Coloring Graphs and Beyond

Joint work with Soheil Anbouhi

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Weisfeiler-Lehman Test[WL68]

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start with $c(v) = c^{(0)}(v)$, and
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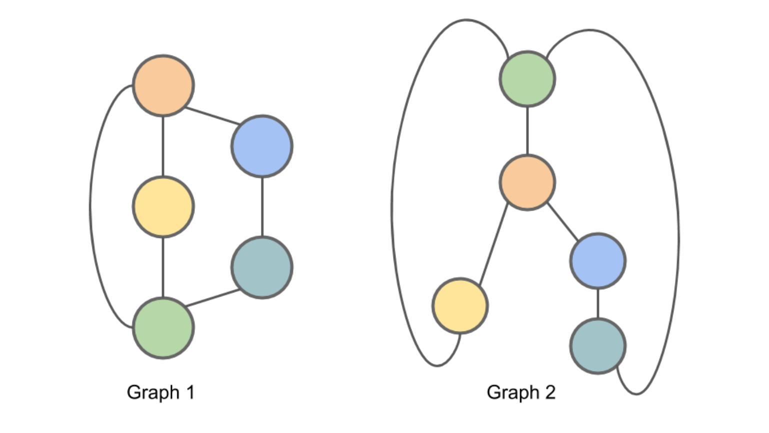
Weisfeiler-Lehman Test

If two graphs have different colorings, then the graphs are not isomorphic. Test is inconclusive if coloring of graphs is the same[MBHSL19]

Weisfeiler-Lehman Test[WL68]



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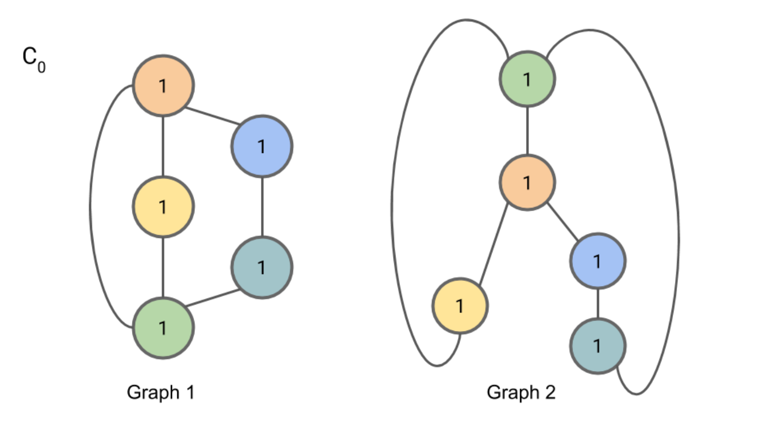

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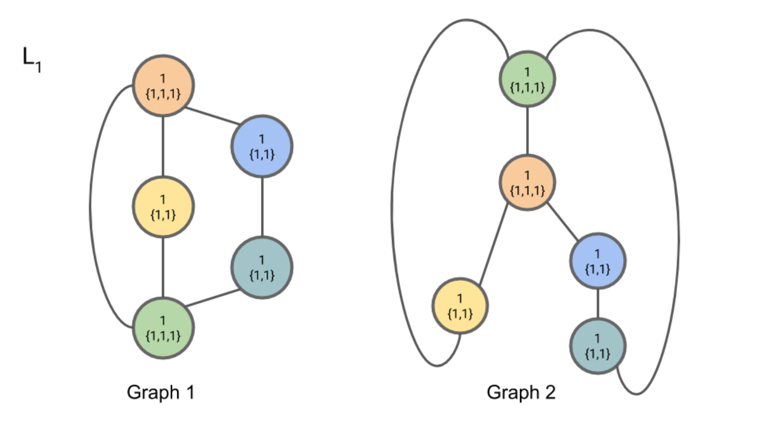

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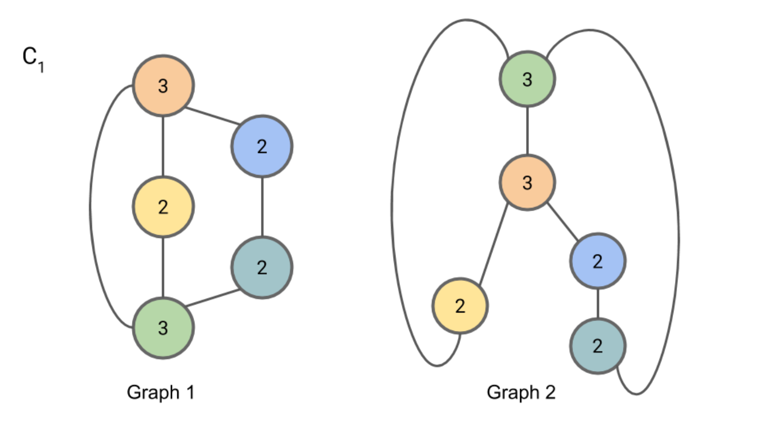

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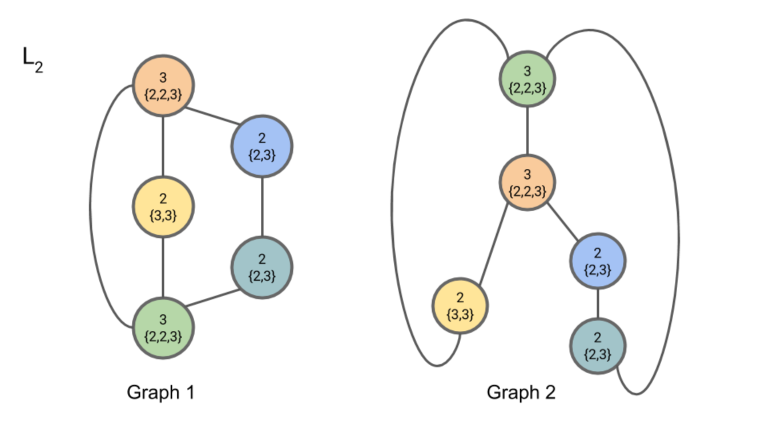

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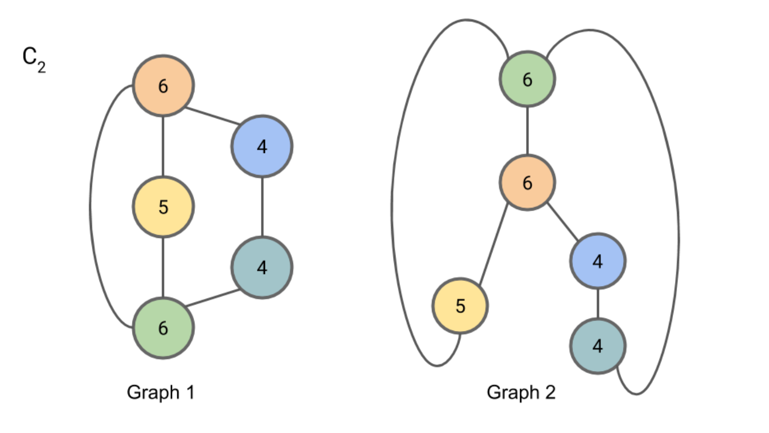

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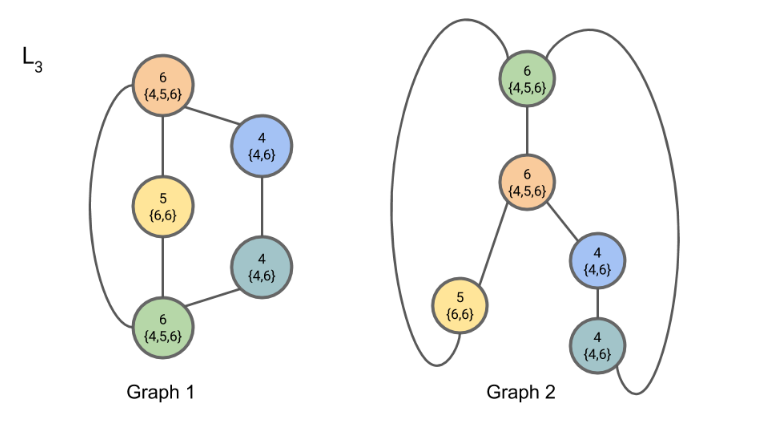

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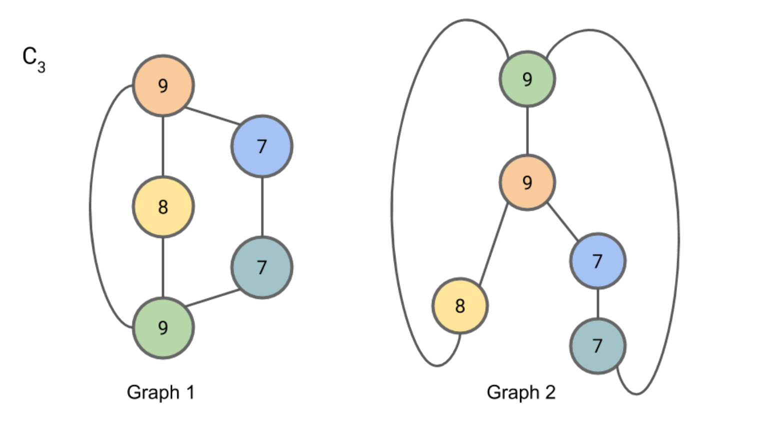

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Weisfeiler-Leman Algorithm[WL68]

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A **coloring** of a graph $G = (V, E)$ at iteration t is a function $c^{(t)} : V \longrightarrow \mathbb{N}$. A (perfect) **hashing** is any injective function.

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Algorithm Weisfeiler-Leman (WL) or Naive vertex refinement[WL68]

Input: (V, E, X_V) Here, $x_v \in \mathbb{Z}_2^d$
$c(v) = c^{(0)}(v) \longleftarrow hash(x_v)$
while $c^{(t)}(v) = c^{(t+1)}(v)\ \forall v \in V$ **do**
  $c^{(t+1)}(v) \longleftarrow \mathrm{hash}\left(c^{(t)}(v), \{\!\{c^{(t)}(w) : w \in N(v)\}\!\}\right)$
Output: $c^{(T)}(v)\ \forall v \in V$

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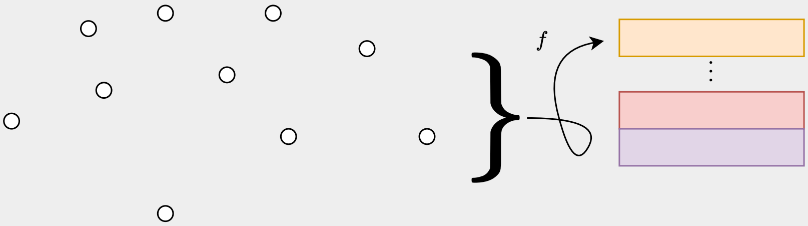
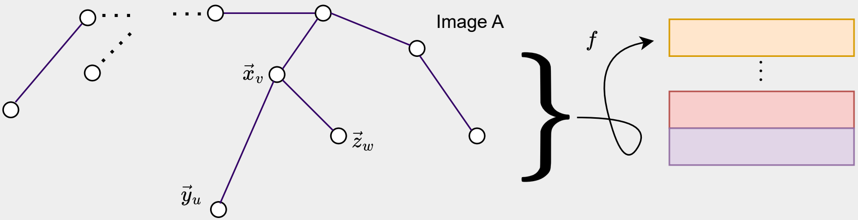
Secretly message passing!

Neural Networks



Message passing in Graph Neural Networks



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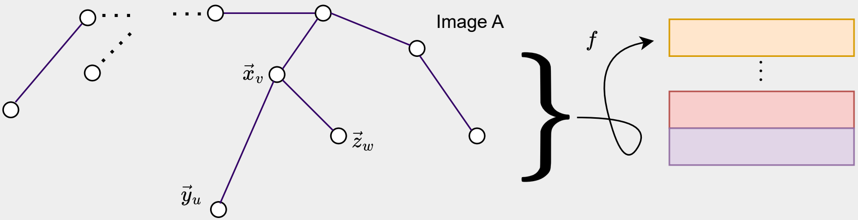

$$x_v^{(k+1)} = \mathrm{COMBINE}\left(x_v^{(k)}, \mathrm{AGGREGATE}^{(k+1)}\left(\left\{x_u^{(k)} : u \in N(v)\right\}\right)\right)$$

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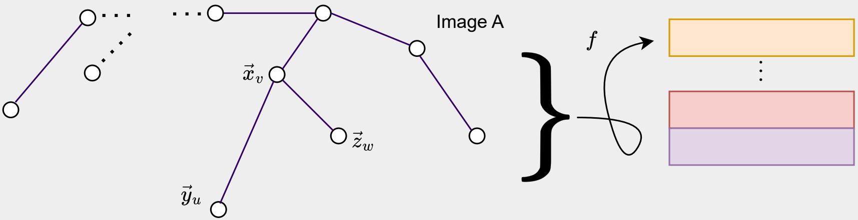

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$$F^{out} = \psi \circ ((AW + I)\, F).$$

$$\psi : \mathbb{R} \longrightarrow \mathbb{R}$$

Examples of Message Passing

AGGREGATE	COMBINE	Ref
$\mathrm{MAX}\left(\left\{\sigma\left(W_1.x_u^{(k)}\right)\right\}, u \in N(v)\right)$	$W_2.\left[x_v^{(k)}, a_v^{(k+1)}\right]$	GraphSAGE[HYL17]
$W_1.\mathrm{MEAN}\left(x_u^{(k)}, u \in N(v) \cup \{v\}\right)$	$\sigma\left(\left\{W_2.a_v^{(k+1)}\right\}\right)$	GCN[KW08]

Message passing in Graph Neural Networks

How powerful are graph neural networks?[MBHSL19, XHLJ18]

Theorem

Let G_1 and G_2 be any two non-isomorphic graphs. If a graph neural network $f : \mathcal{G} \longrightarrow \mathbb{R}^d$ maps G_1 and G_2 to different embeddings, the Weisfeiler-Leman graph isomorphism test also decides G_1 and G_2 are not isomorphic. Converse holds if COMBINE and AGGREGATE are injective[XHLJ18].

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Proof sketch

Compare

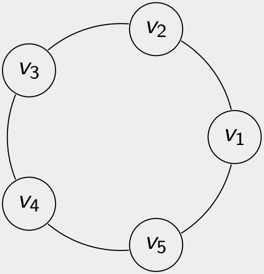
$x_v^{(k+1)} = \mathrm{COMBINE}\Big(x_v^{(k)}, \mathrm{AGGREGATE}^{(k+1)}\Big(\Big\{x_u^{(k)} : u \in N(v)\Big\}\Big)\Big)$

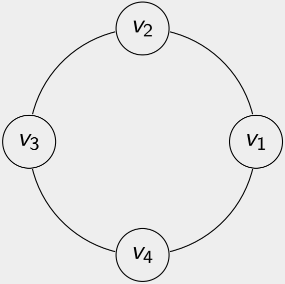
with

$c^{(t+1)}(v) = \mathrm{hash}\big(c^{(t)}(v), \{\!\{c^{(t)}(w) : w \in N(v)\}\!\}\big)$

Limits of WL Test

WL Test fails to distinguish the following graphs:





k-Weisfeiler-Leman Algorithm

Algorithm k-Weisfeiler-Leman (k-WL)

Input: (V, E, X_V) Here, $x_v \in \mathbb{Z}_2^d$
$c\left(\overrightarrow{v}\right) = c^{(0)}\left(\overrightarrow{v}\right) \longleftarrow hash\left(x_{\overrightarrow{v}}\right)$
while $c^{(t)}\left(\overrightarrow{v}\right) = c^{(t+1)}\left(\overrightarrow{v}\right) \forall \overrightarrow{v} \in V^k$ **do**
    $c_i^{(t+1)}\left(\overrightarrow{v}\right) \longleftarrow \{\!\{c^{(t)}\left(\overrightarrow{w}\right) : w \in N_i\left(\overrightarrow{v}\right)\}\!\} \; \forall \overrightarrow{v} \in V^k$
    $c^{(t+1)}\left(\overrightarrow{v}\right) \longleftarrow \text{hash}\left(c^{(t)}\left(\overrightarrow{v}\right), c_1^{(t+1)}\left(\overrightarrow{v}\right), \ldots, c_k^{(t+1)}\left(\overrightarrow{v}\right)\right) \; \forall \overrightarrow{v} \in V^k$
Output: $c^{(T)}\left(\overrightarrow{v}\right) \; \forall \overrightarrow{v} \in V^k$

where $\text{hash}(x_{\overrightarrow{v}}) = \text{hash}(x_{\overrightarrow{w}})$ iff **(a)** $x_{v_i} = x_{w_i}$ and **(b)** $(v_i, v_j) \in E$ iff $(w_i, w_j) \in E$.
N.B.: $N_i\left(\overrightarrow{v}\right) = \{(v_1, \ldots, v_{i-1}, u, v_{i+1}, \ldots, v_k) : u \in V\}$.

Weisfeiler-Leman Hierarchies

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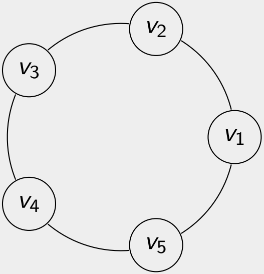

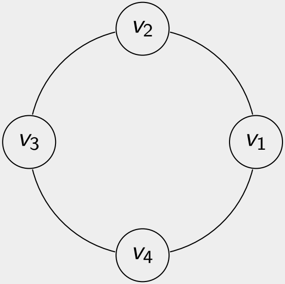

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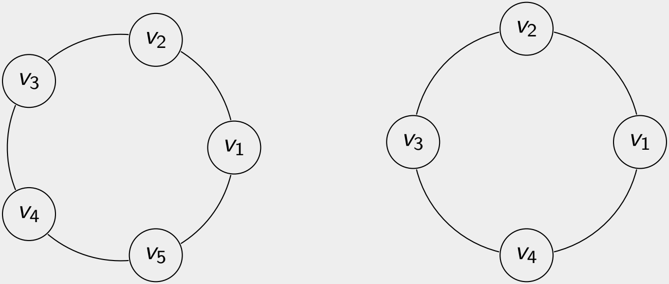

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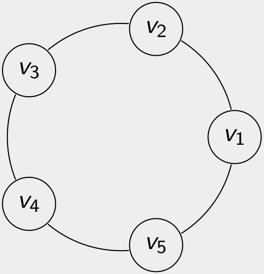

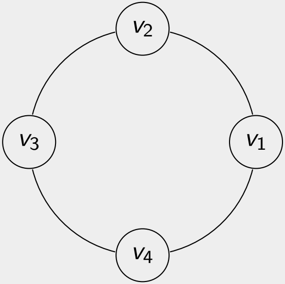

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However.. for every k, there is an infinite family of graphs for which the k-WL test fails[CFI92]

Message Passing on Simplicial Complexes

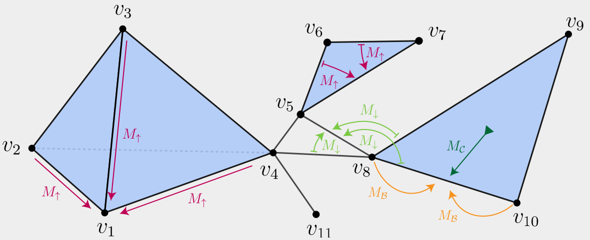

Image from [BFW+21]

Simplicial WL [BFW+21]: $c^{t+1}(\sigma) =$hash of coloring at t of σ and..

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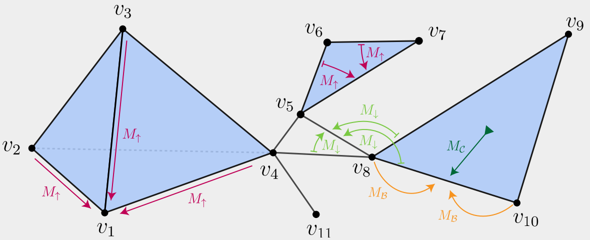

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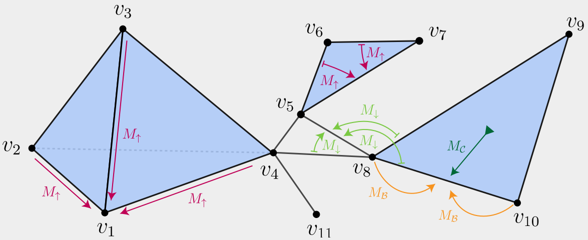

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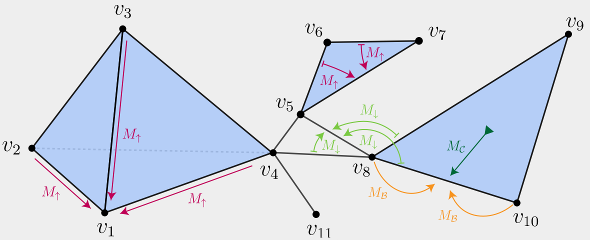

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Lemma

For each $k \leq n$ and $a : V(G)^k \longrightarrow \mathbb{N}$ and $c : \mathcal{K} \longrightarrow \mathbb{N}$, where dim$\mathcal{K} = n$, SWL is strictly stronger than k-WL.

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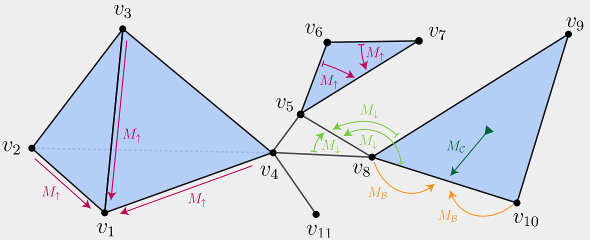

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Lemma

For each $k \leq n$ and $a : V(G)^k \longrightarrow \mathbb{N}$ and $c : \mathcal{K} \longrightarrow \mathbb{N}$, where dim$\mathcal{K} = n$, SWL is (almost) strictly stronger than k-WL.

Can we get better directions?

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Algorithm Directed Weisfeiler-Leman (DWL)[MG21]

1: **Input**: (V, E, X_V) Here, $x_v \in \mathbb{Z}_2^d$
2: $c(v) = c^{(0)}(v) \longleftarrow hash(x_v)$
3: **while** $c^{(t)}(v) = c^{(t+1)}(v)\ \forall v \in V$ **do**
4: $c^{(t+1)}(v) \longleftarrow \text{hash}\left(\begin{array}{c} c^{(t)}(v), \{\!\{c^{(t)}(w) : w \in N_{\text{in}}(v)\}\!\}, \\ \{\!\{c^{(t)}(u) : w \in N_{\text{out}}(u)\}\!\} \end{array}\right)$
5: **Output:** $c^{(T)}(v)\ \forall v \in V$

DWL is strictly stronger than WL[BFW$^+$21]

Yes, we can

$$G_1 \rightrightarrows G_0 \qquad \textbf{Directed Graph}$$

Yes, we can

$$\begin{tikzcd} G_1 \arrow[r, bend left, shift left] \arrow[r, bend left] & G_0 \arrow[l, bend left] \end{tikzcd}$$

Directed Graph

Yes, we can

$$\begin{tikzcd}
G_1 \arrow[r, shift left=2] \arrow[r, shift left=4] & G_0 \arrow[l, shift left=2]
\end{tikzcd}$$

Directed Graph

$$\begin{tikzcd}
\cdots \arrow[r, shift left=2] \arrow[r, shift left=4] \arrow[r, shift left=6] \arrow[r, shift left=8] \arrow[r, shift left=10] & X_3 \arrow[l, shift left=2] \arrow[l, shift left=4] \arrow[l, shift left=6] \arrow[l, shift left=8] \arrow[r, shift left=2] \arrow[r, shift left=4] \arrow[r, shift left=6] \arrow[r, shift left=8] & X_2 \arrow[l, shift left=2] \arrow[l, shift left=4] \arrow[l, shift left=6] \arrow[r, shift left=2] \arrow[r, shift left=4] \arrow[r, shift left=6] & X_1 \arrow[l, shift left=2] \arrow[l, shift left=4] \arrow[r, shift left=2] \arrow[r, shift left=4] & X_0 \arrow[l, shift left=2]
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Simplicial Set

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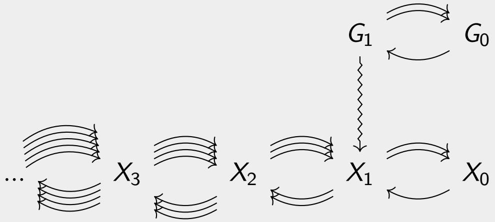

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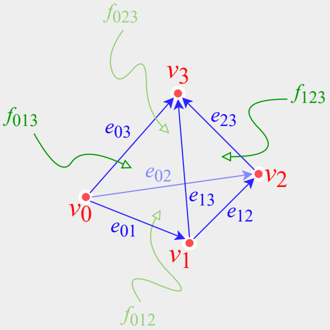

$\nu_0, \nu_1, \nu_2, \nu_3 \in X_0$

$e_{01}, e_{02}, e_{03}, e_{12}, e_{13}, e_{23} \in X_1$

$f_{012}, f_{013}, f_{023}, f_{123} \in X_2$

$g_{0123} \in X_3$

Simplicial Set WL

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Update rules for SSWL

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Update rules for SSWL

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Simplicial Set Weisfeiler-Leman Algorithm

SSWL is strictly stronger than SWL[BFW+21]

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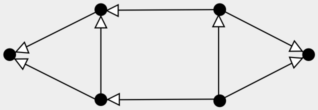
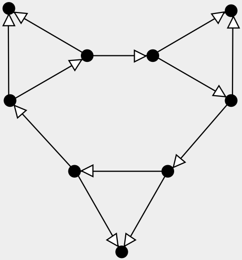
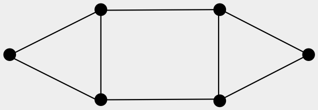
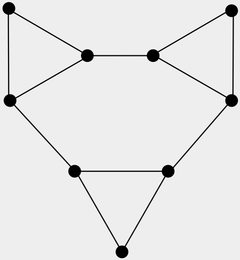




Simplicial Set Weisfeiler-Leman Algorithm

SSWL is strictly stronger than SWL[BFW$^+$21]





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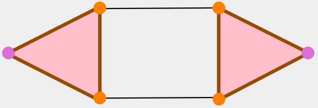
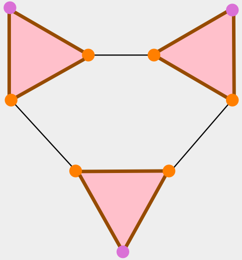
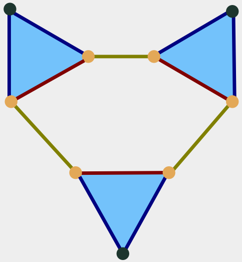




Simplicial Set Weisfeiler-Leman Algorithm

SSWL is strictly stronger than SWL[BFW$^+$21]



Message Passing with Higher Dimensional Data

Summary:

$$\begin{array}{ccc} DWL & \sqsubset & WL \\ & & \sqcup \\ & & 3\text{-WL} \\ & & \sqcup \\ & & SWL \end{array}$$

Message Passing with Higher Dimensional Data

Summary:

$$\begin{array}{ccc} DWL & \sqsubset & WL \\ \sqcup & & \sqcup \\ ? & & k\text{-WL} \\ \sqcup & & \sqcup \\ SSWL & \sqsubset & SWL \end{array}$$

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Thank you!