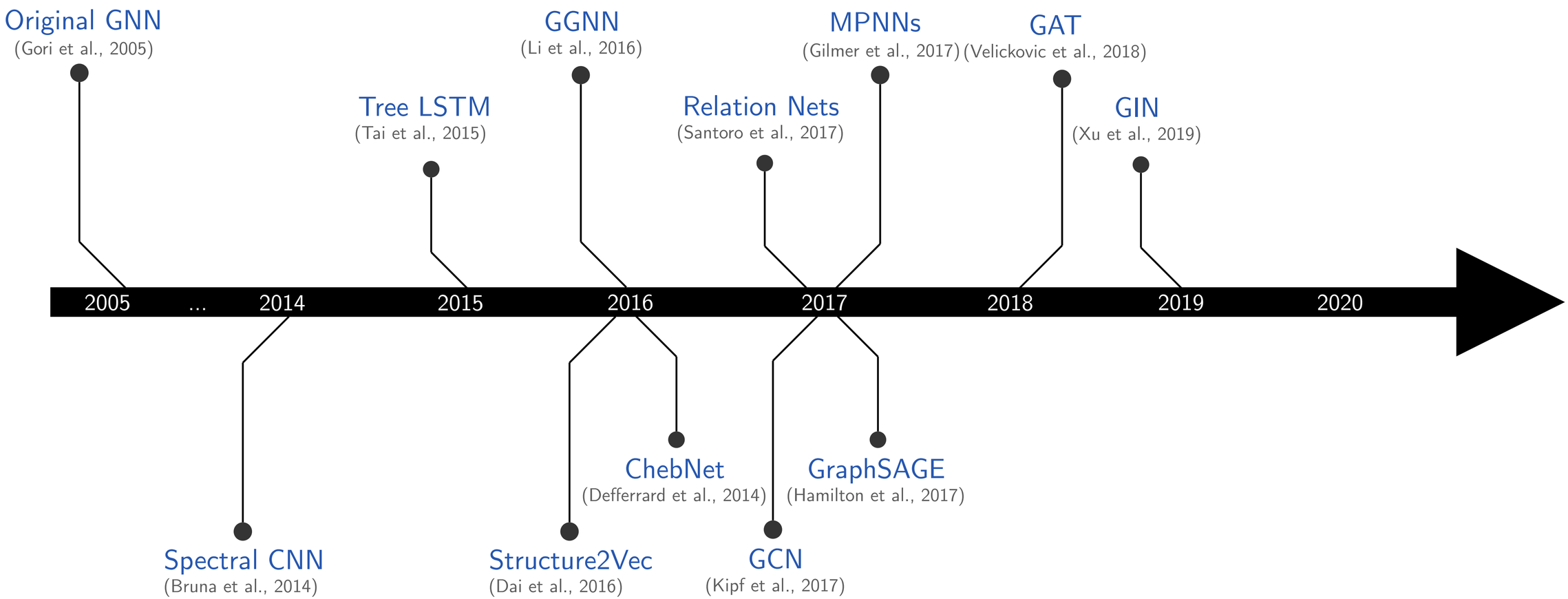

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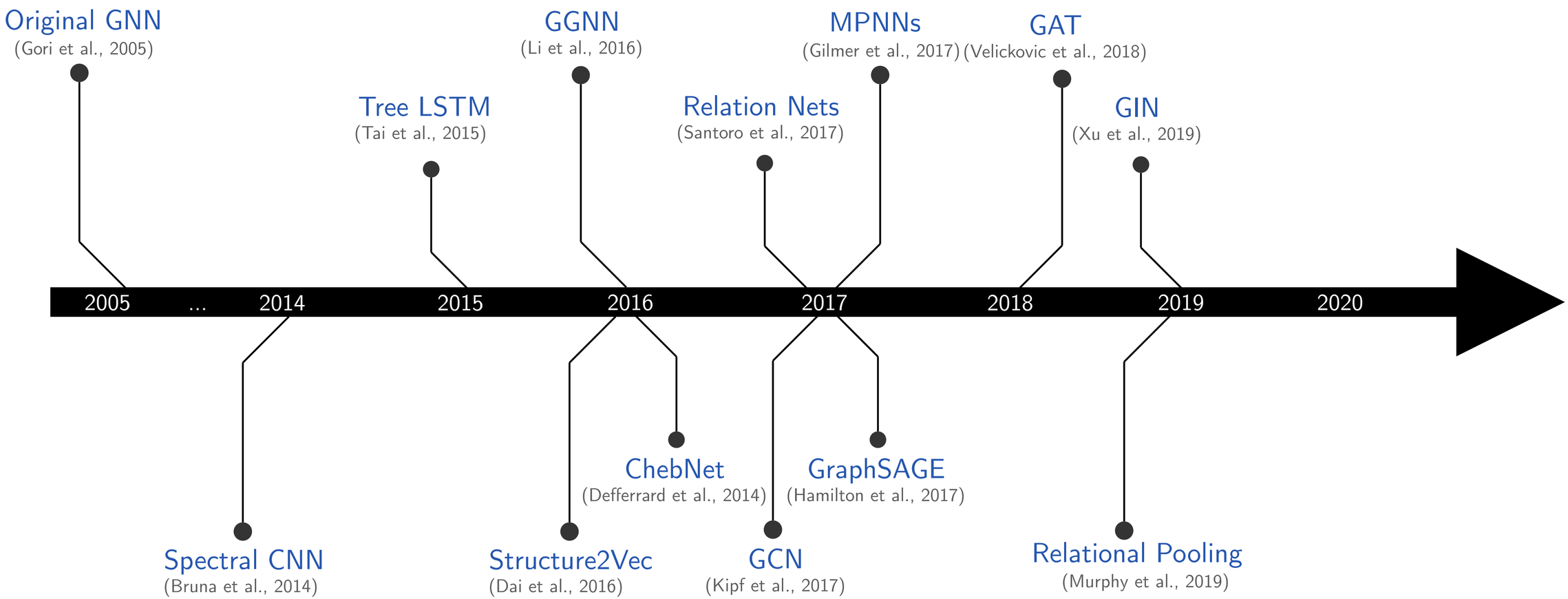

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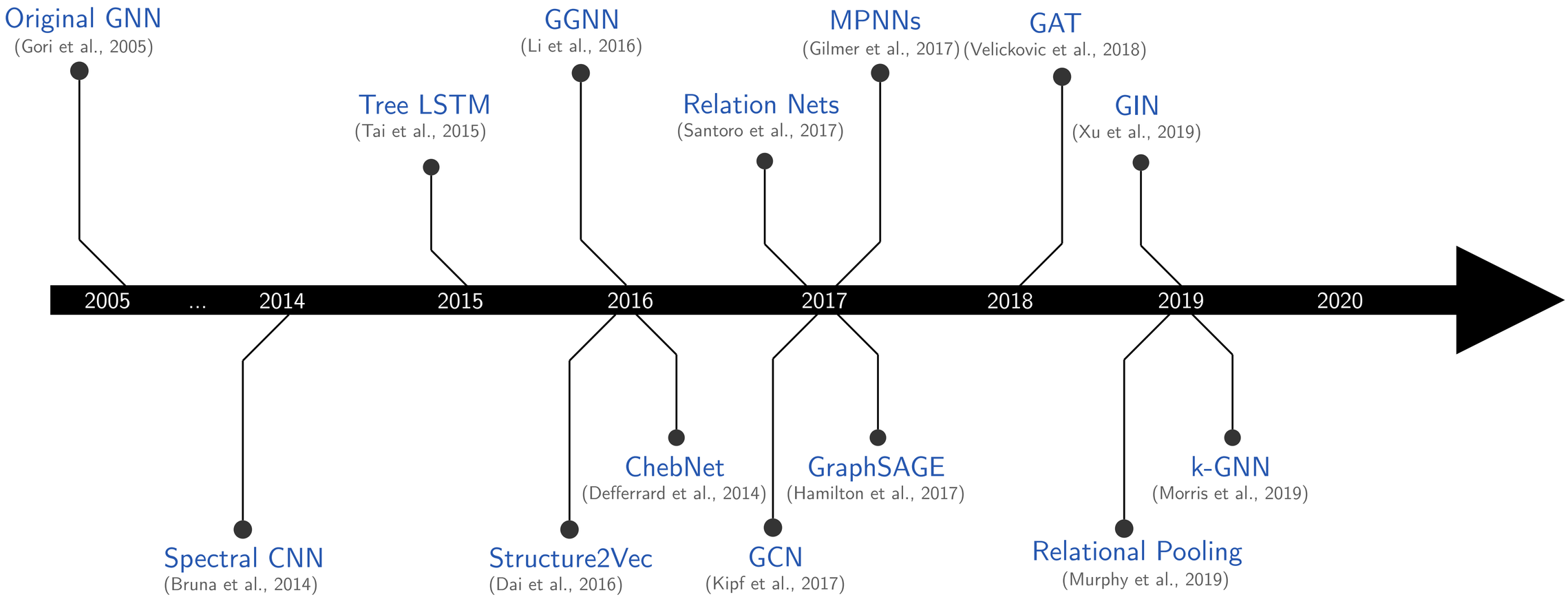

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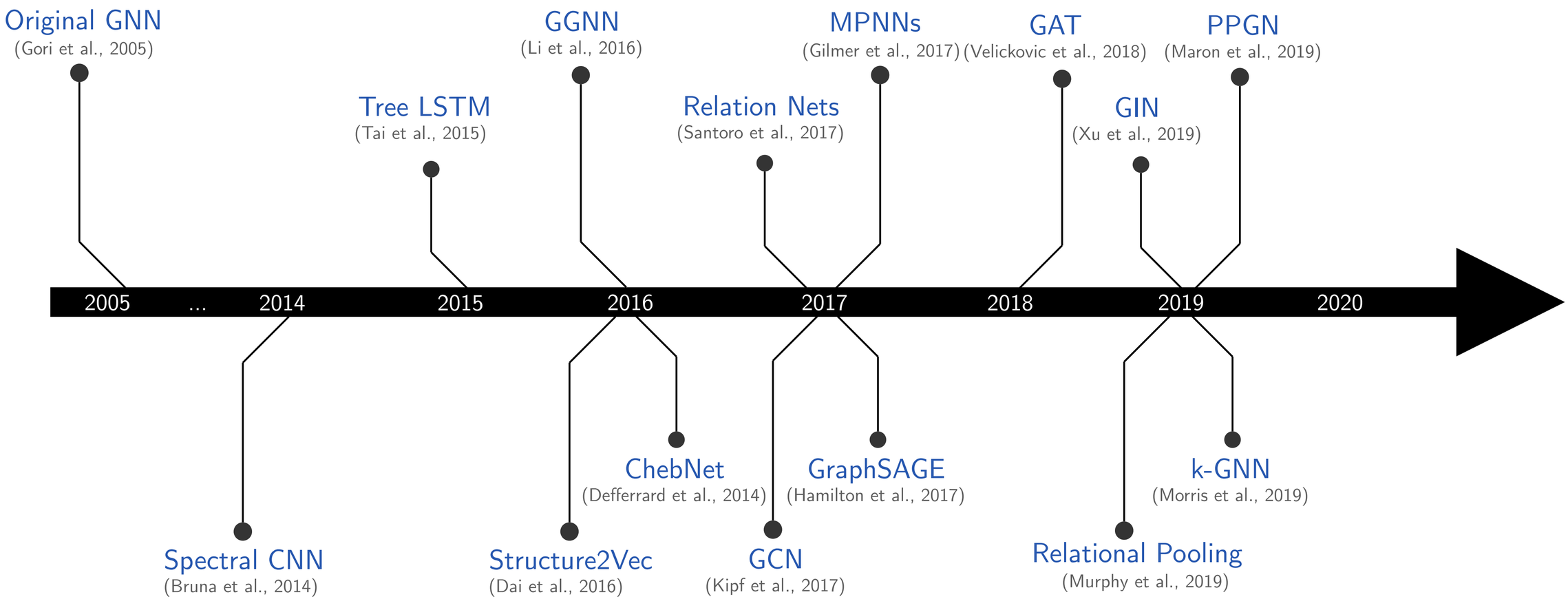

Graph Convolutional Networks

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Briefly, let f and h be two functions. Then, the convolution operation is defined as follows:

$$(f \star h)(\mathbf{x}) = \int_{\mathbb{R}^d} f(\mathbf{y})\, h(\mathbf{x} - \mathbf{y})\, d\mathbf{y}.$$

Intuitively, this means that the function h "slides" over the function f for every value $\mathbf{x}$, and returns a value reflecting the similarity between the two functions around the value $\mathbf{x}$.

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Convolution can be mapped to the frequency domain, such that the integration operation reduces to point-wise multiplication over the Fourier transforms of both functions:

$$(f \star h)(\mathbf{x}) = \mathscr{F}^{-1}(\mathscr{F}(f(\mathbf{x})) \circ \mathscr{F}(h(\mathbf{x}))),$$

where $\mathscr{F}, \mathscr{F}^{-1}$ denote the Fourier and inverse Fourier transform, respectively.

Properties of Convolution

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Convolutions are translation-equivariant:

$$f(t+a) \star g(t) = f(t) \star g(t+a) = (f \star g)(t+a),$$

which means that translating a signal and then convolving it is equivalent to convolving the signal and then translating the result.

Convolution allows for a more localised processing of information, and this offers a strong inductive bias.

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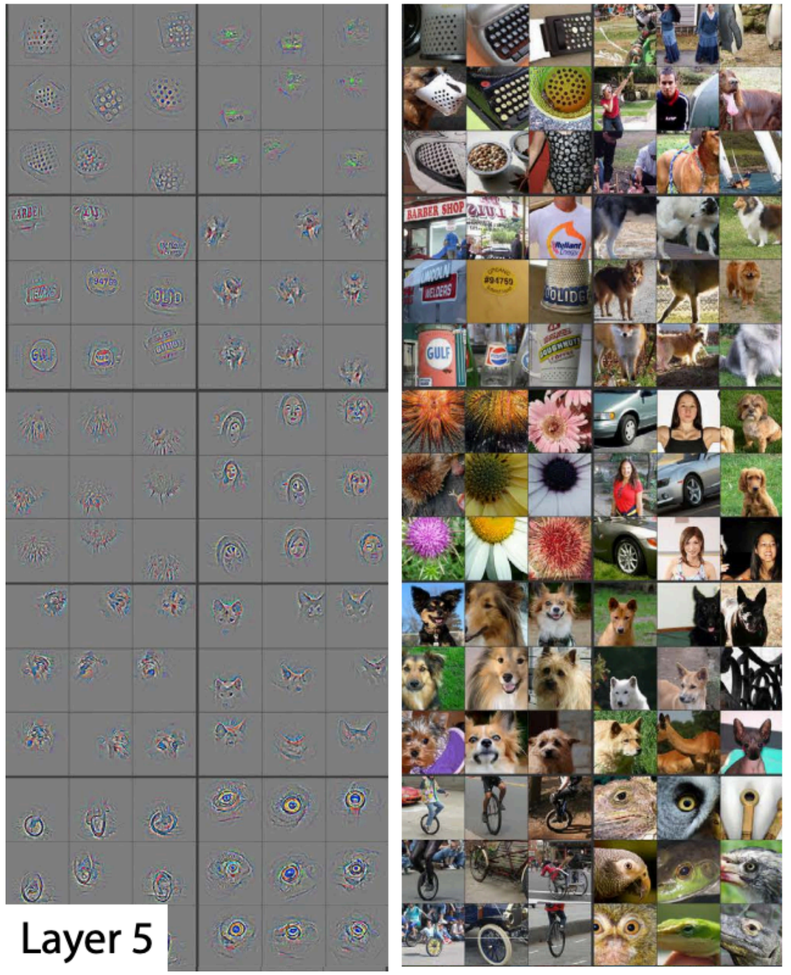

Excerpt from Figure 2 of (Zeiler and Fergus, 2014).

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Question: Can we lift convolutions to the graph domain, to take advantage of their inductive bias?

Recall the basic MPNN model from Lecture 3, defined as:

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

Can we interpret this model in terms of convolutions?

Revisiting the Basic Model

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

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

where $\mathbf{H}^{(t)} \in \mathbb{R}^{|V_G| \times d}$ denotes the matrix of node representations at layer t and $\mathbf{A}^{G}$ is the adjacency matrix of G, and will omit the superscript G, for brevity.

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Convolution can be done based on spectral properties of the graph, and in this case, this is defined via the adjacency matrix!

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Problem: For general graphs, commutativity with the adjacency matrix (i.e., translation-equivariance) does not necessarily imply commutativity with the Laplacian!

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These matrices share the same eigenvectors! We observe the following relationship:

$$\mathbf{L}_{sym} = \mathbf{I} - \mathbf{A}_{sym} \Rightarrow \mathbf{L}_{sym} = \mathbf{U}\mathbf{\Lambda}\mathbf{U}^{\top} \text{ and } \mathbf{A}_{sym} = \mathbf{U}(\mathbf{I} - \mathbf{\Lambda})\mathbf{U}^{\top},$$

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Defining filters based on one of these matrices implies commutativity with the other, which is a very convenient and desirable property!

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Based on graph convolutions, the basic graph convolutional network (GCN) model is defined as follows:

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In this basic GCN, the node base embedding is treated identically to messages from other nodes, and the combine and aggregate functions are intertwined. Recall that this can hinder the expressiveness of the model, and there are variants of GCNs without self-loops.

Gated Graph Neural Networks

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This mode of operation suggests yet another abstraction: View node embedding updates during message passing as a sequential process!

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- This is typically done with recurrent neural models, and a popular model is the Gated Recurrent Unit (GRU) defined as:

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\mathbf{R}^t &= \sigma(\mathbf{X}^t \mathbf{W}_{xr} + \mathbf{H}^{(t-1)} \mathbf{W}_{hr} + \mathbf{b}_r), \\
\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), \\
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- Briefly, the idea it to maintain a state in memory, and then based on the new state and input, decide to retain or update your state.

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Therefore, the state abstraction for nodes in a graph gives rise to 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, such as GRU, that accepts the current state, the aggregation of messages, and yields an update.

Gated Graph Neural Networks

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This yields a model known as the gated graph neural networks (Li et al., 2016), where the representation $\mathbf{h}_u$ for each node $u \in V$ is iteratively updated as:

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

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Several variants to the base GGNN model have been developed by simply modifying any of the three aforementioned components.

Multi-layer perceptrons have been used for message computation; other gated units, such as LSTM, Layer-Norm LSTM, have also been applied instead of GRU; finally, we have the usual choices for different aggregation functions.

Graph Isomorphism Networks

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- **Max**: Allows to highlight a relevant element in the neighbourhood, but has very limited discriminative ability. If we consider an ordering red $<$ yellow $<$ green, then green will be returned for any neighborhood involving at least 1 green node.

Aggregation and Expressiveness

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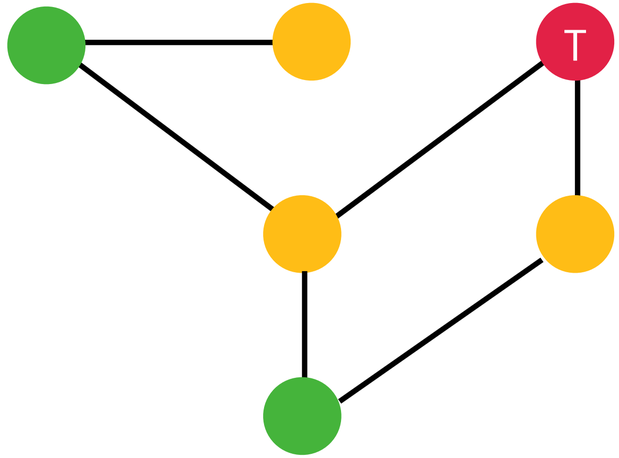

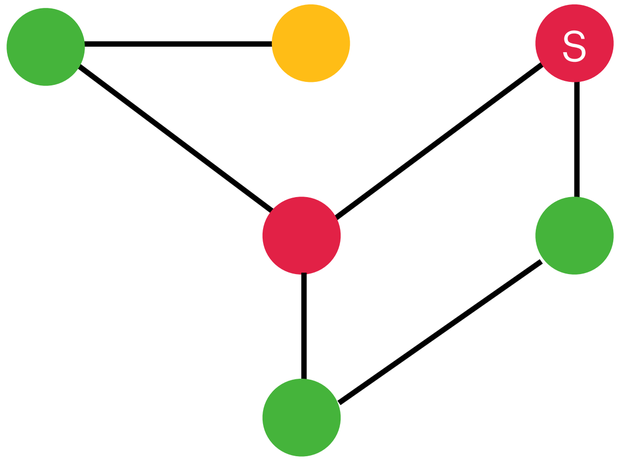

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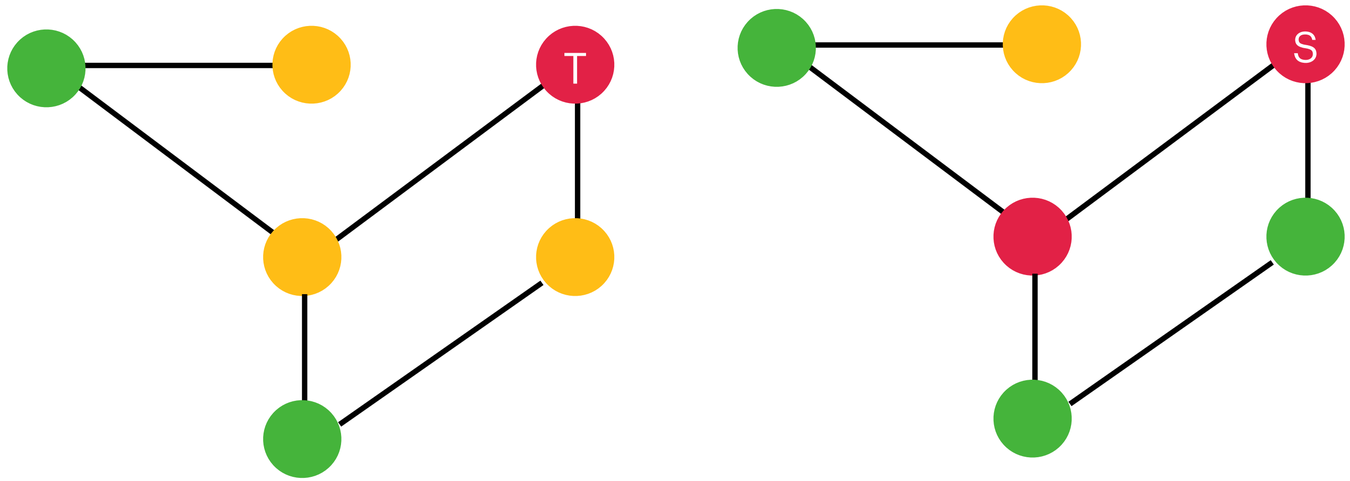

In order to be more generally applicable, an aggregation function must be able to distinguish between distinct neighbourhoods, and return different results given different neighbourhood multisets.

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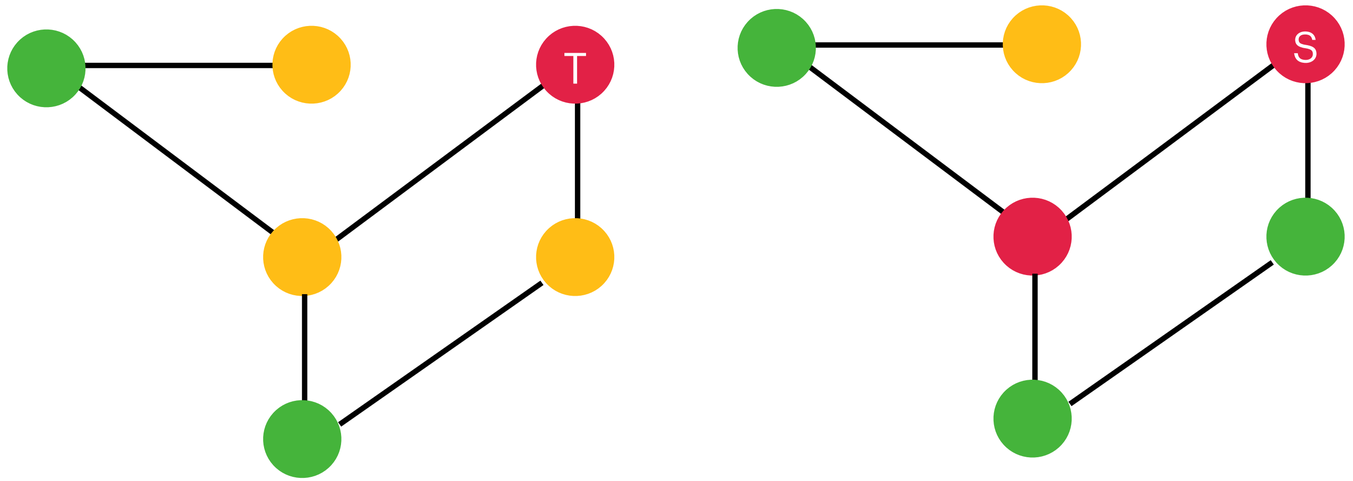


In order to be more generally applicable, an aggregation function must be able to distinguish between distinct neighbourhoods, and return different results given different neighbourhood multisets.

More formally, the aggregation function must be injective relative to the neighbourhood. In fact, it is shown that MPNNs are at their maximal expressiveness if the aggregation function being used is injective (Xu et al.,2019).

Aggregation and Expressiveness

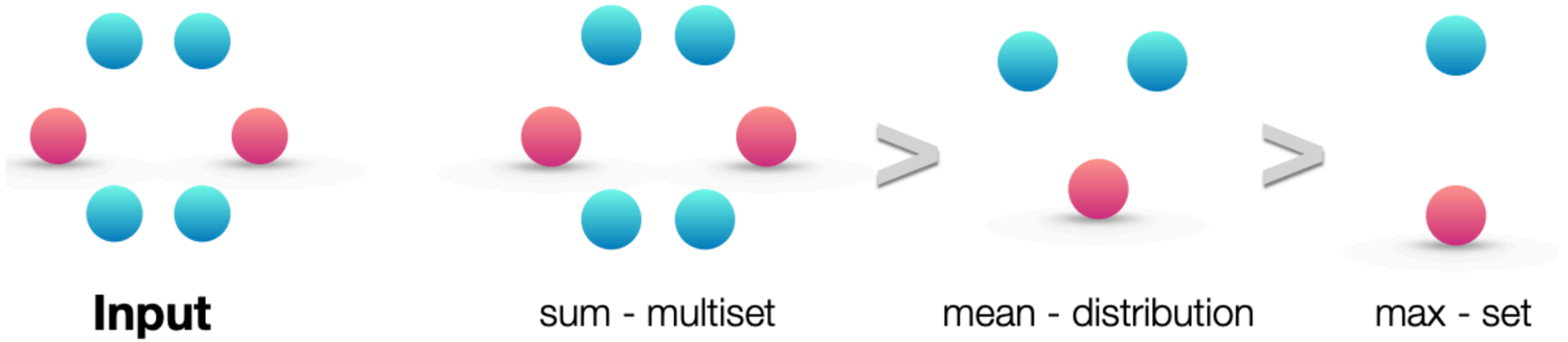
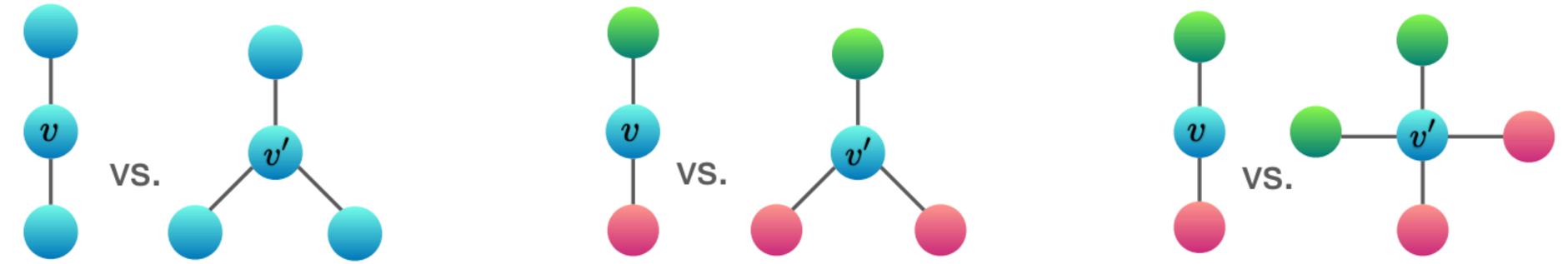


Figure 2: **Ranking by expressive power for sum, mean and max aggregators over a multiset.** Left panel shows the input multiset, *i.e.*, the network neighborhood to be aggregated. The next three panels illustrate the aspects of the multiset a given aggregator is able to capture: sum captures the full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

— In terms of injectiveness sum > mean > max. (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)

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

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

is unique for each pair (c, X), where $c \in X$ and $X \subset \mathcal{X}$ is a multiset of bounded size. Moreover, any function g over such pair (c, X) can be decomposed as:

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

for some function ψ.

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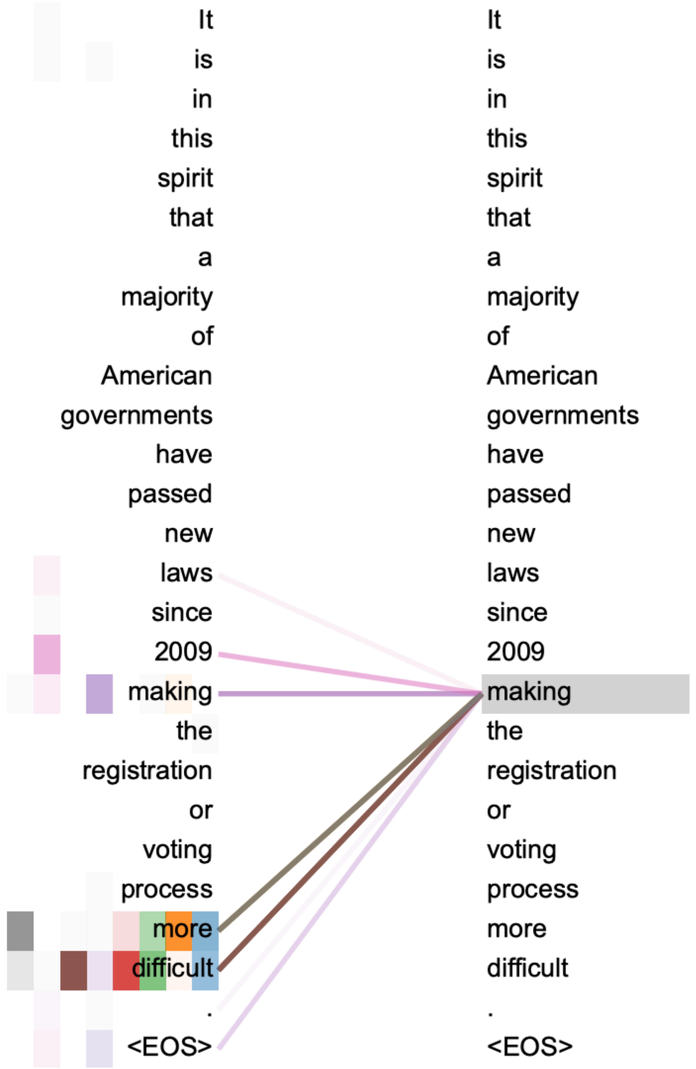
The scaling up of the current node representation distinguishes this node from the neighbour nodes.

Graph Attention Networks

Attention: Refresher



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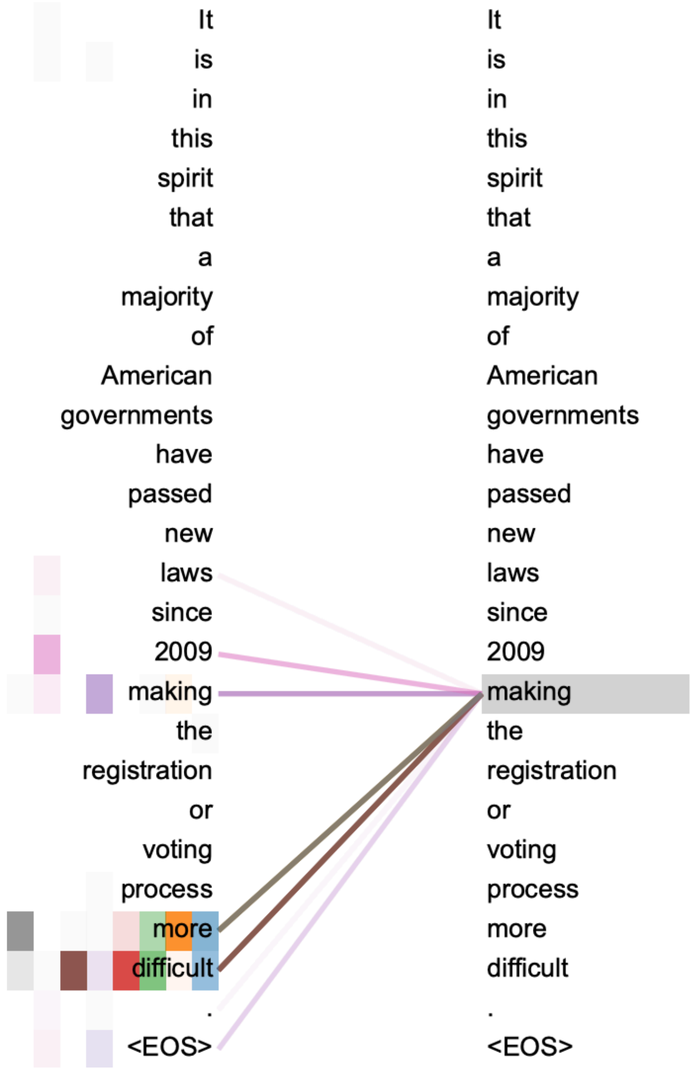

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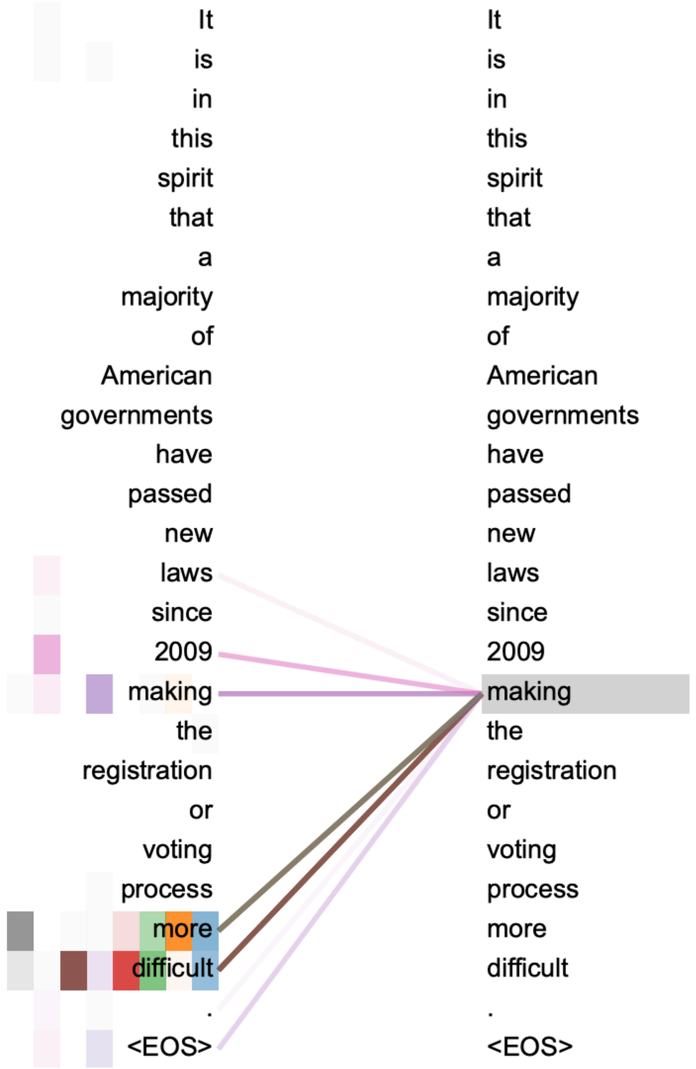

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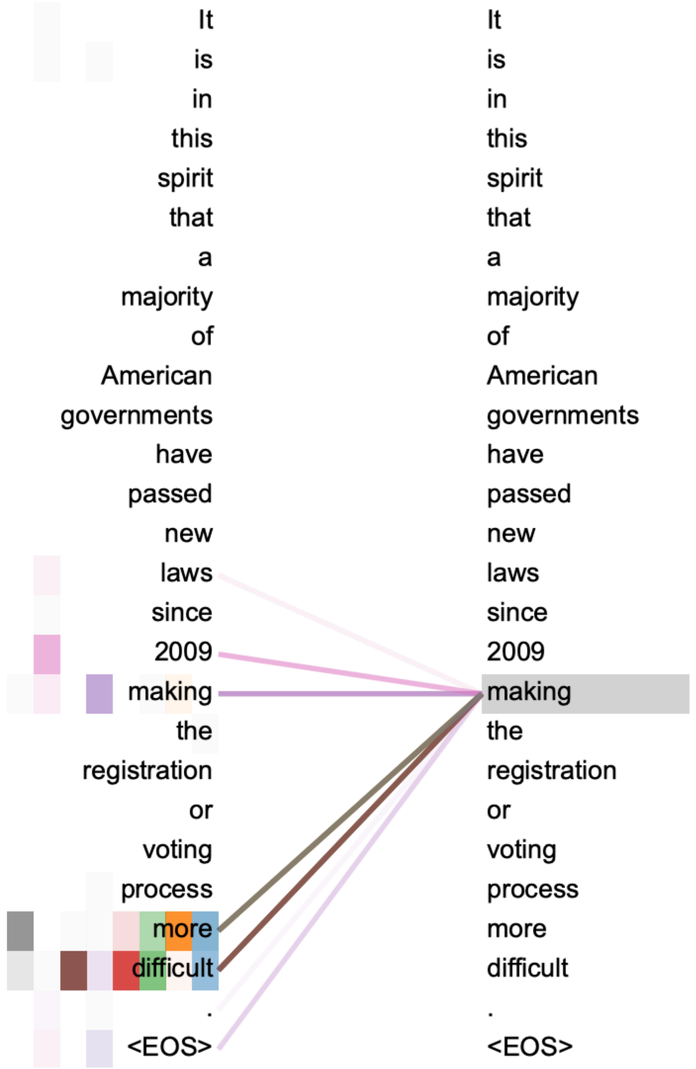

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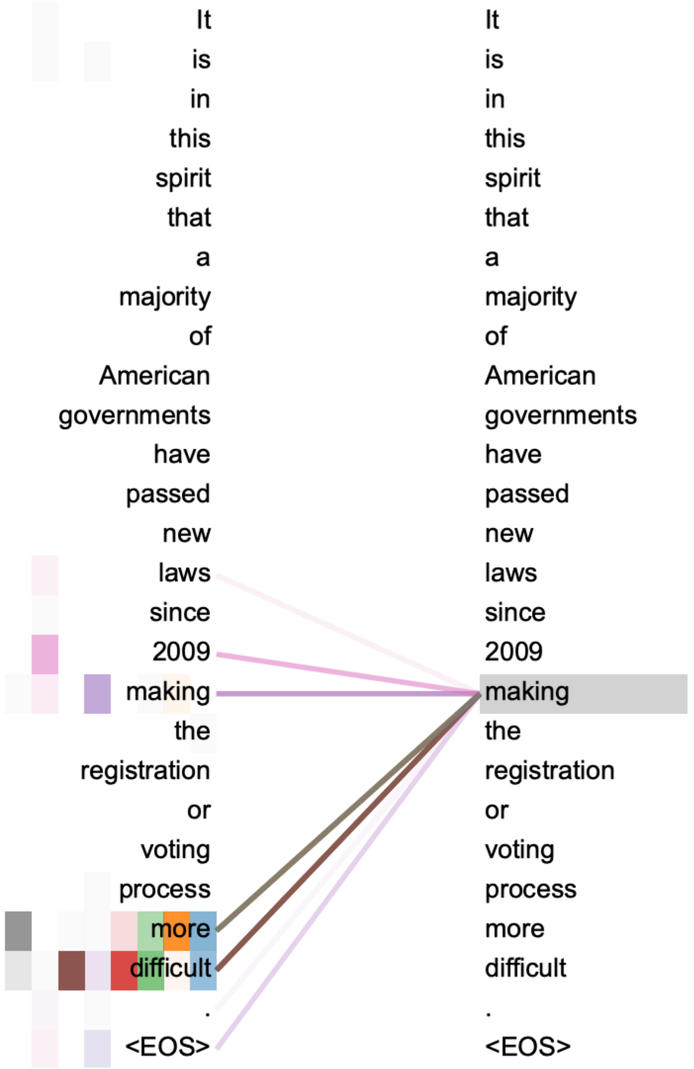
"Many of the attention heads attend to a distant dependency of the verb 'making', completing the phrase 'making...more difficult'. Attentions here shown only for the word 'making'. Different colours represent different heads."



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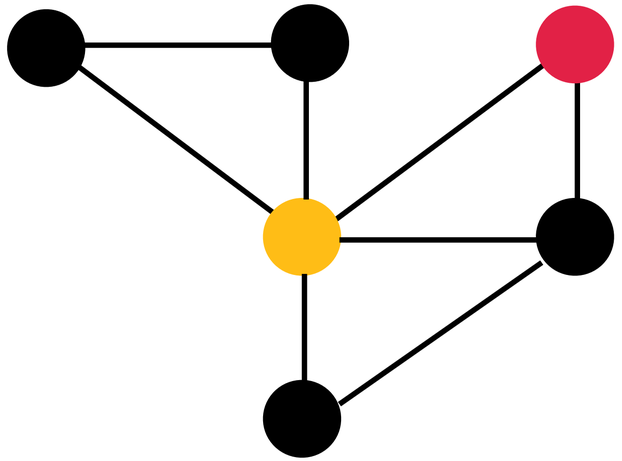

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This intuition underlies the development of graph attention networks (GAT) (Velickovic et al., 2018), which uses weighted sum aggregation, and a pairwise node attention mechanism during message passing;

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

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This can be seen as an extension of the base MPNN model with self-loops. Having self-loops is fine here, as the discrimination of nodes is happening through the attention mechanism. We can of course generalise this:

$$\mathbf{h}_u^{(t)} = combine\Big(\mathbf{h}_u^{(t-1)}, \sum_{v \in N(u)} \alpha_{(u,v)}\, \mathbf{h}_v^{(t-1)}\Big).$$

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- Attention for computing the global readout following, or during, message passing.
- Attention across different message passing iterations, similarly to sequence models. For instance, a GGNN model can compute its update by attending to its previous states at earlier iterations, much like standard sequence models.

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Briefly, the transformer architecture (Vaswani et al., 2017) defines neural network layers entirely based on the attention operation, and generates, at each layer, a representation for every position in the input data by using multiple attention heads to compute attention weights between all pairs of positions in the input, which are then aggregated with weighted sums based on these attention weights.

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Briefly, the transformer architecture (Vaswani et al., 2017) defines neural network layers entirely based on the attention operation, and generates, at each layer, a representation for every position in the input data by using multiple attention heads to compute attention weights between all pairs of positions in the input, which are then aggregated with weighted sums based on these attention weights.

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A Relation to Transformer Model

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We can therefore view the basic Transformer model as a GNN model with multi-head attention, if we further assume that the GNN receives a fully connected graph as input.

Discussions and Limitations

Over-smoothing

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"*If a GCN is deep with many convolutional layers, the output features may be over-smoothed and vertices from different clusters may become indistinguishable.*"

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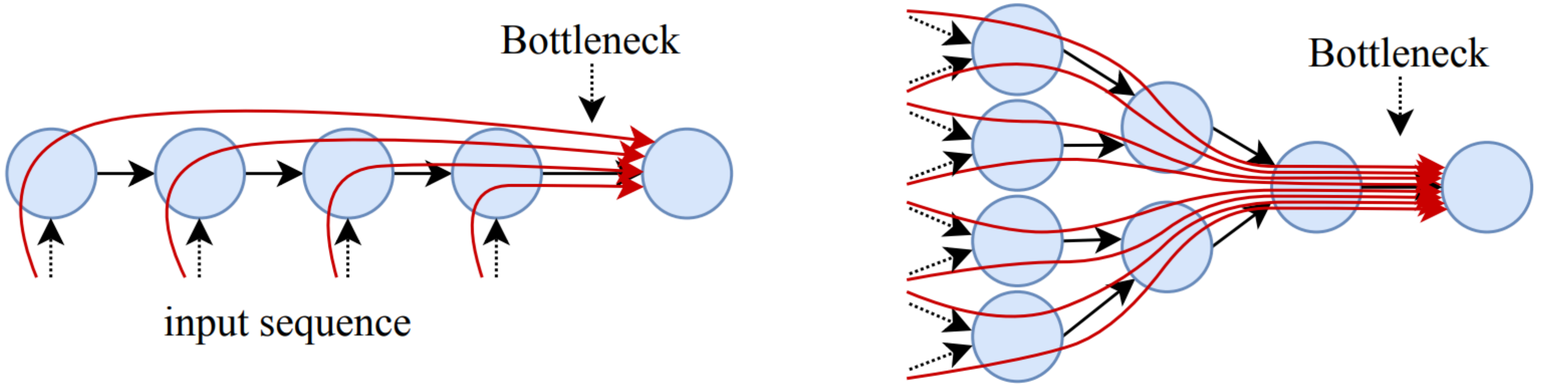
This is not a solution to the problem, but rather a way to alleviate the problem in practice.

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.

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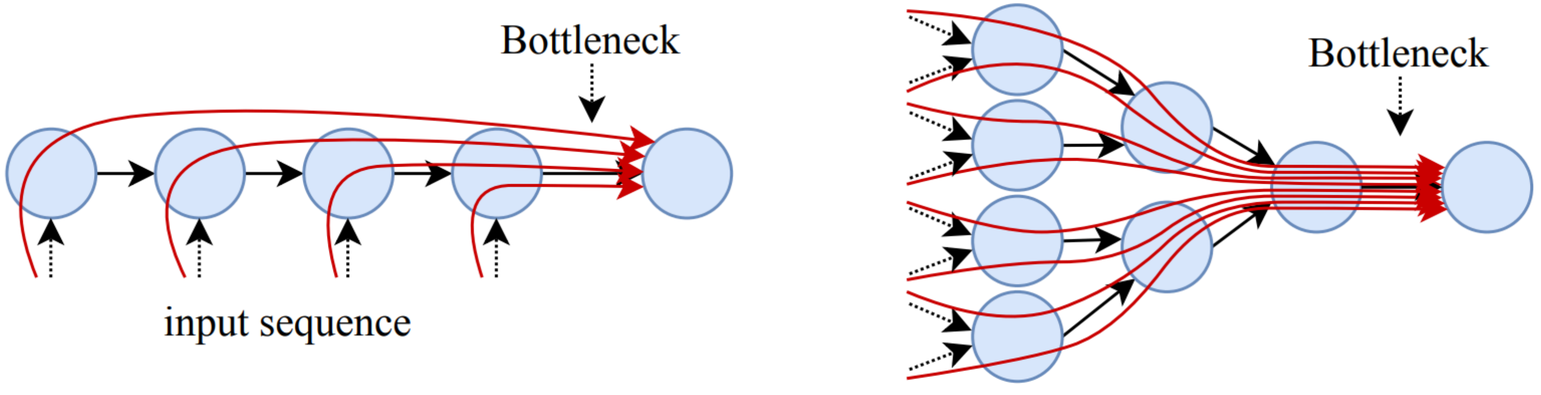

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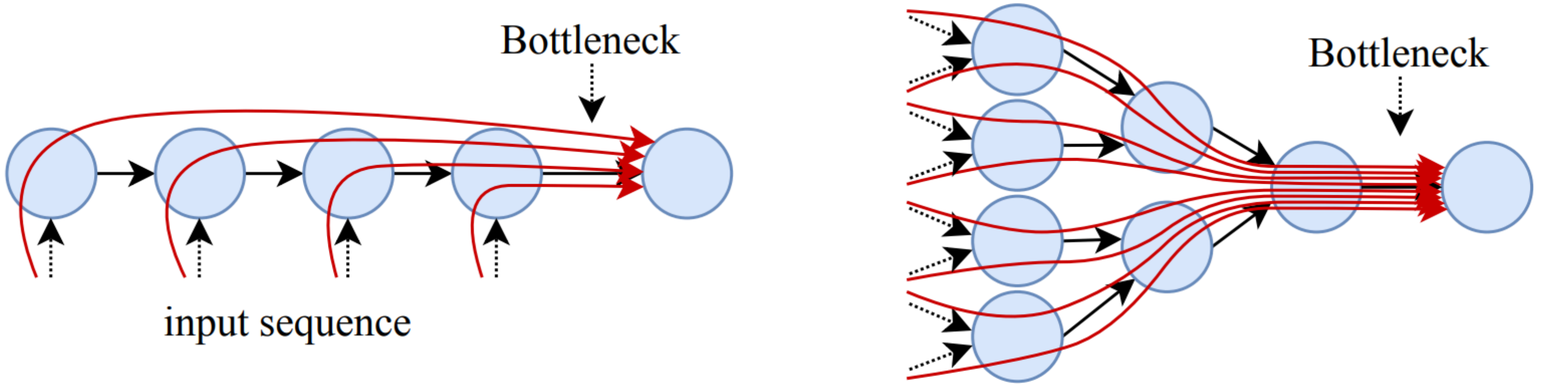

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"As the number of layers increases, the number of nodes in each node's receptive field grows exponentially. This causes over-squashing: information from the exponentially-growing receptive field is compressed into fixed-length node vectors. Consequently, the graph fails to propagate messages flowing from distant nodes; the model learns only short-range signals from the training data; and overall, generalises poorly at test time."

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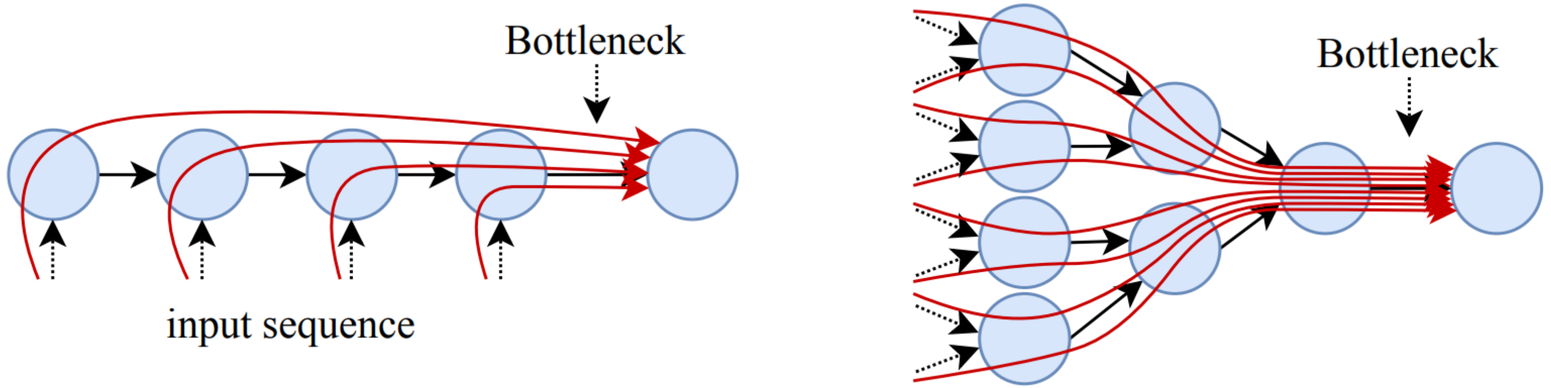

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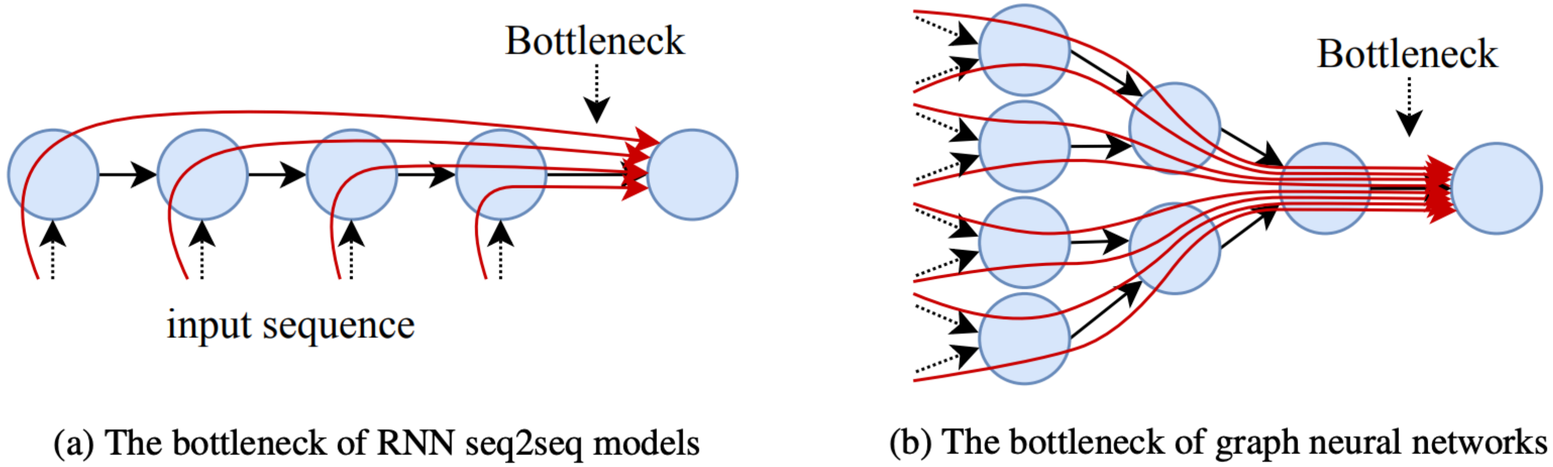

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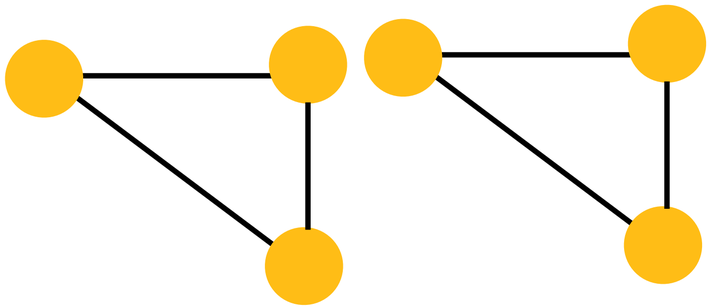
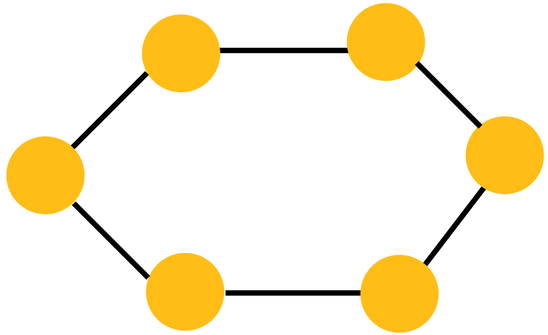
The model then performs poorly when the prediction task depends on long-range interactions, and it is easy to imagine tasks that require long-range dependencies: consider the reachability task on graphs, which requires as many iterations as the diameter of the graph, as otherwise it will suffer from under-reaching (i.e., not receiving information from some nodes).

Expressiveness





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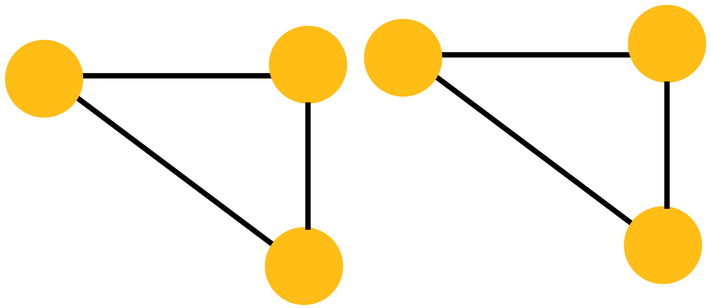

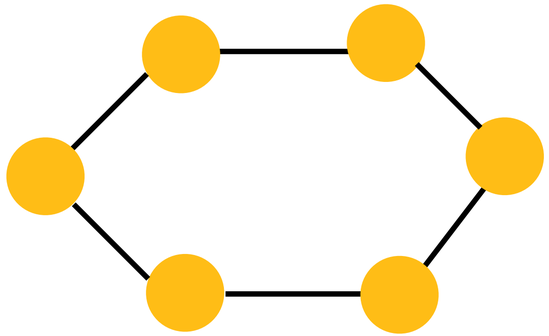

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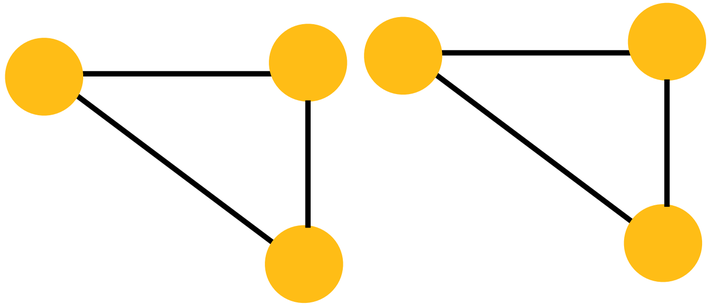

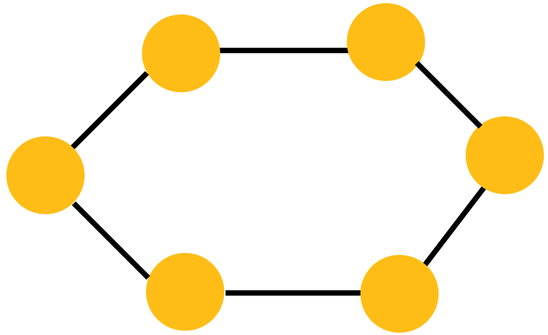

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This is an important limitation, which will be the topic of the next lecture.

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- There are a plethora of other GNN models; some cannot be classified as MPNNs: Lecture 6.

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