Lecture 6: Higher-Order Graph Neural Networks

Relational Learning

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Overview

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- The Weisfeiler-Lehman hierarchy

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  - Provably powerful graph networks

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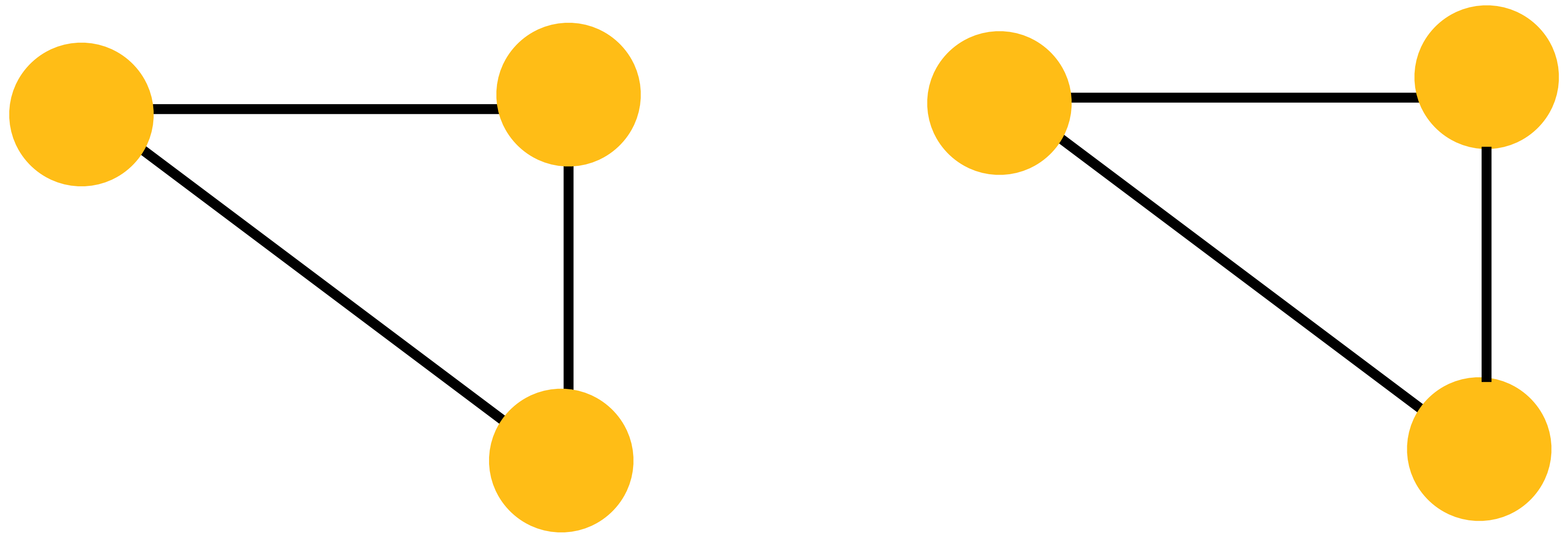
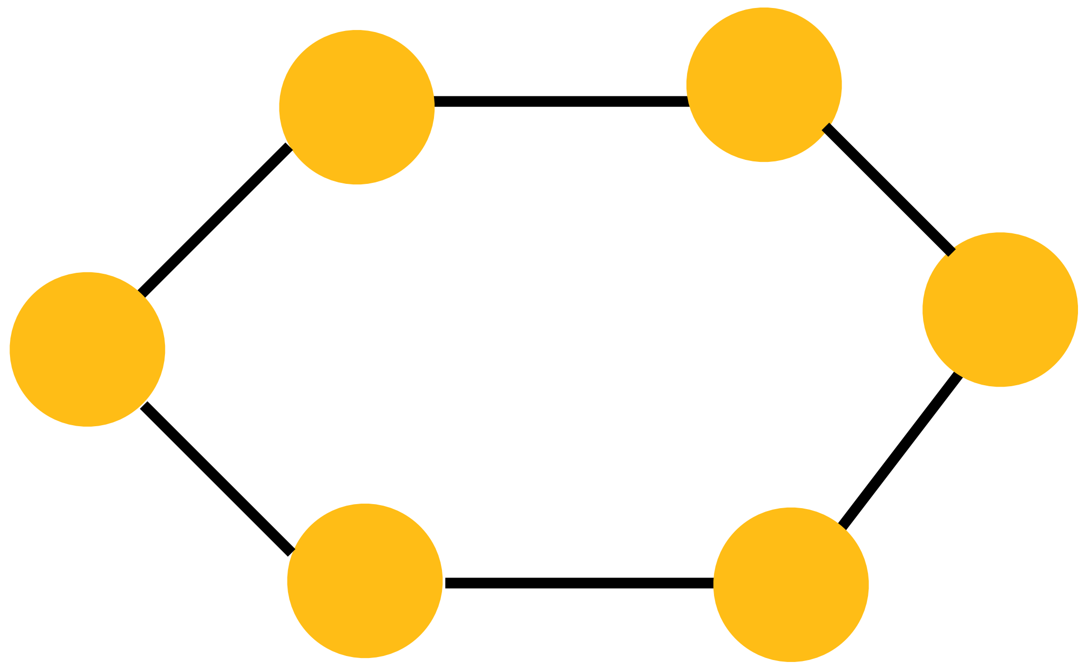
One way of achieving more expressive models is through a richer message passing approach — and this is related to Weisfeiler-Lehman hierarchy.

The Weisfeiler-Lehman Hierarchy

A Tale of Two Graphs





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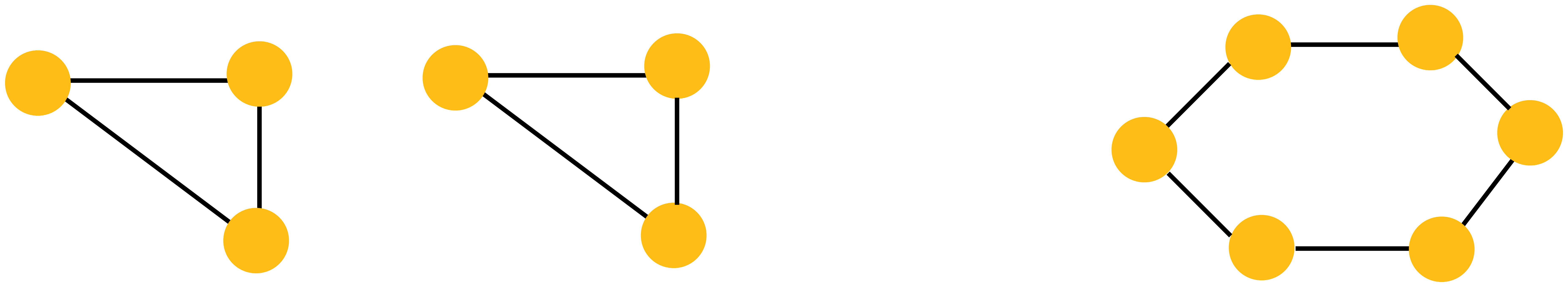

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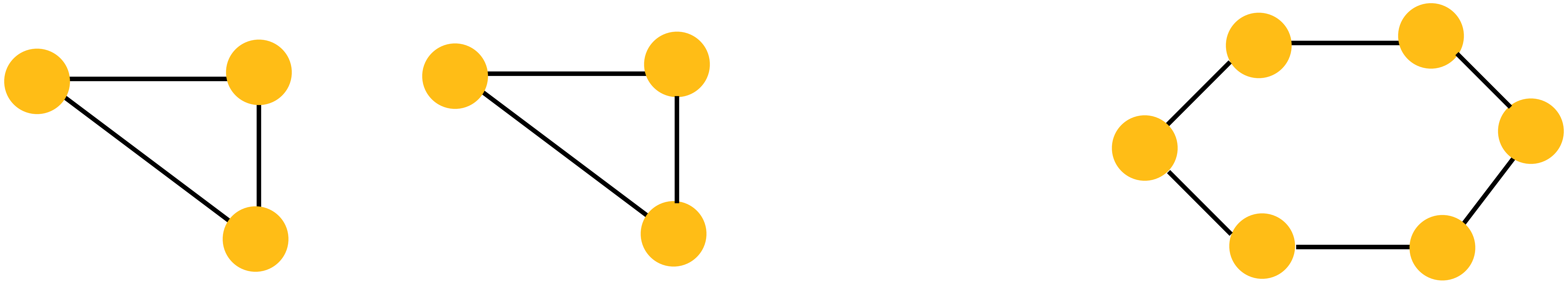

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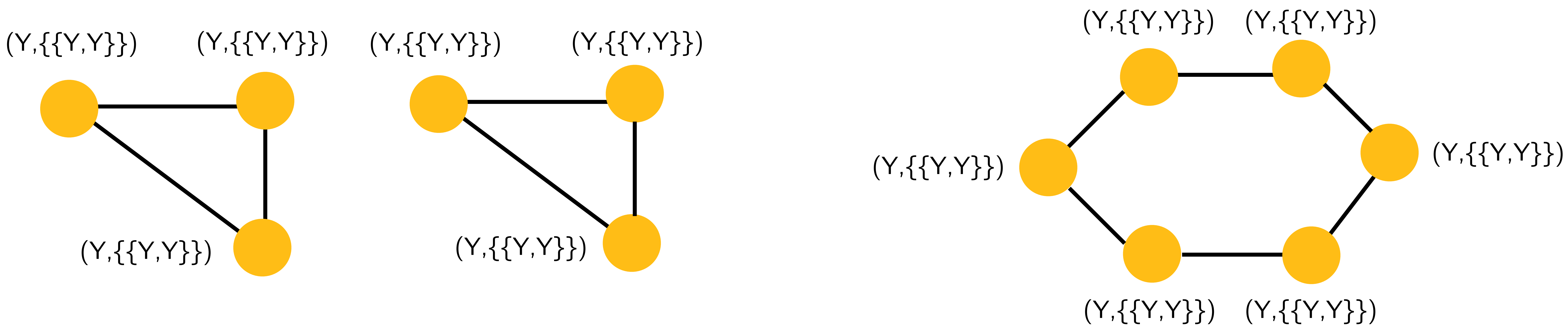

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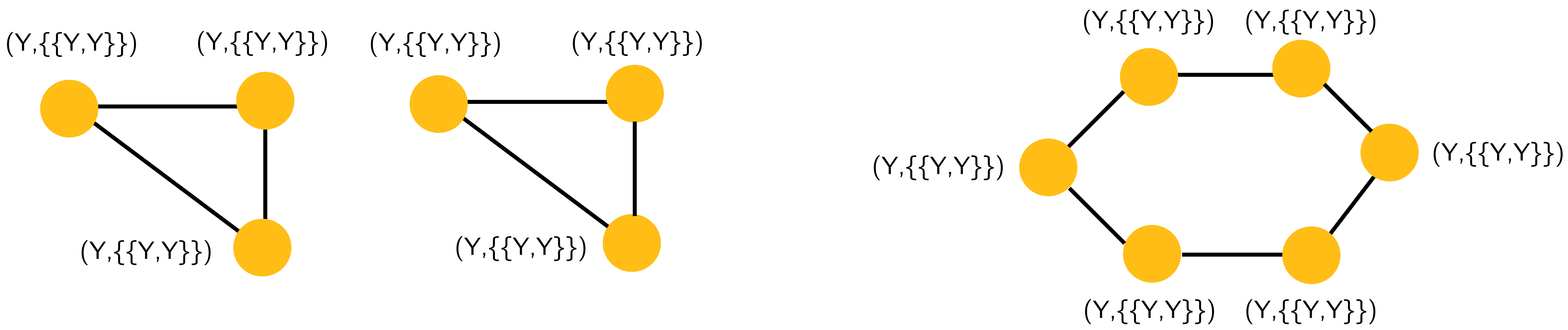

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What if we extend the 1-WL algorithm to consider, e.g., pairs of nodes when colouring?

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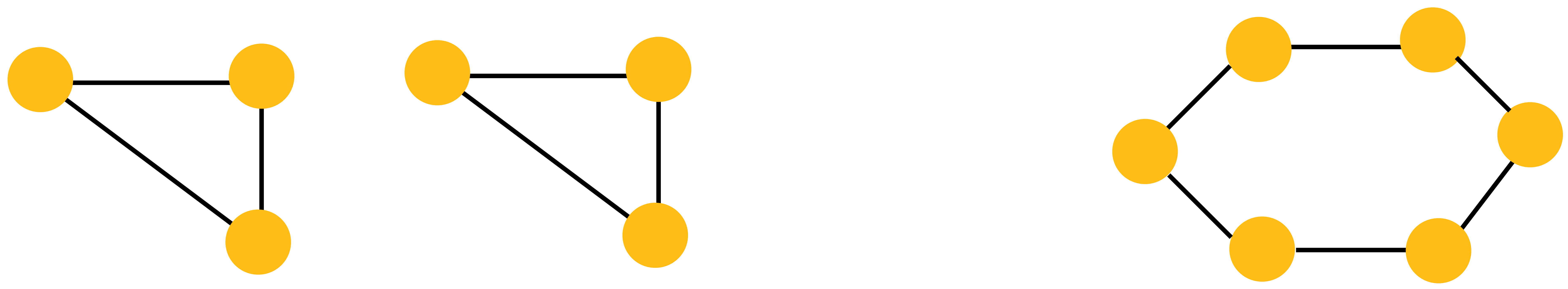

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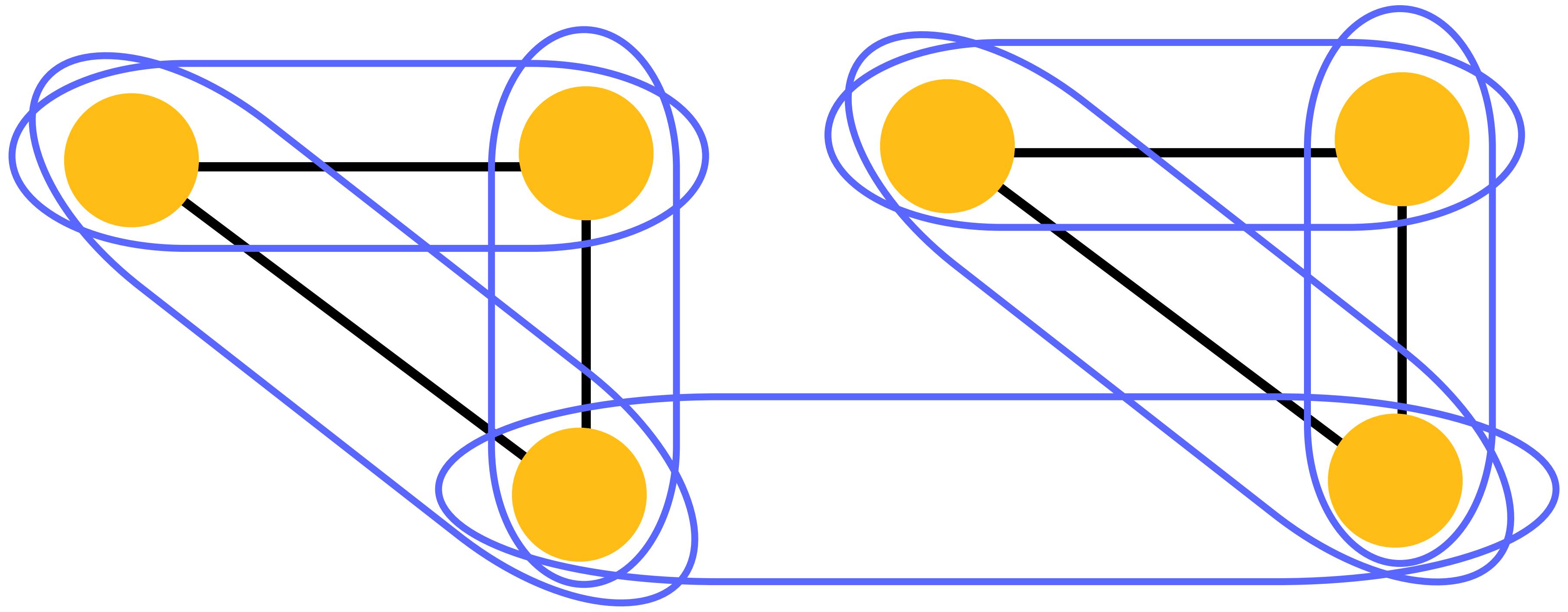

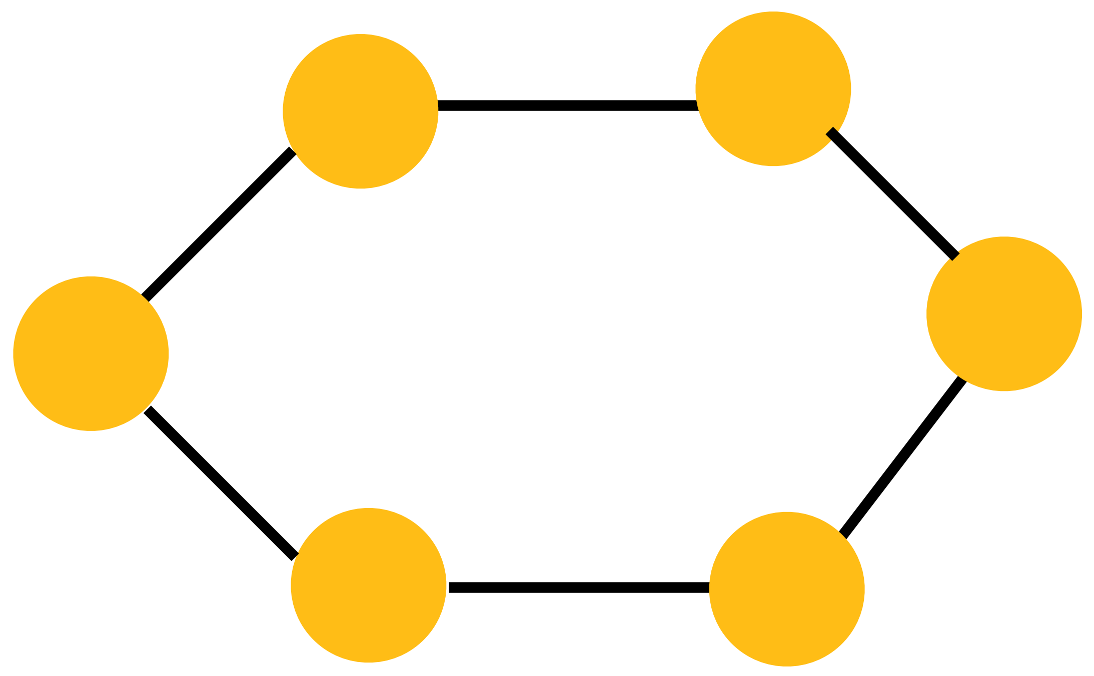

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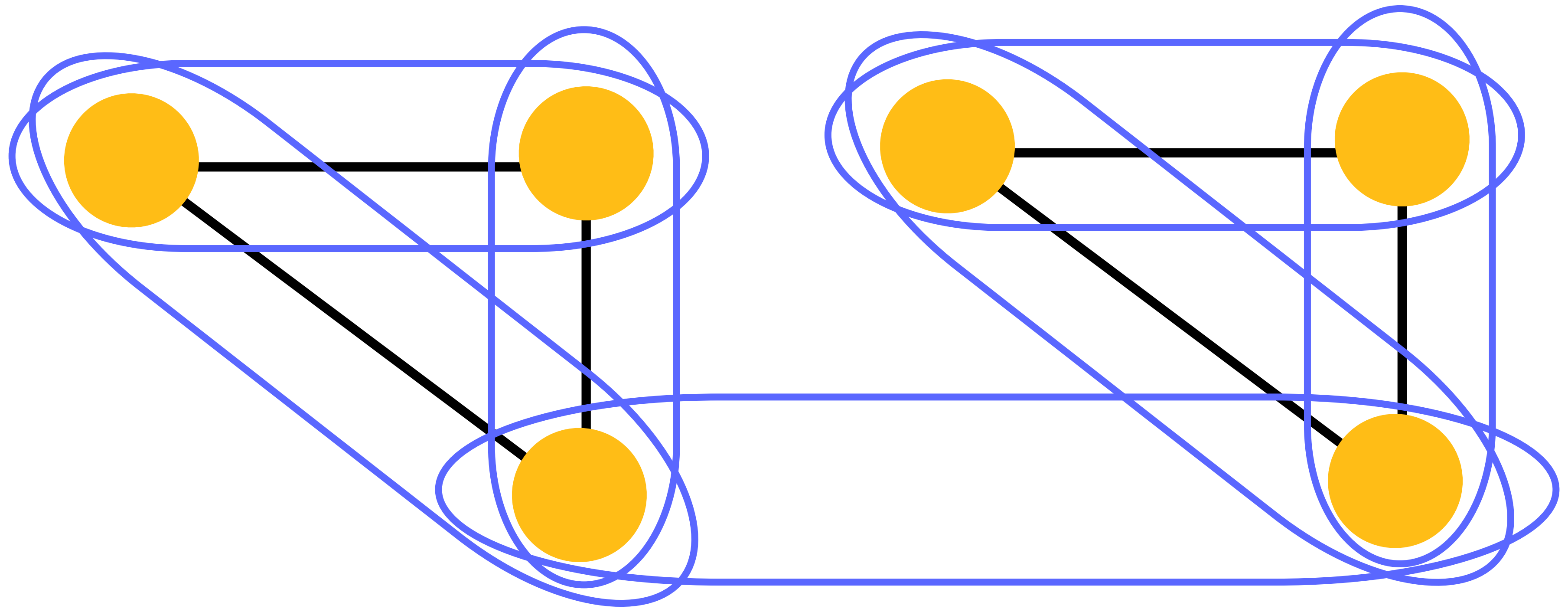

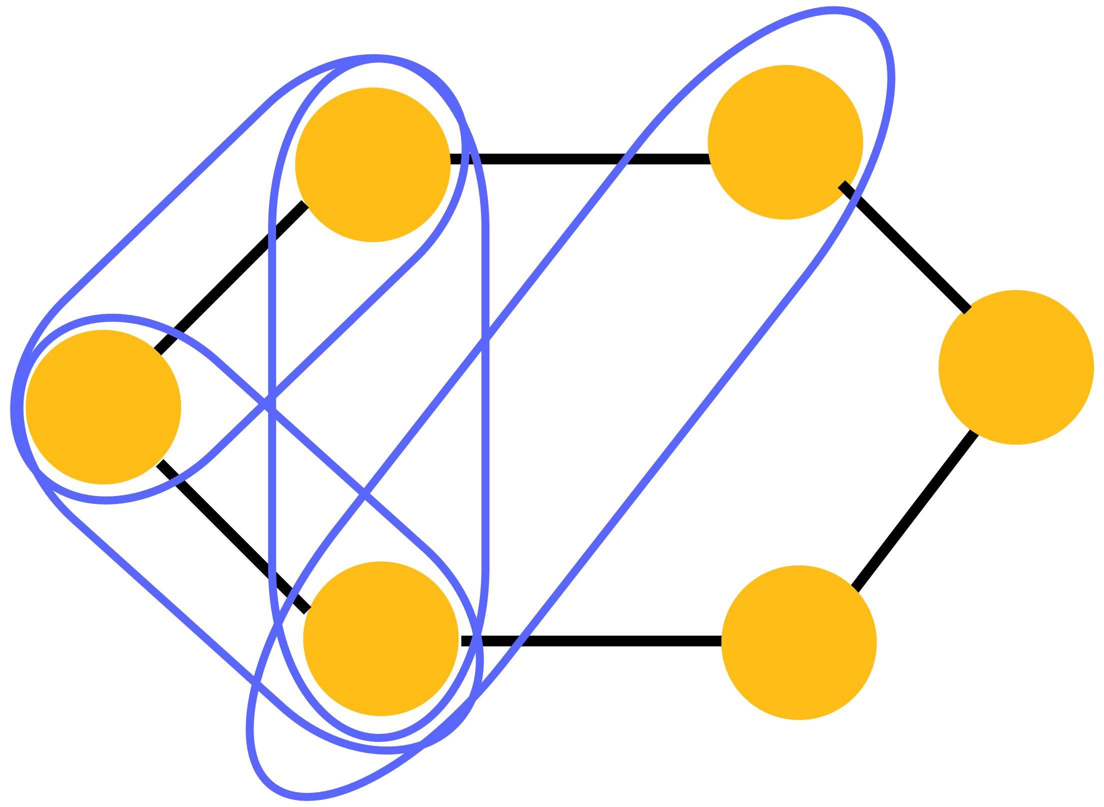

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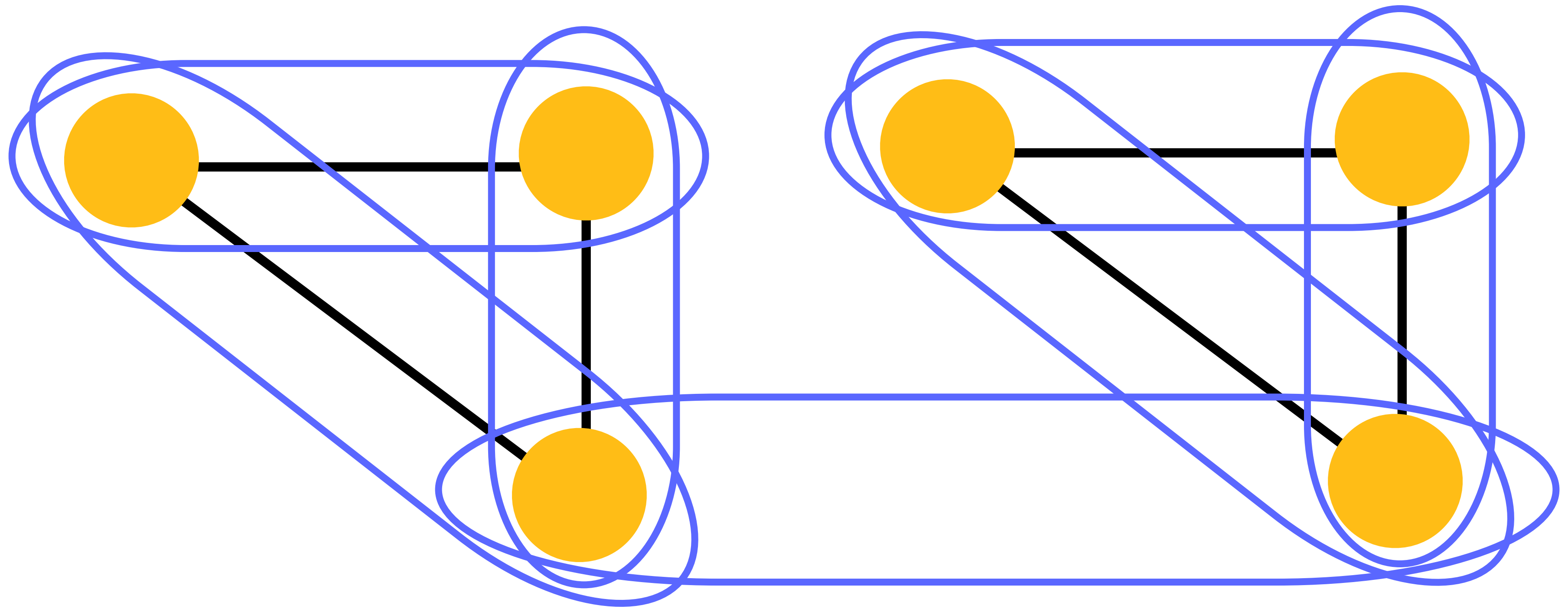

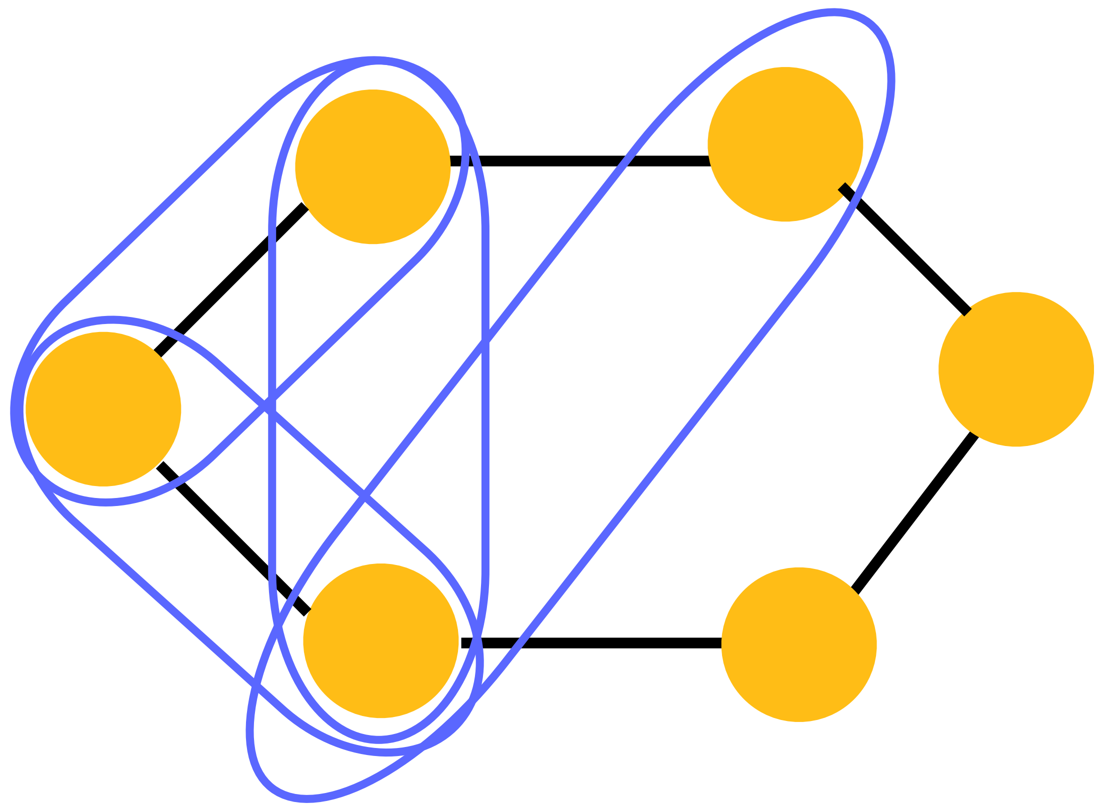

This extended algorithm is called the 2-dimensional WL algorithm, and it can distinguish these two graphs!

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We denote a k-tuple as $t = (u_1, \ldots, u_k)$, and define a substitution as $t[v/i] = (u_1, \ldots, u_{i-1}, v, u_{i+1}, \ldots, u_k)$.

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$$\forall t, t' \in V_G^k : \lambda^{(j+1)}(t) = \lambda^{(j+1)}(t') \text{ if and only if } \lambda^{(j)}(t) = \lambda^{(j)}(t').$$

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We will always refer to the folklore version of this algorithm in the sequel, unless stated explicitly otherwise.

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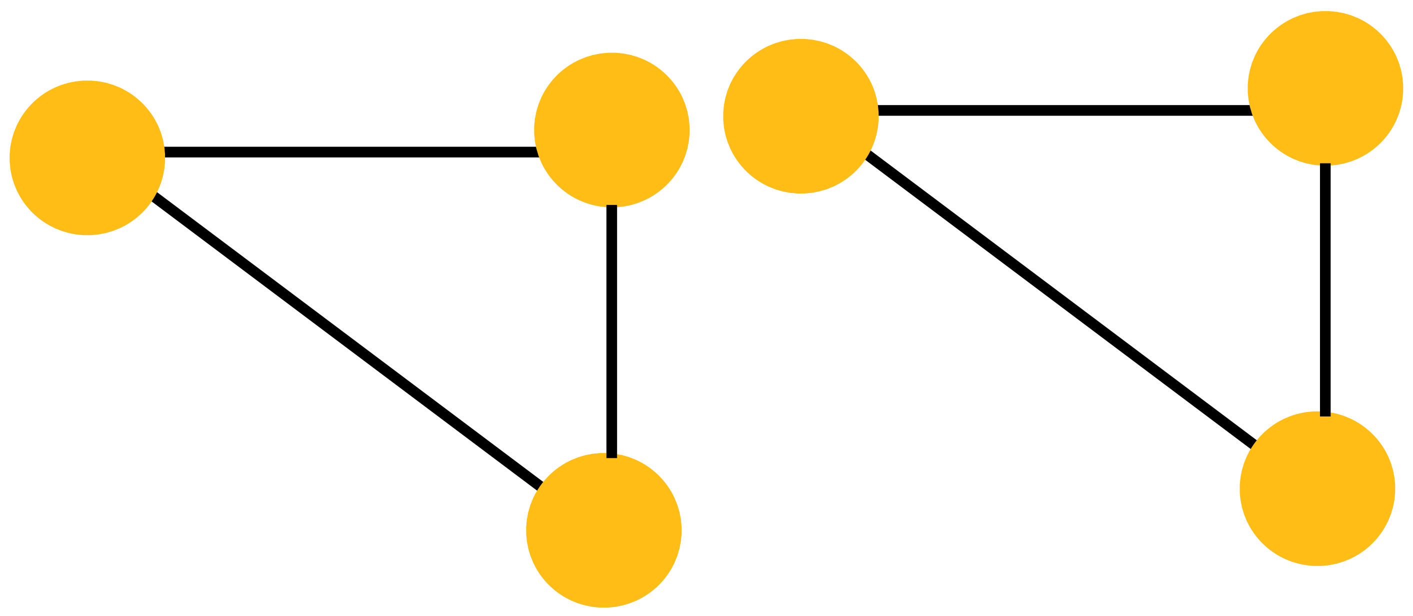

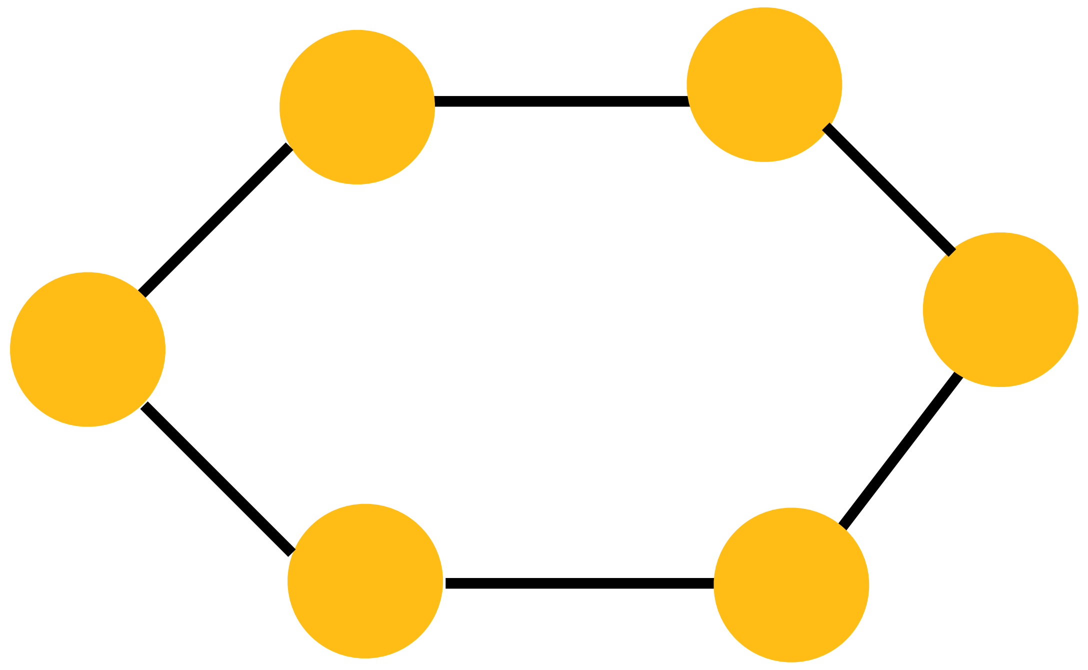

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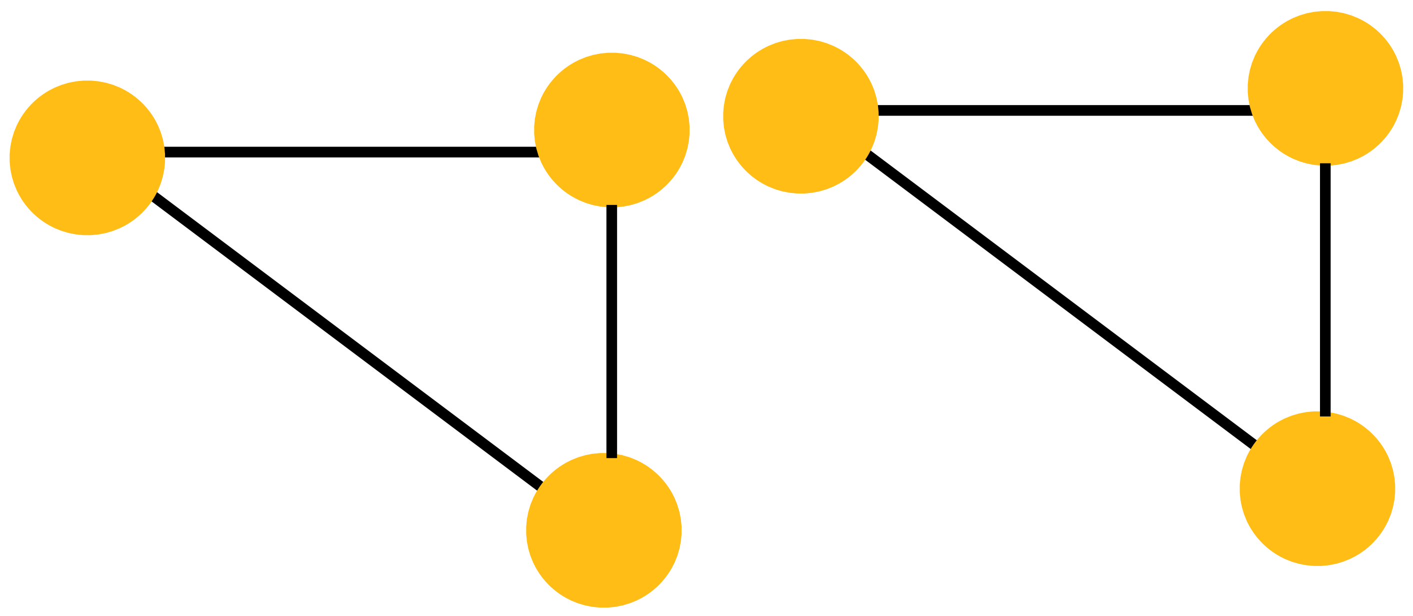

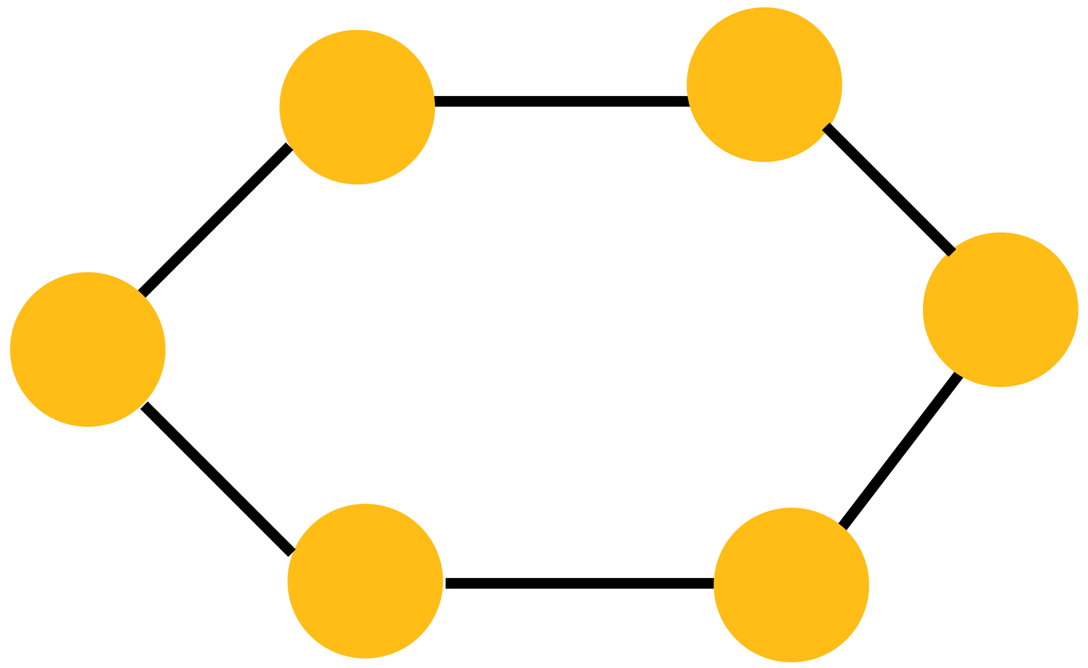

Recall that for all $k \geq 2$ two graphs G and H satisfy the same C^k-sentences if and only if $(k-1)$-WL does not distinguish them (Cai et al., 1992).

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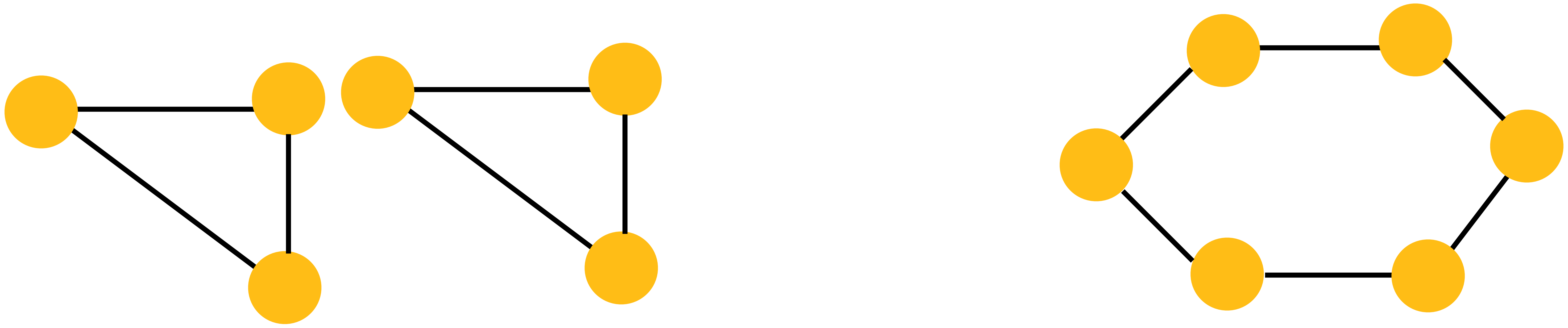

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To see why separator and non-separator nodes can be distinguished for the given graphs with 2-WL, it is sufficient to formalise this as a logical node classifier in C^3:

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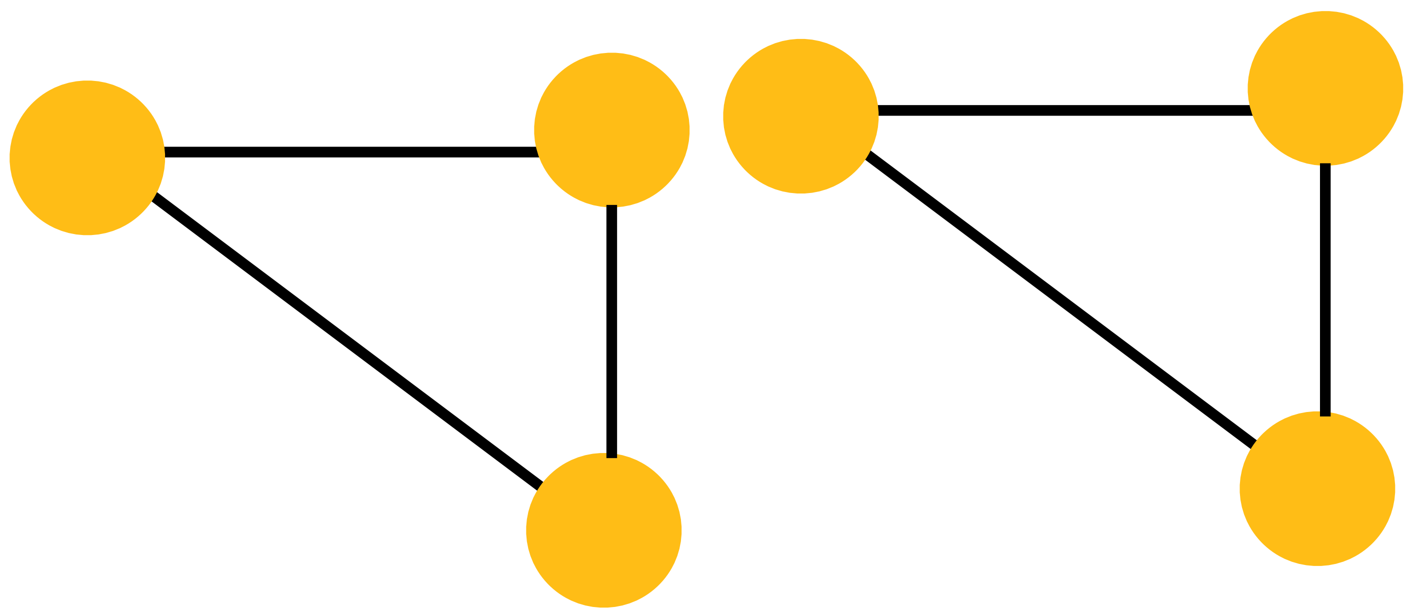

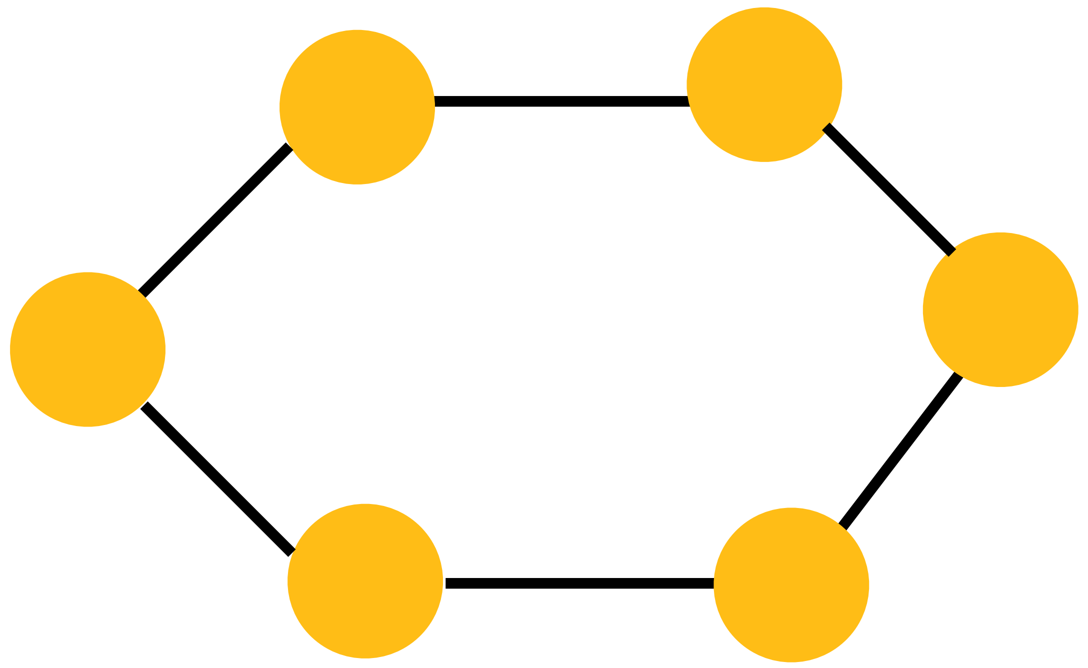

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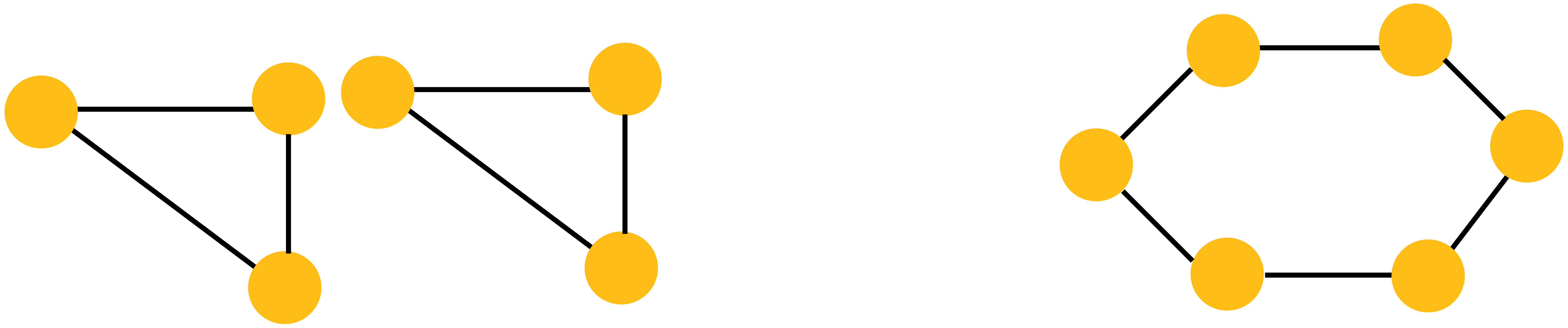

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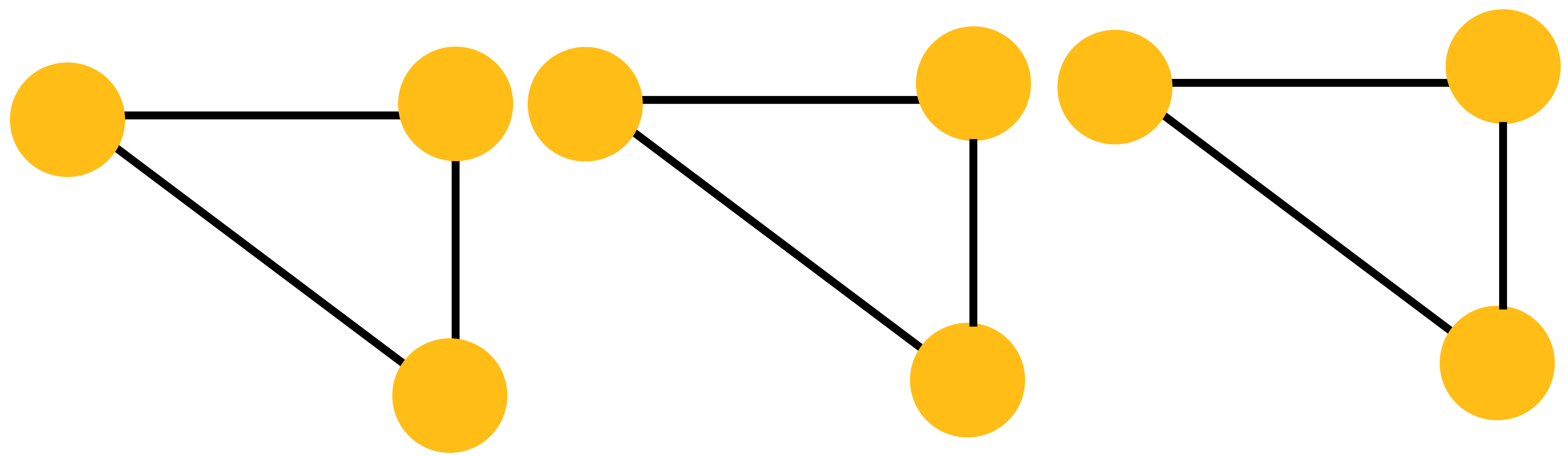
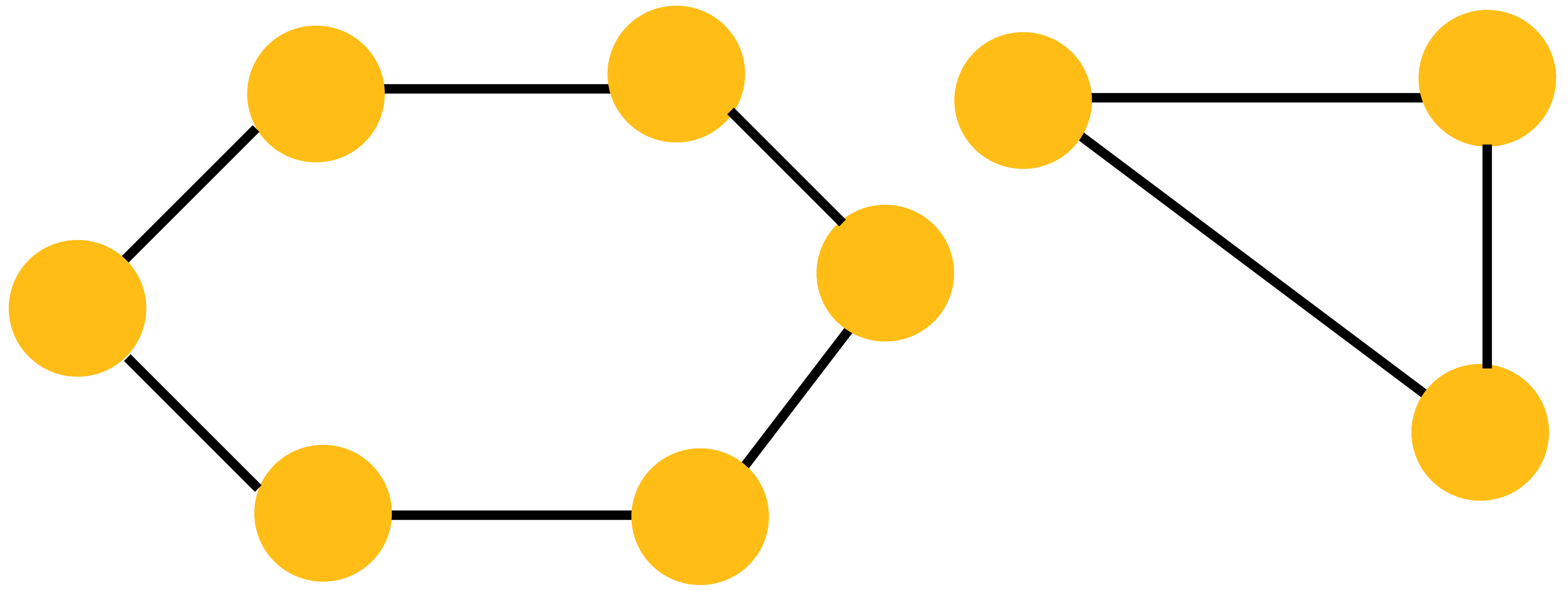
It is easy to see that the graph on the left hand side satisfies $\Phi(u)$ for any node u, and the graph on the right hand side does not. That is, there are C^3-sentences, distinguishing these graphs, and so must 2-WL.

Higher-Order Graph Neural Networks

Higher-Order Message Passing Neural Networks

Weisfeiler-Lehman: From 1-GNNs to k-GNNs





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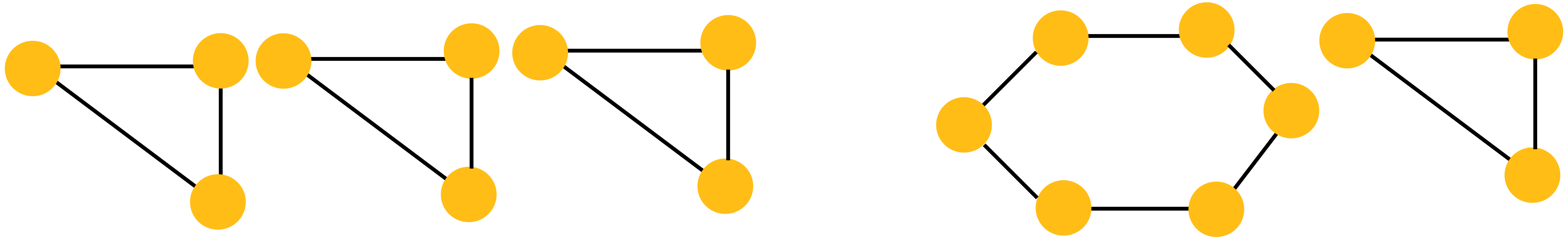

The k-GNN model (Morris et al., 2019) is a generalisation of MPNNs based on the $(k-1)$-dimensional WL algorithm.

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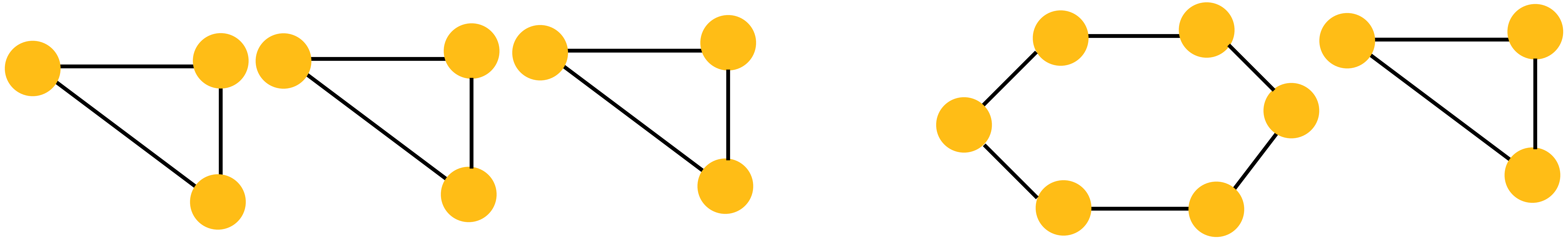

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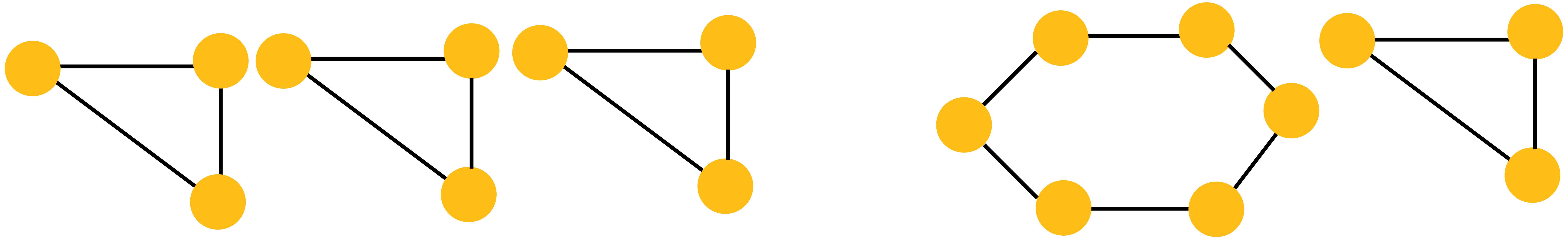

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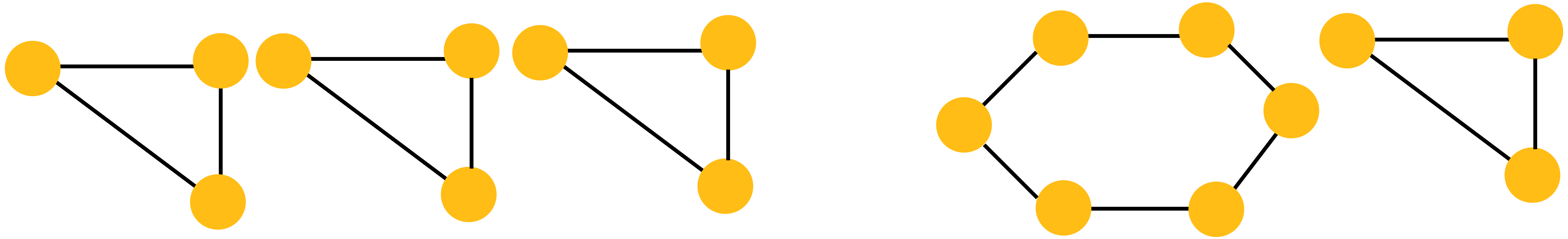

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This form of message passing can capture structural information that is not visible at the node-level.

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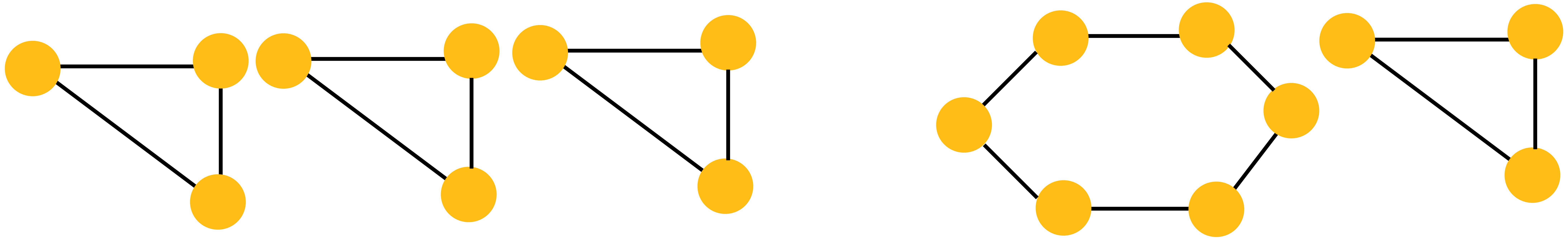

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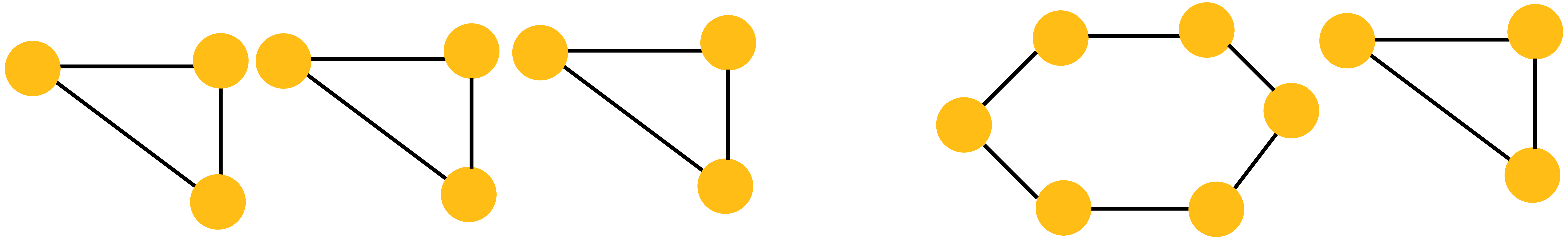

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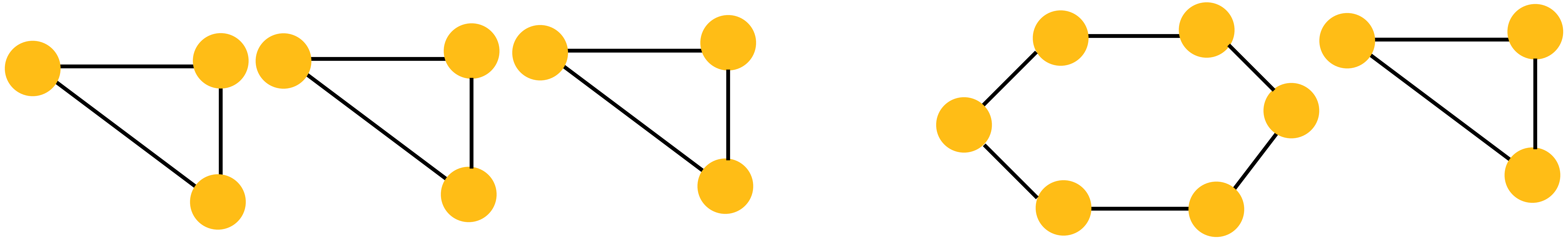

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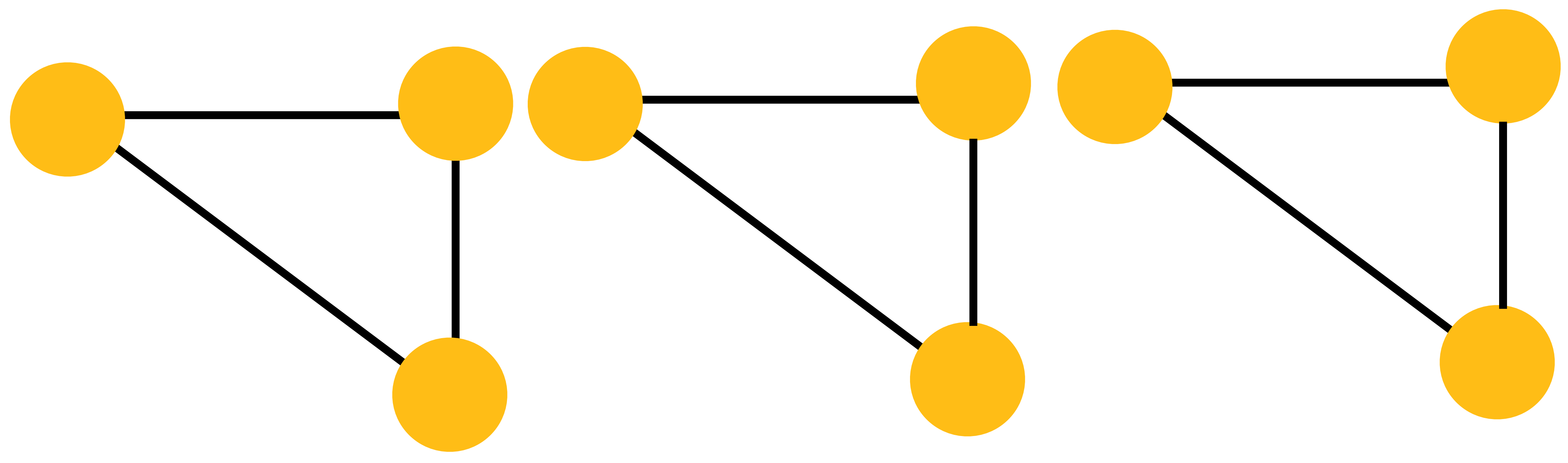

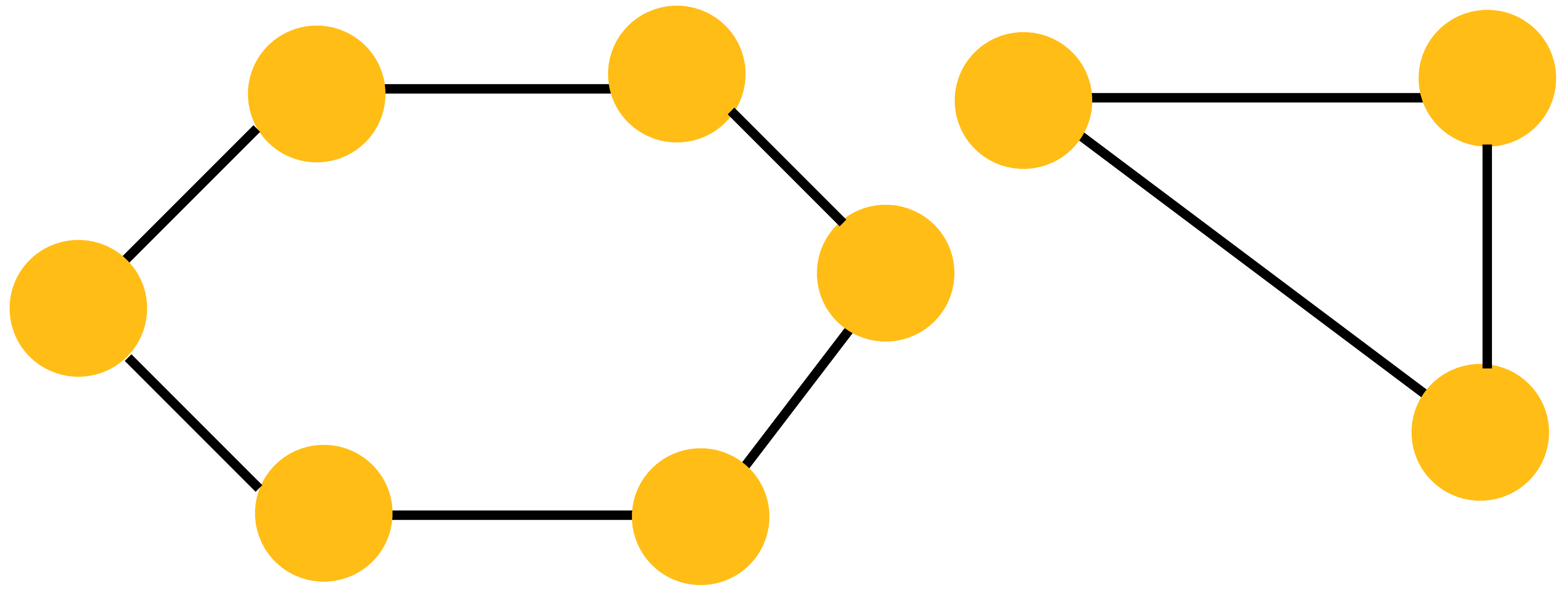

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This formula states that there are at least three triangles, which is satisfied by the graph on the left hand side but not by the graph on the right hand side. k-GNNs with $k \geq 3$ are strictly more powerful than MPNNs.

Hierarchical Variants

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Hierarchical variants of k-GNNs, called 1-k-GNNs, aim to combine graph representations learned at different granularities. The idea is to apply message passing starting from one-hot indicator vectors as initial features, and applying the usual node-level message passing (1-WL), and afterwards using the resulting representations to learn better representations for pairs of nodes, with a higher-order message passing (2-WL), etc., illustrated in Figure 1 of (Morris et al., 2019), as shown above.

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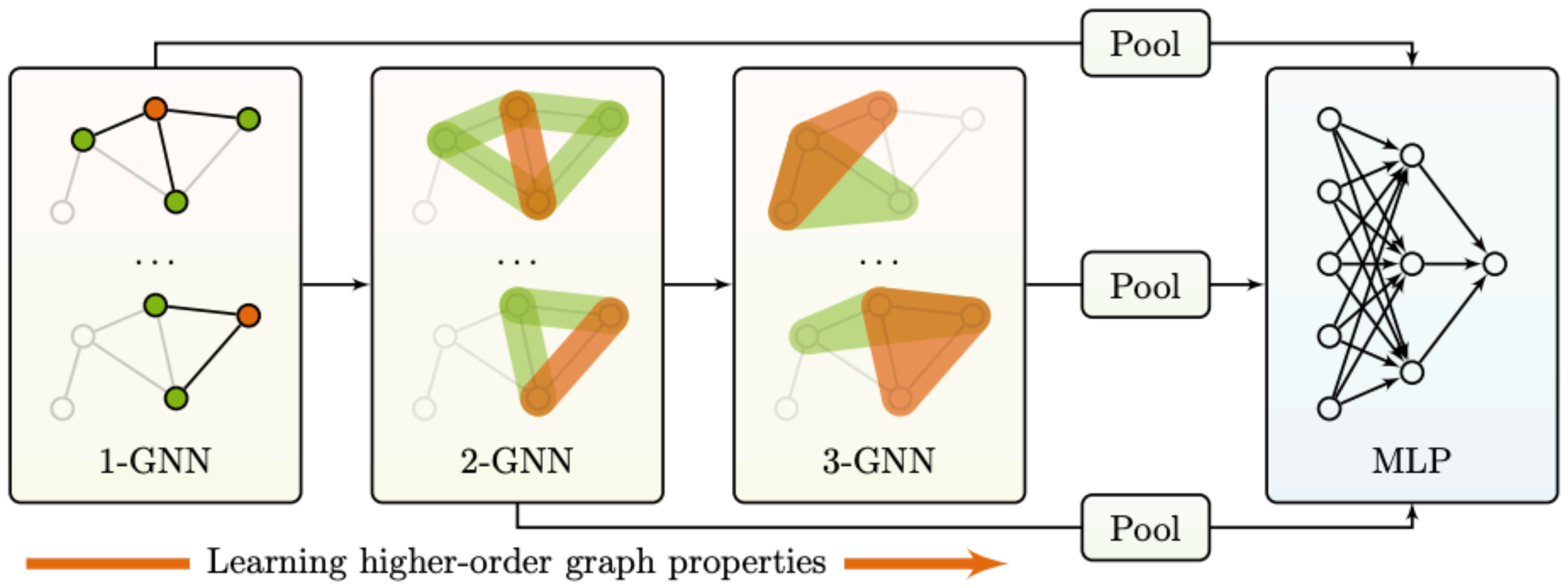

(a) Hierarchical 1-2-3-GNN network architecture

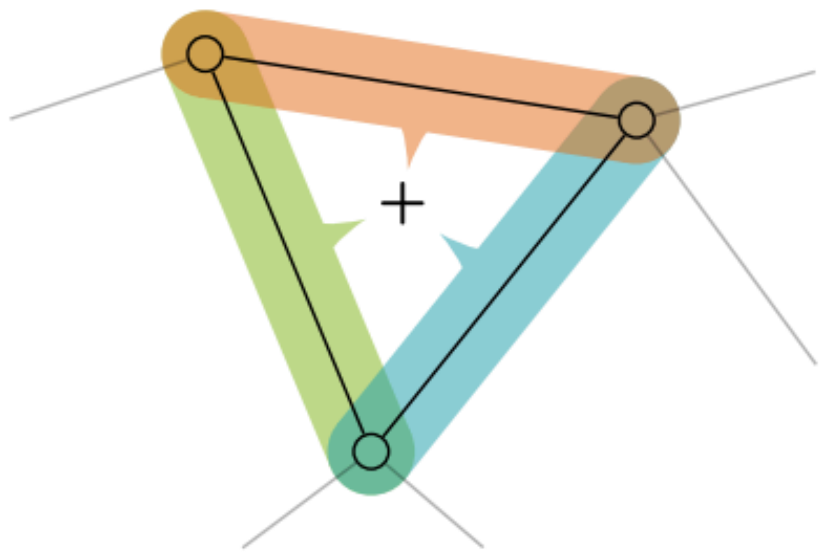

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Figure 1: Illustration of the proposed hierarchical variant of the k-GNN layer. For each subgraph S on k nodes a feature f is learned, which is initialized with the learned features of all $(k-1)$-element subgraphs of S. Hence, a hierarchical representation of the input graph is learned.

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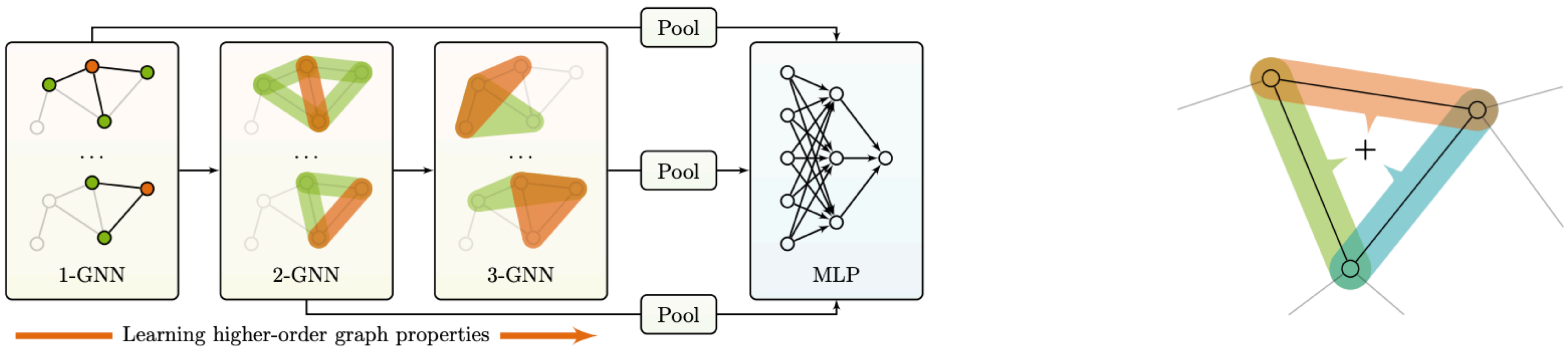

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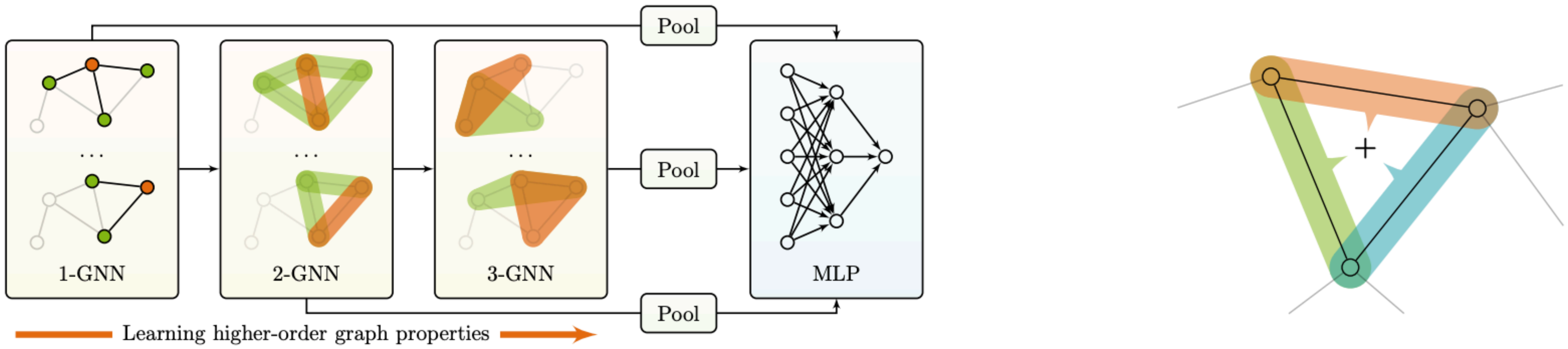

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In this hierarchical approach the initial messages in a k-GNN are based on the output of lower-dimensional GNNs, which allows the model to effectively capture graph structures of varying granularity.

Many real-world graphs inherit a hierarchical structure in this sense, and so a hierarchical message passing approach is potentially helpful — and this is empirically confirmed in the evaluation of (Morris et al., 2019).

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This can hurt the inductive bias, especially when node level features are very important for the task at hand!

Invariant/Equivariant Graph Networks

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Formally, we consider an order $(k+1)$-tensor $\mathbf{T} \in \mathbb{R}^{|V|^k \times d}$ where the first k channels of this tensor are indexed by the nodes of the graph. We write $\mathbf{P} \star \mathbf{T}$ to denote a permutation of the first k channels of this tensor according the node permutation matrix $\mathbf{P}$.

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A linear invariant layer can be defined as $\mathscr{L} : \mathbb{R}^{|V|^k \times d_1} \mapsto \mathbb{R}^{d_2}$ such that for all permutations $\mathbf{P}$:

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Based on this abstraction, invariant k-order GNN model (Maron et al., 2019b), or k-IGNs, is defined as:

$$F = \text{MLP} \circ \mathscr{H} \circ \mathscr{L}_d \circ \sigma \circ \cdots \circ \sigma \circ \mathscr{L}_1,$$

where $\mathscr{L}_1, \ldots, \mathscr{L}_d$ are equivariant linear layers (with up to k different channels), $\mathscr{H}$ is an invariant layer, and σ denotes element-wise non-linearity. Figure 1 of (Maron et al., 2019c) illustrates the model.

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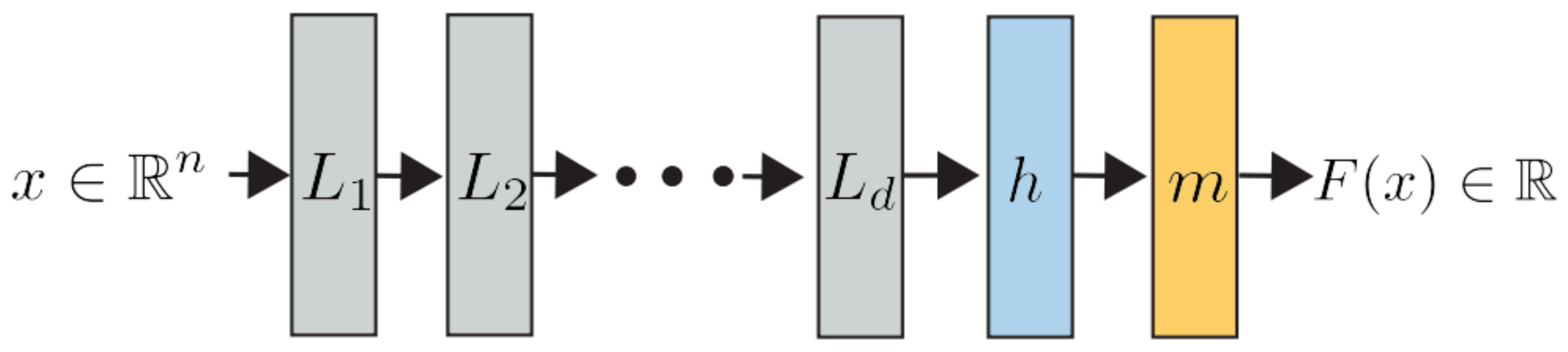

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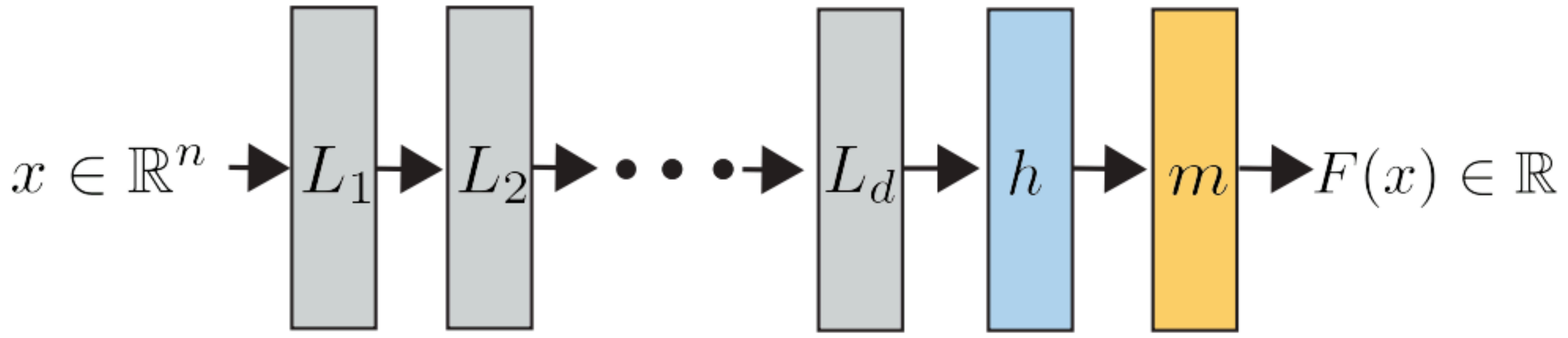

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The input to the k-order invariant GNN is a tensor $\mathbf{T} \in \mathbb{R}^{|V|^2 \times d}$, where the first two channels correspond to the adjacency matrix of the graph and the remaining channels encode the initial node features.

The model is called k-order, as it allows equivariant layers with k channels, and this directly correlates with the expressive power of the model.

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Invariant networks are shown to be universal (Maron et al., 2019c), but with tensor orders of $O(|V|^2)$!

More specifically, invariant networks are universal with tensor order $\dfrac{n(n-1)}{2}$. An alternative proof is given by (Keriven and Peyré, 2019), who also showed a universality result for the equivariant case.

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Finally, these models are also prohibitive to run for large values of k, due to their very large memory and computational requirements.

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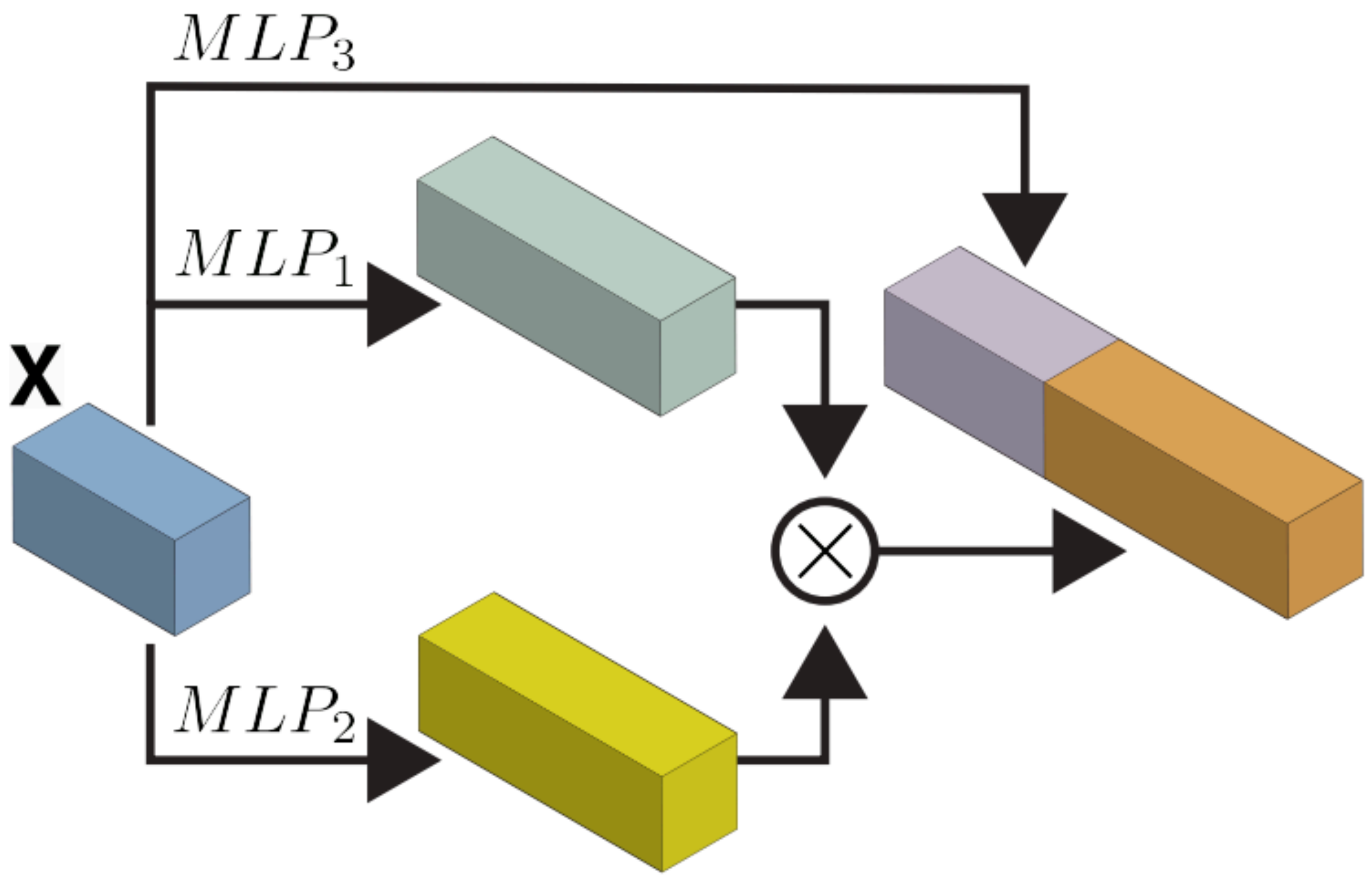

Figure 2: Block structure.

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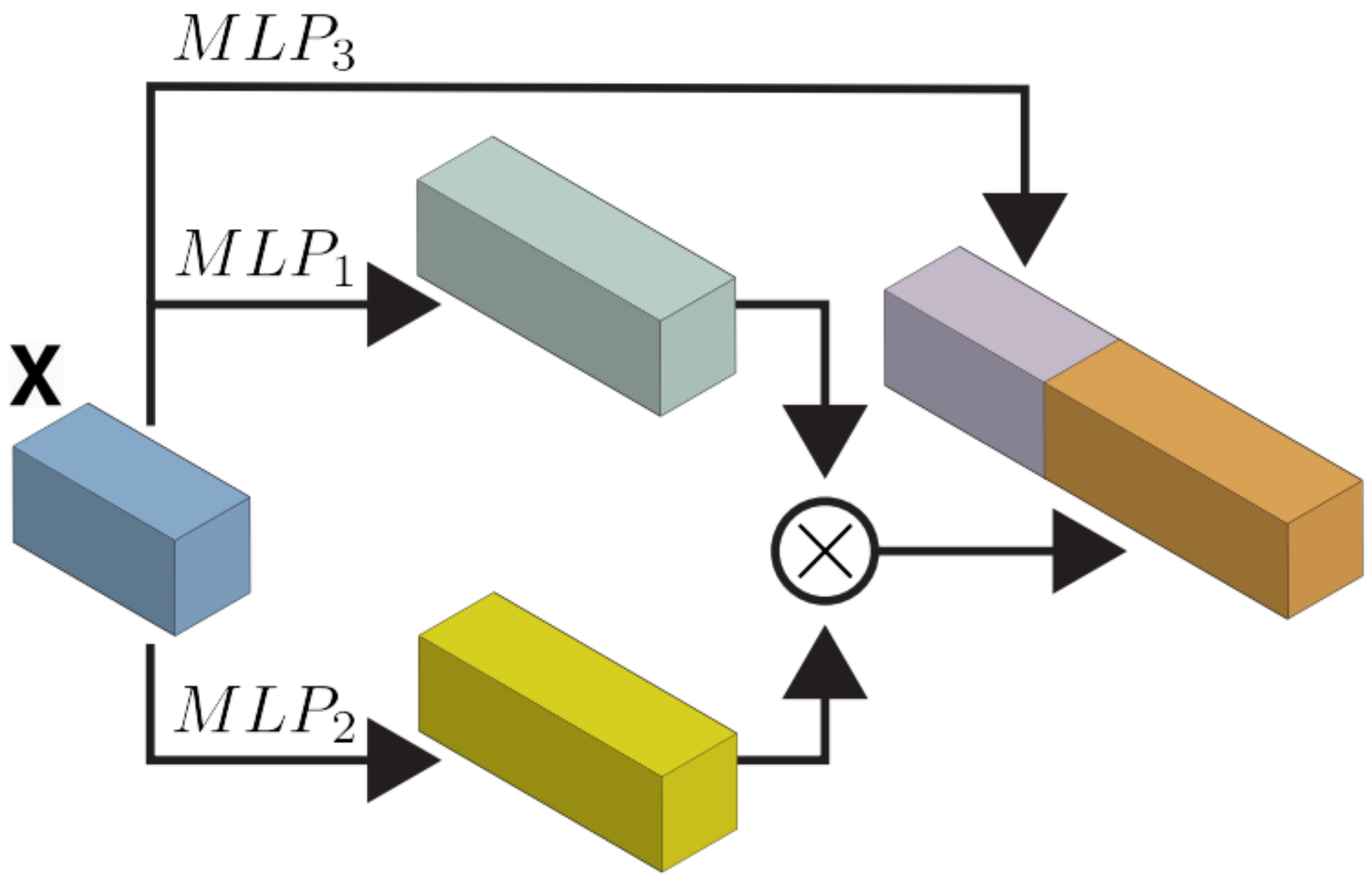

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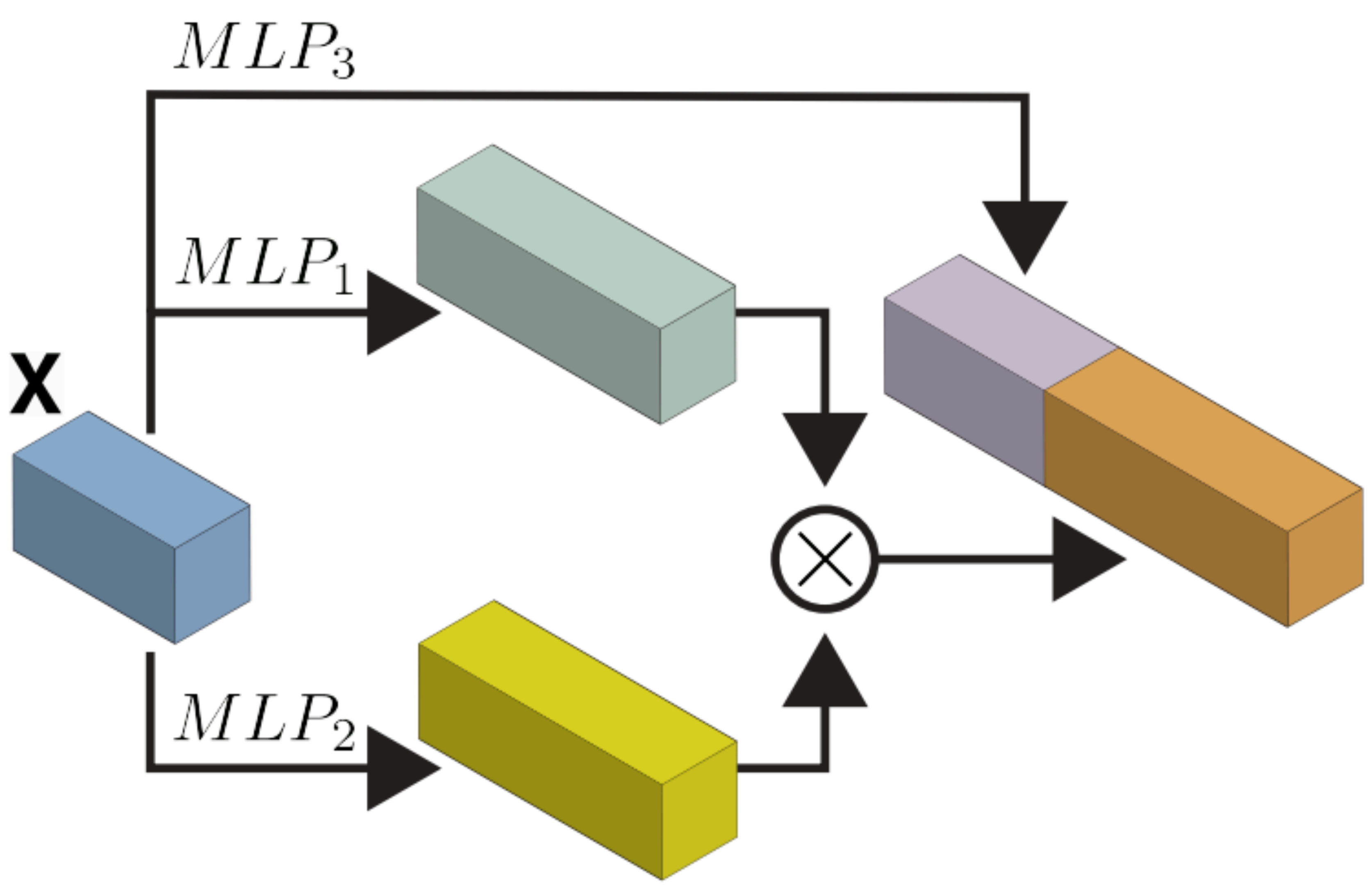

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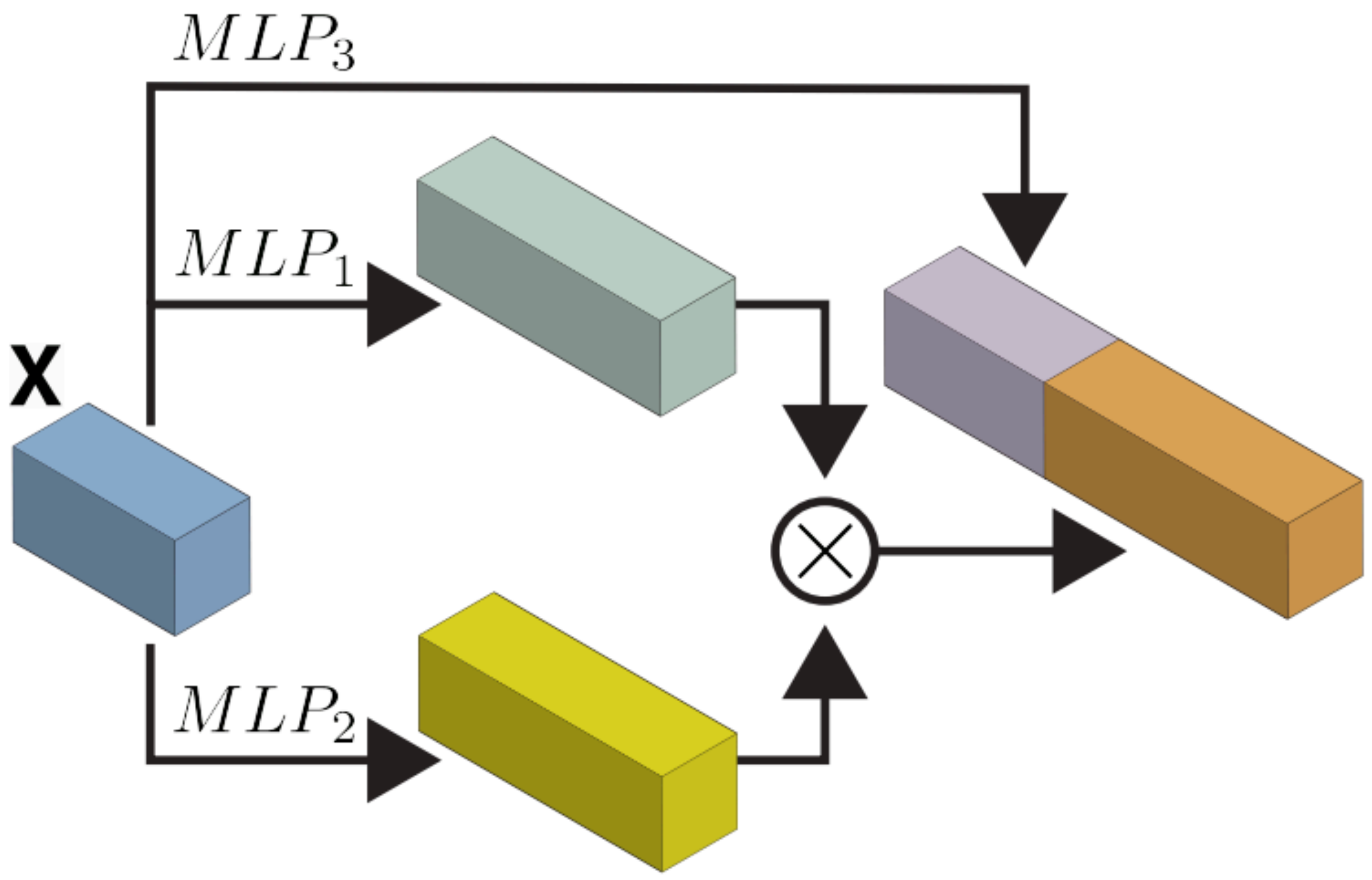
Briefly, given an input $\mathbf{T} \in \mathbb{R}^{|V| \times |V| \times d}$ the idea is to apply MLP to each feature of the input tensor independently (i.e., 3 MLPs), and then perform matrix multiplication between matching features.



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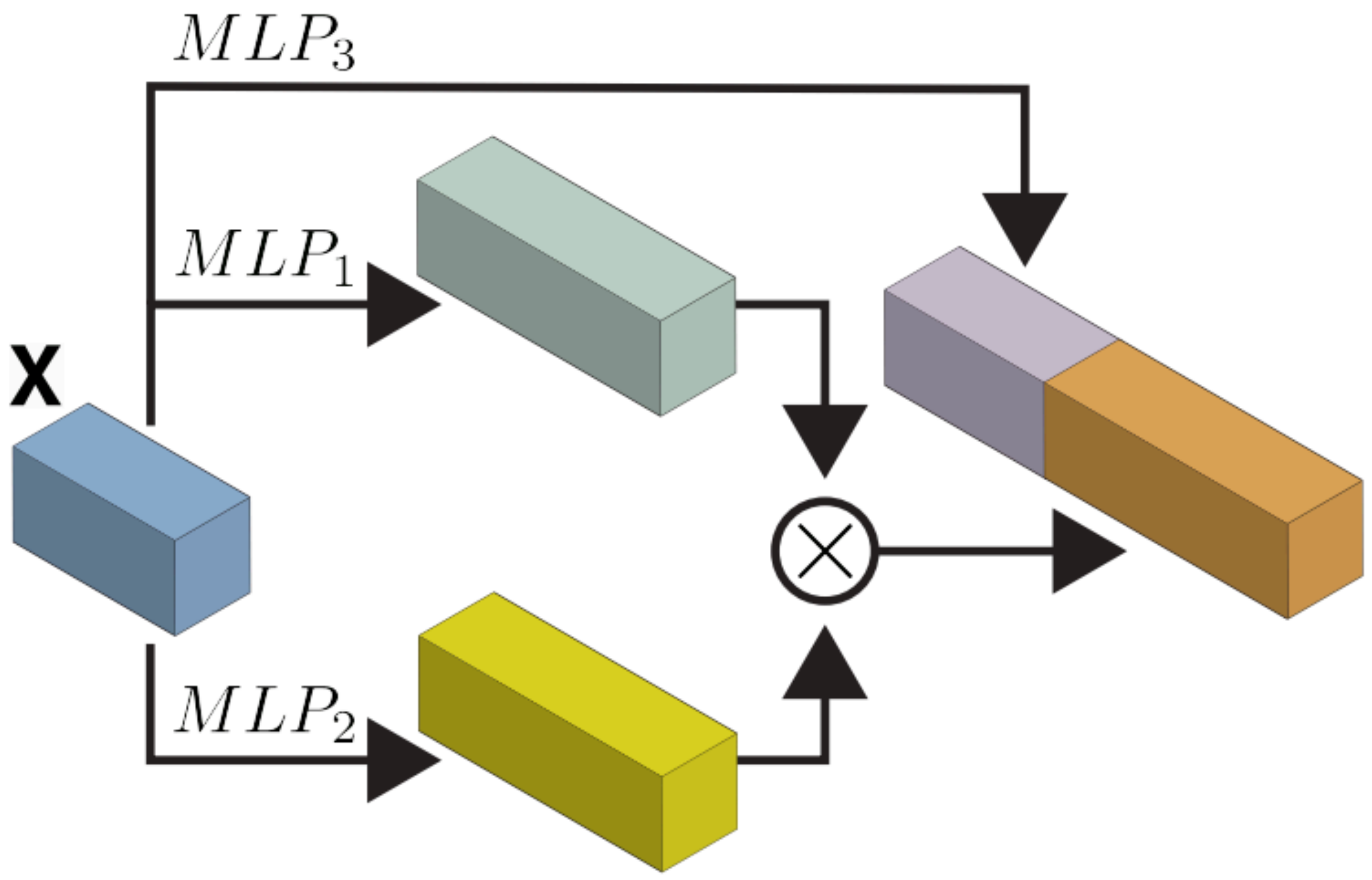

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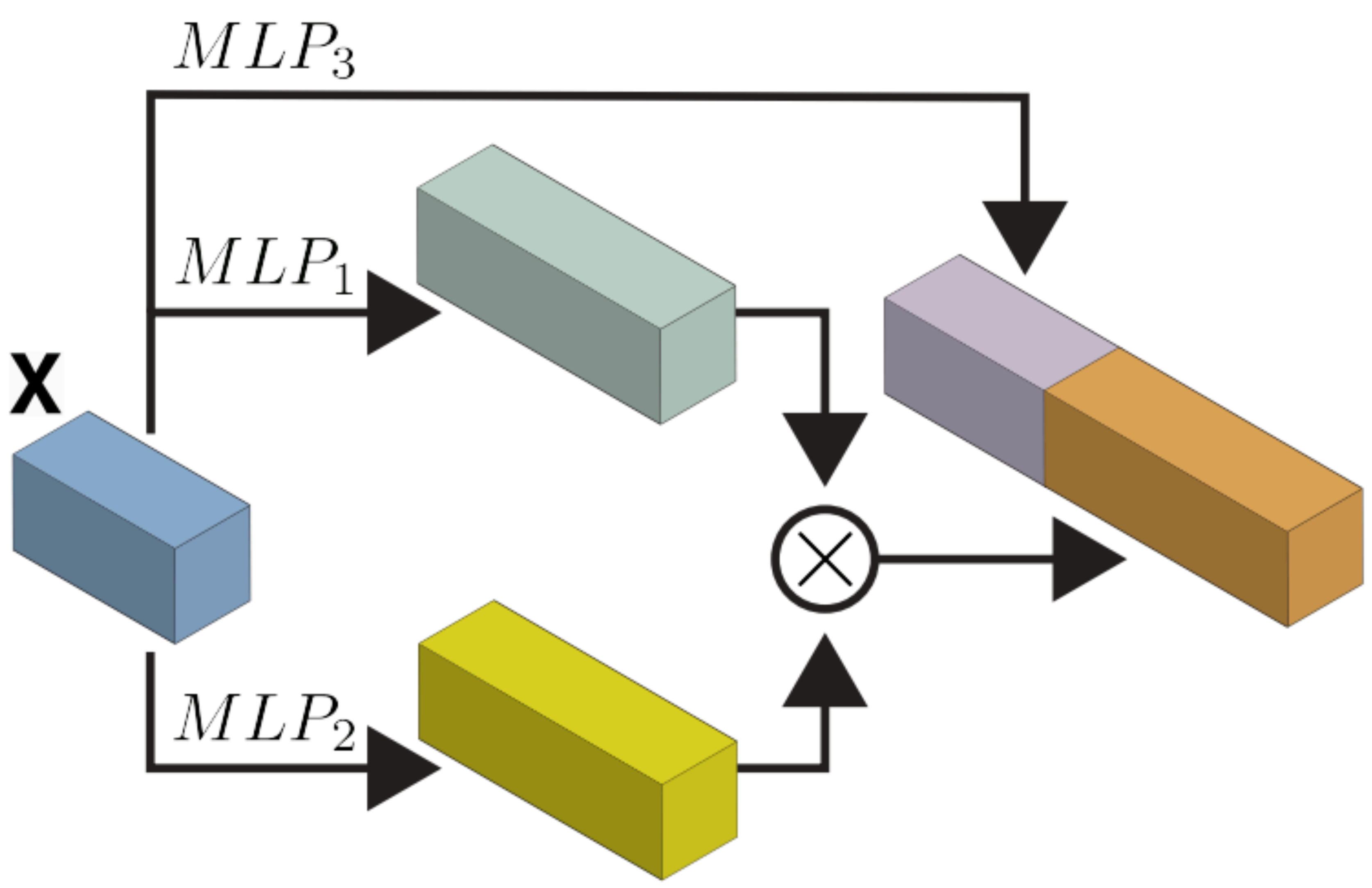

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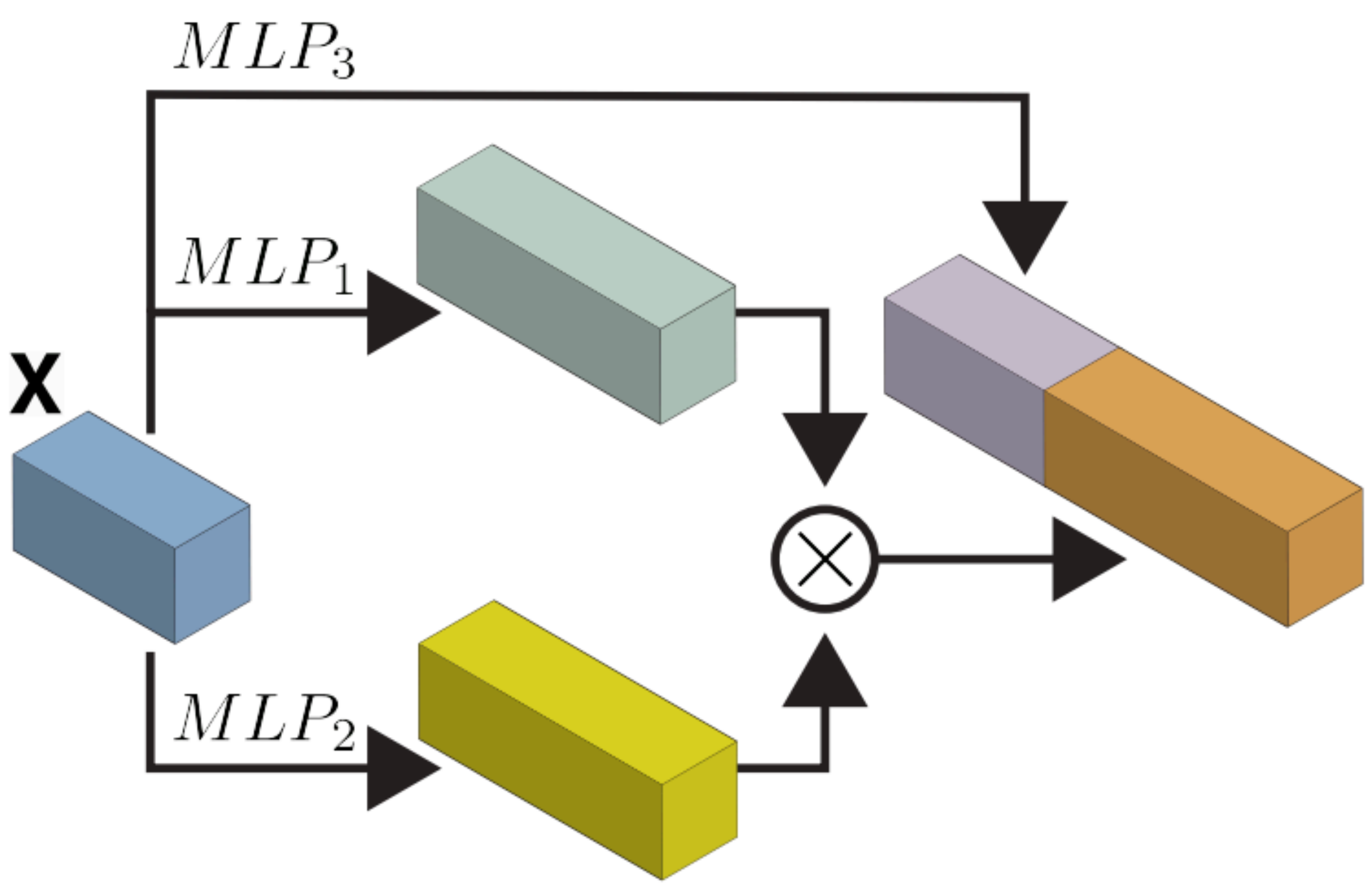
Furthermore, PPGNs are strictly more powerful than MPNNs. In fact, PPGNs can distinguish any pair of graphs that can be distinguished by folklore 2-WL.



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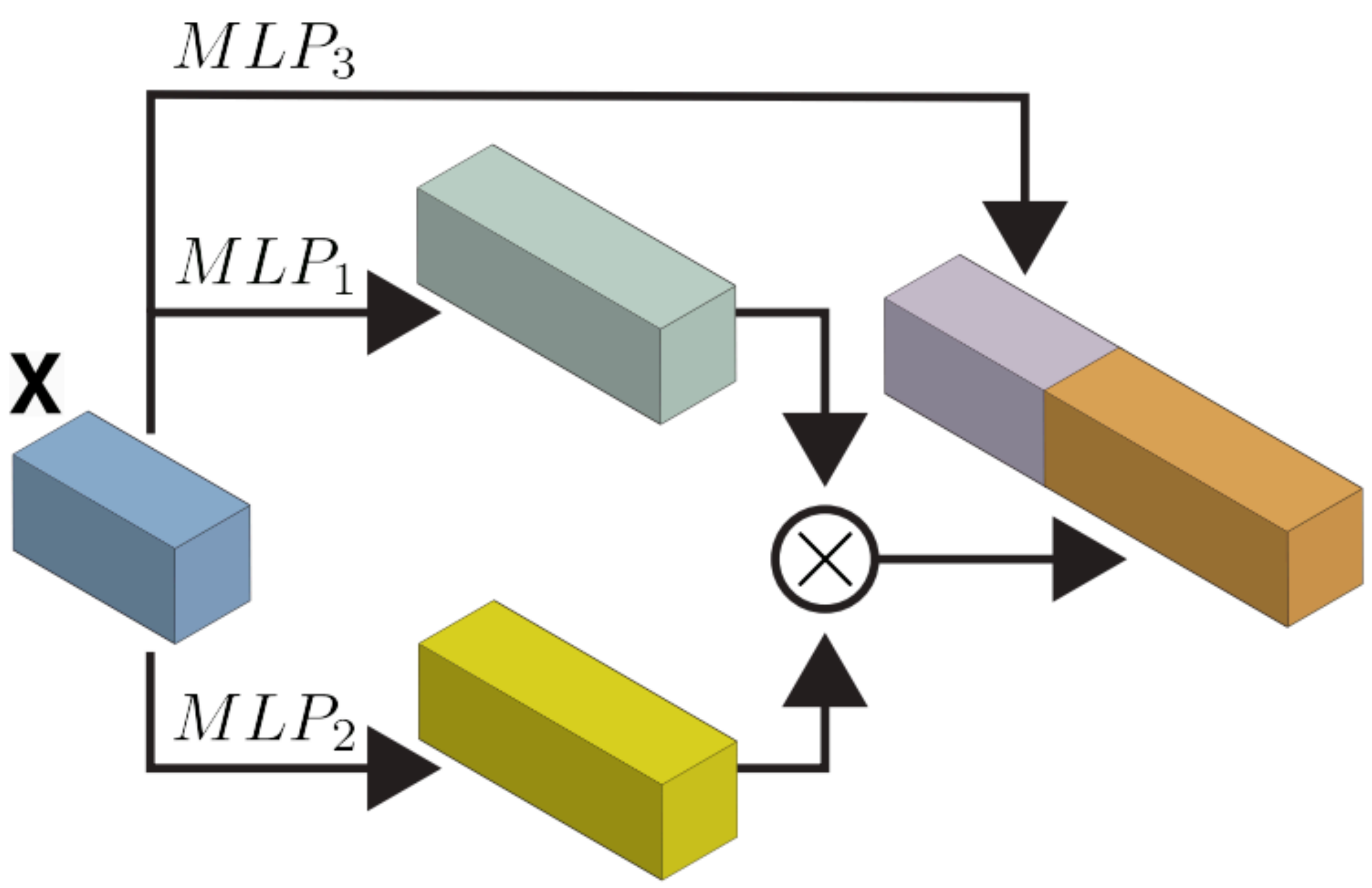

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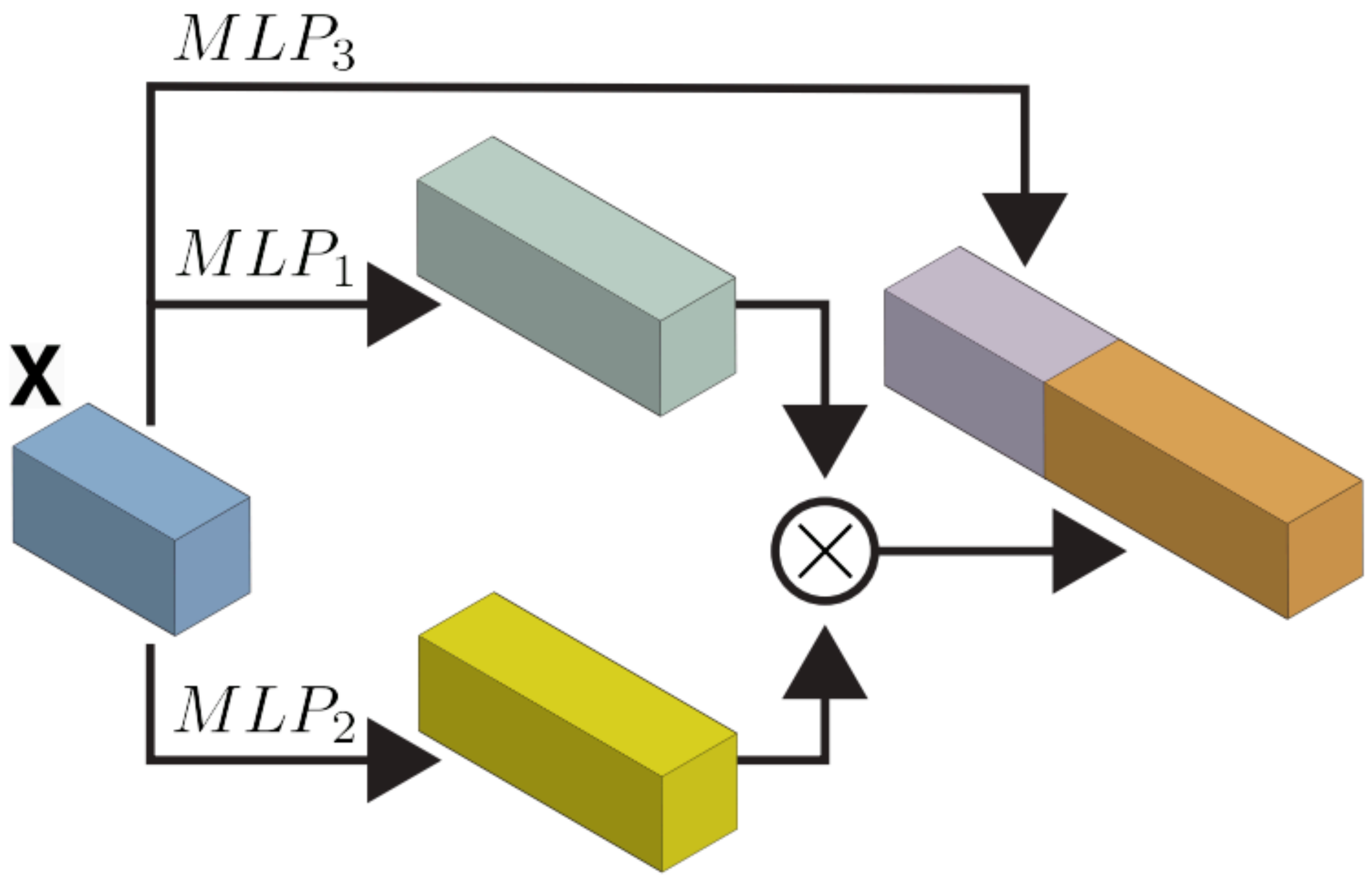
PPGNs have therefore the same power as 3-GNNs, but the strong point is that they maintain only $O(n^2)$ embeddings, which makes them more memory-efficient than 3-GNNs.



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1. 1-WL edge cases typically correspond to data that is highly regular, whereas real-world data is overwhelmingly uneven and variable, e.g., knowledge graphs, where some entities are connected to hundreds of other entities, and others connect to very few, if any.

2. Real-world graphs are also typically large, and involve thousands, and potentially millions, of nodes. At this scale, the limitations of 1-WL are less likely to surface, as it is highly probable that some local substructure within the large graph can help distinguish it. In fact, 1-WL can distinguish almost all graphs as the number of graph nodes tends to infinity (Babai et al., 1980), i.e., it can distinguish these graphs with probability almost 1.

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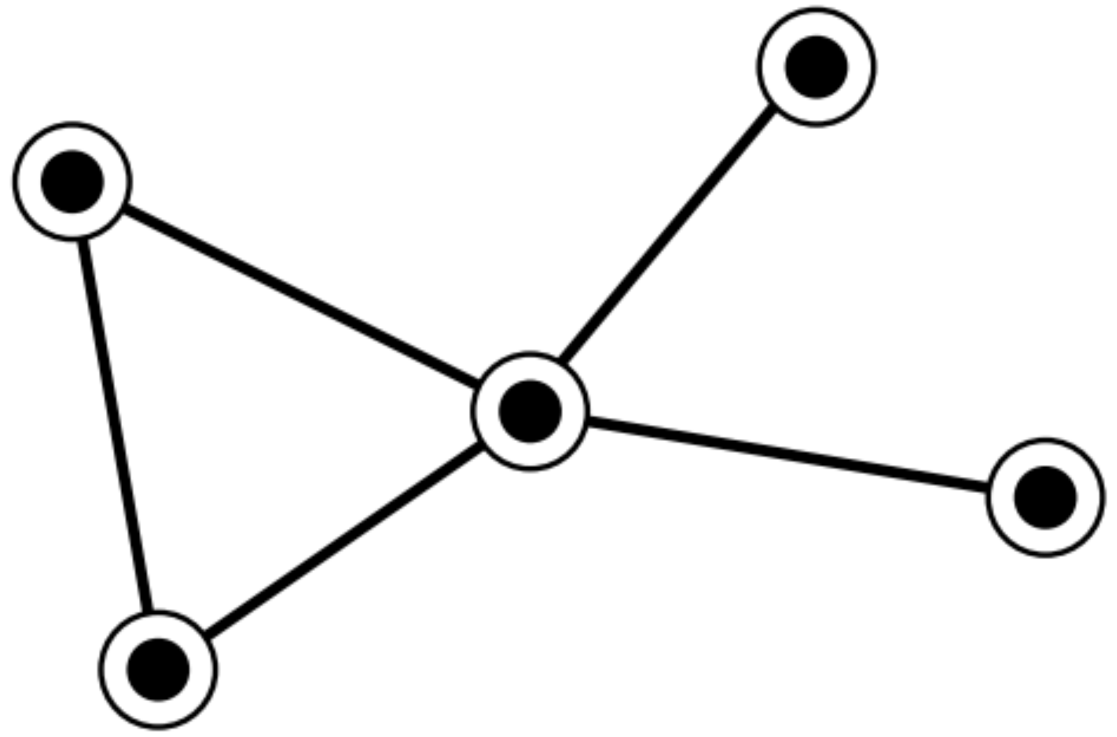

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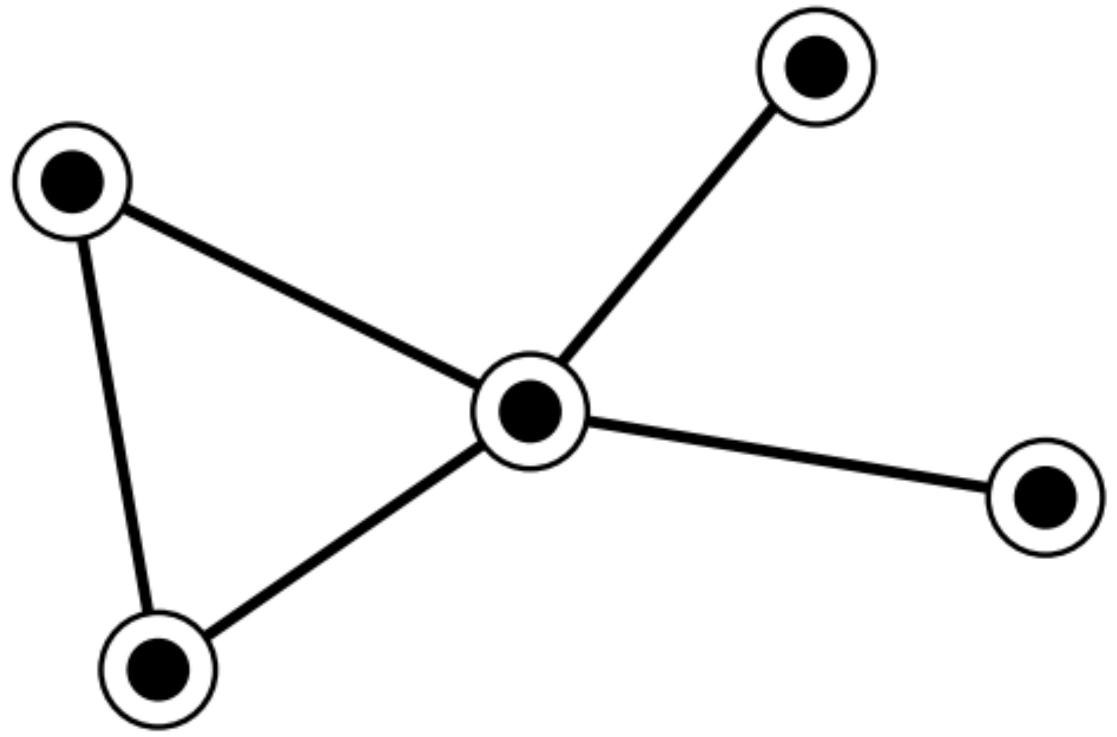

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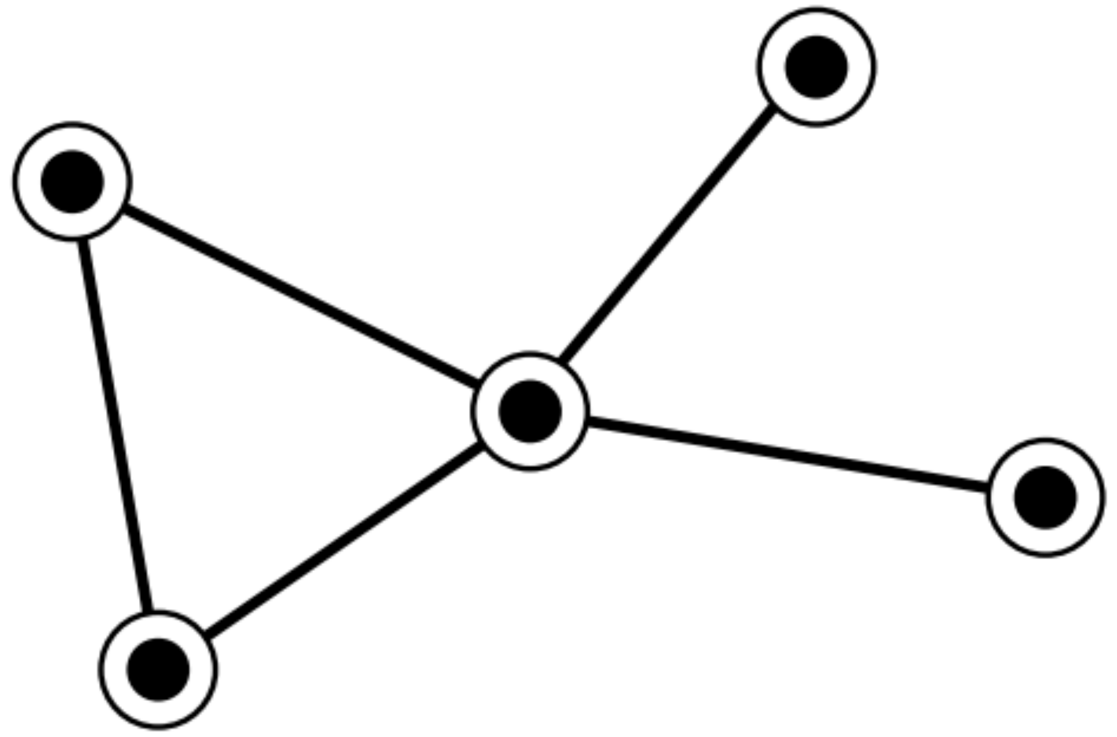

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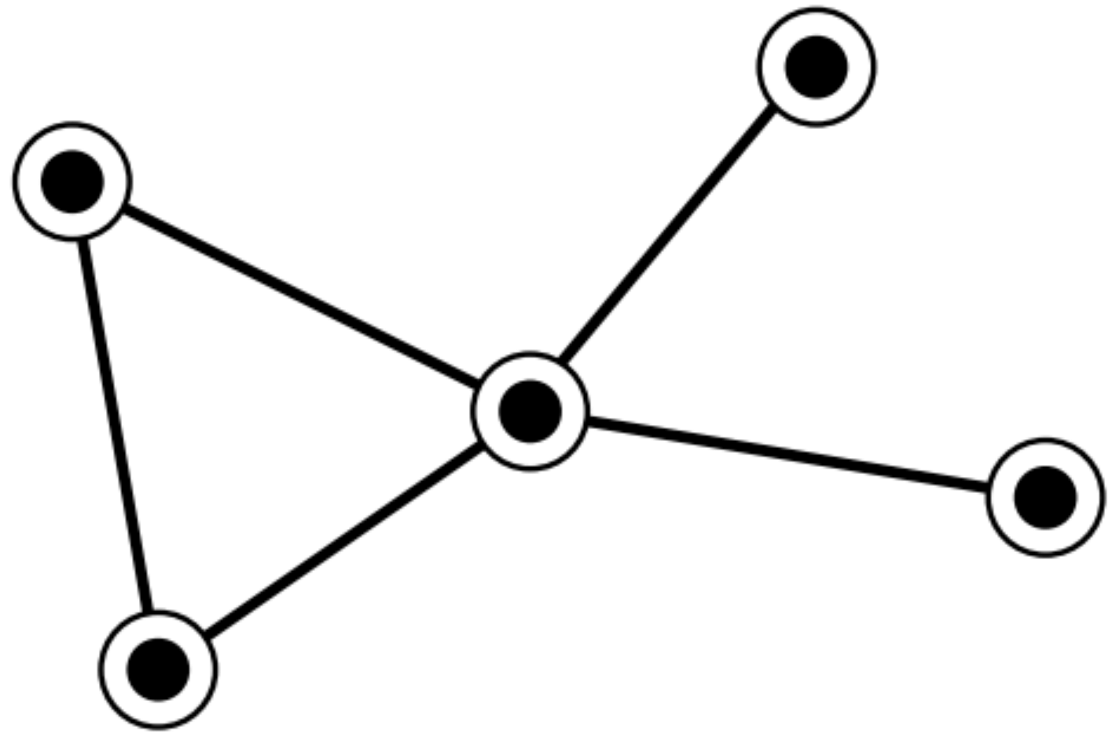

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This has been noted and new synthetic datasets dedicated to quantify the effect of expressive power are proposed (Abboud et al., 2020) with a detailed comparison against higher-order models, as we will see in more detail in Lecture 7.

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where a "connected triple" means a single vertex with edges running to an unordered pair of others."

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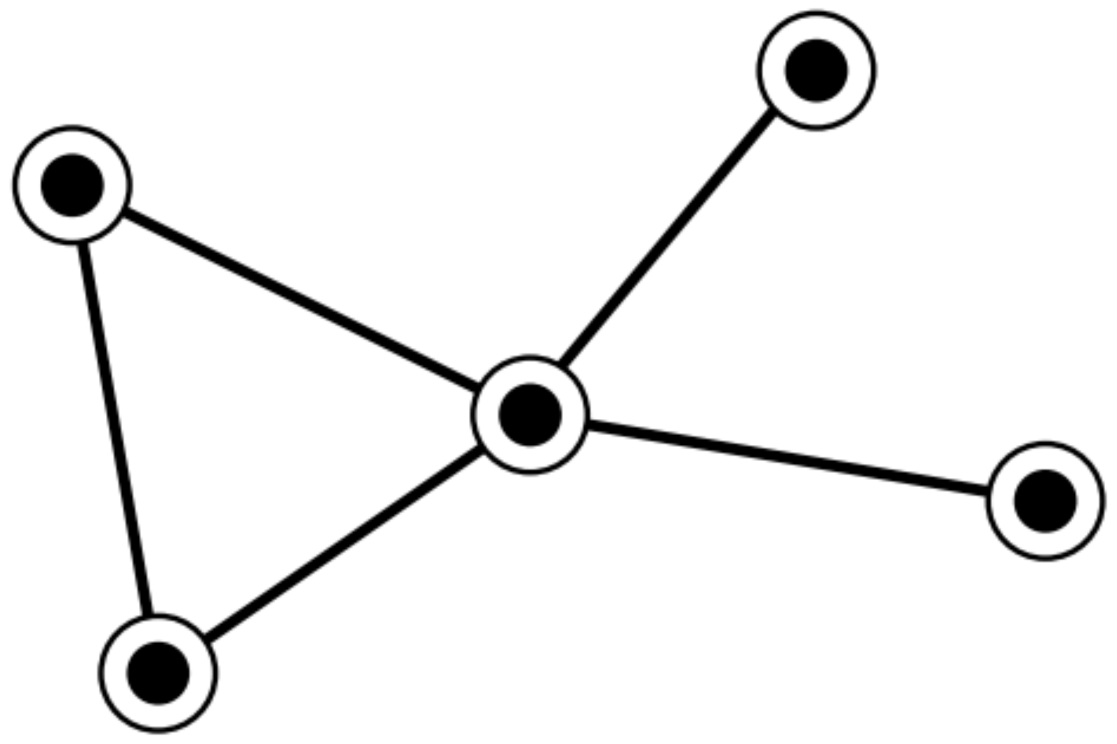

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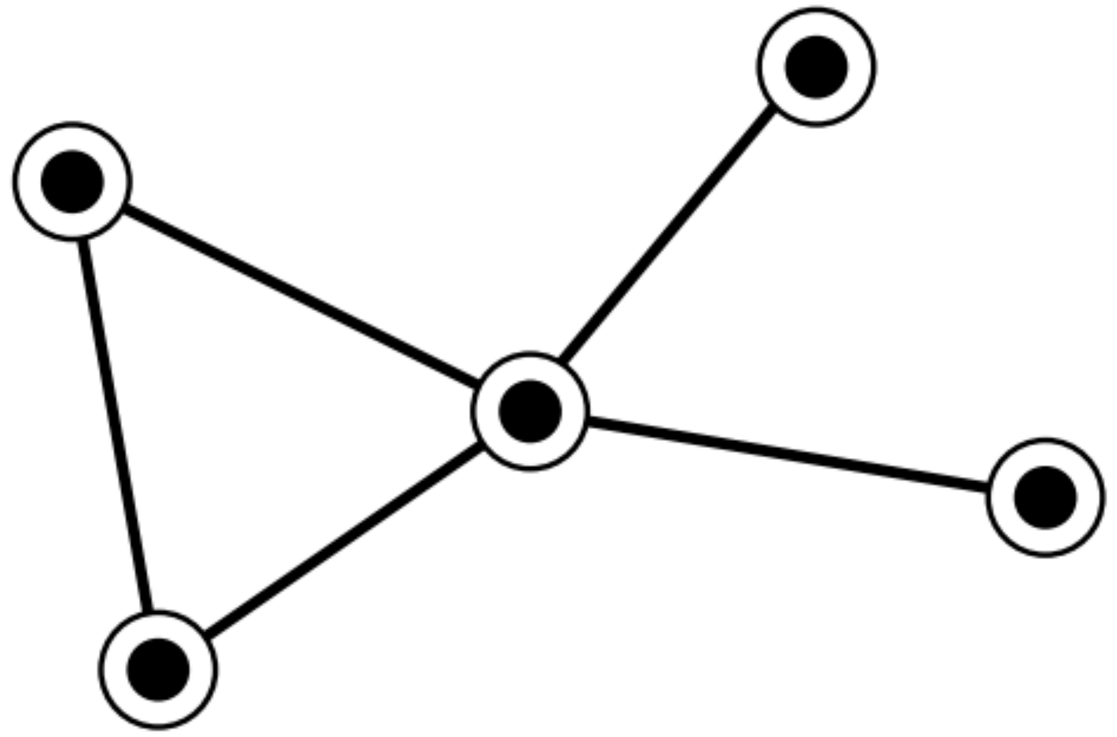

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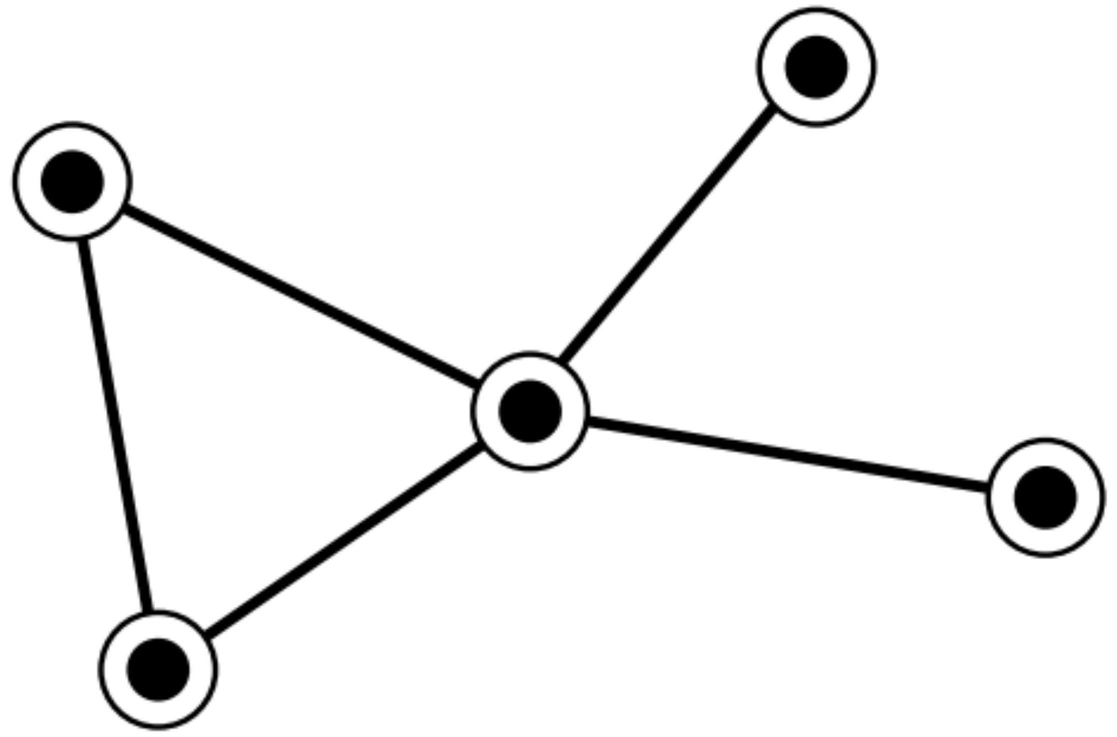

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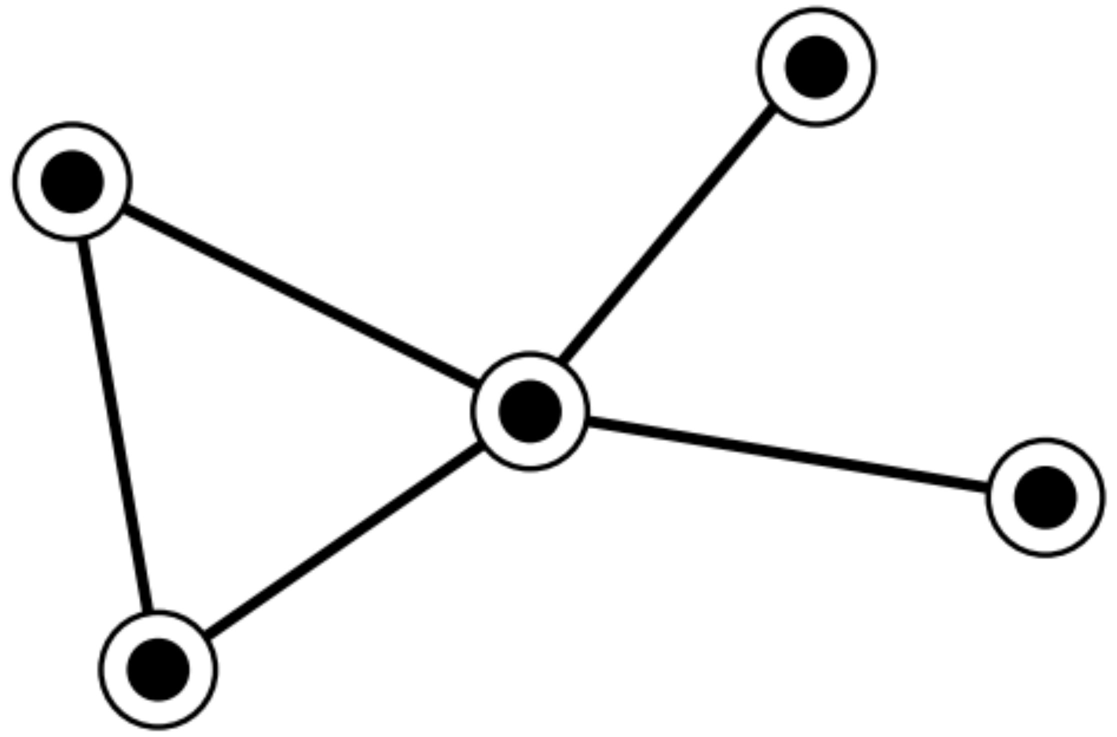

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There are other ways of defining cluster coefficient but they rely on being able to detect triangles.

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For instance, protein graphs exhibit heterophily, as the proteins that interact with one another are usually different from a composition perspective.

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For example, k-GNN, for larger k, would require non-uniform handling of its connected tuples, based on local neighbourhoods, and k-IGN processes all nodes simultaneously, and thus must learn to filter out non-local features!

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- Homophily and heterophily: MPNNs vs higher-order models
- There are other extensions of MPNNs, particularly with random features, yielding more expressive power without the need for higher-order tensors — Lecture 7.

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