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On the Power of the Weisfeiler-Leman Test for Graph Motif Parameters

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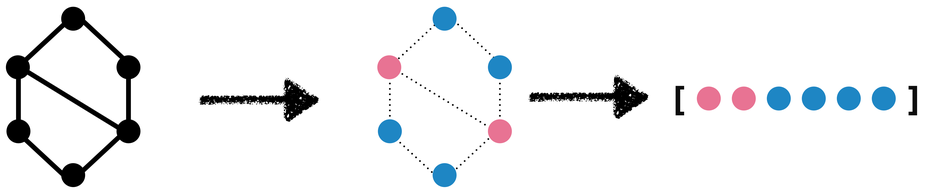
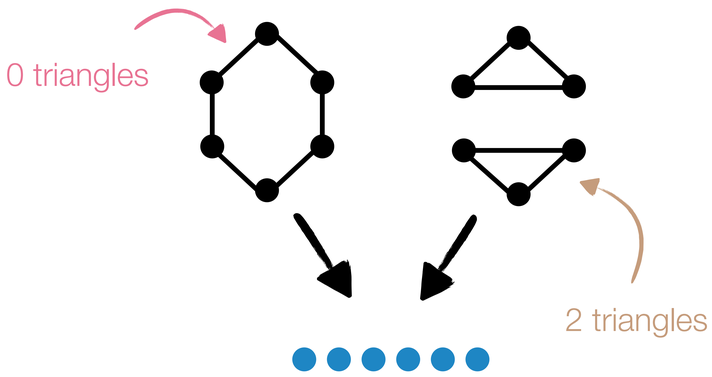
GNNs learn representations:



But there are graphs that always have the same representation!



A GNN can express function f if whenever $f(G) \neq f(H)$, then G and H have different representations.

When can a GNN express a function?

$\Gamma : \mathit{Graphs} \to \mathbb{Q}$ is a graph motif parameter (gmp) if it is of the form:

$$\Gamma(G) = \sum_{F \in \mathscr{F}_\Gamma} \alpha_F \cdot \mathrm{homs}(F, G)$$

finite $\mathscr{F}_\Gamma$ — rational coefficients

Results A

For graphs with vertex and edge labels,
k-WL can express gmp Γ
$\iff$
maximum tree width in $\mathscr{F}_\Gamma \leq k$

Includes e.g., all subgraph counting problems!

Results B

When a GNN can express gmp Γ, then there is a uniform final layer that computes Γ from the individual node representations.

Results C

- When Γ = count occurences of pattern P: Can find the precise k in polynomial time!
- Counting k-graphlets requires $(k-1)$-WL