Weisfeiler-Lehman use Simplicial Sets

PseudoTop Vertex Neural Network

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Outline

- Weisfeiler-Lehman Algorithm and graph neural networks
- The case for higher order relations
- Kan Extensions and Indexing Categories
- Top vertices and pseudotop vertices
- Pseudotop Vertex Neural Network
- Implementation

Weisfeiler-Lehman Algorithm

Definition

A **coloring** of a graph $G = (V, E)$ is a function $c : V \longrightarrow \mathbb{N}$.

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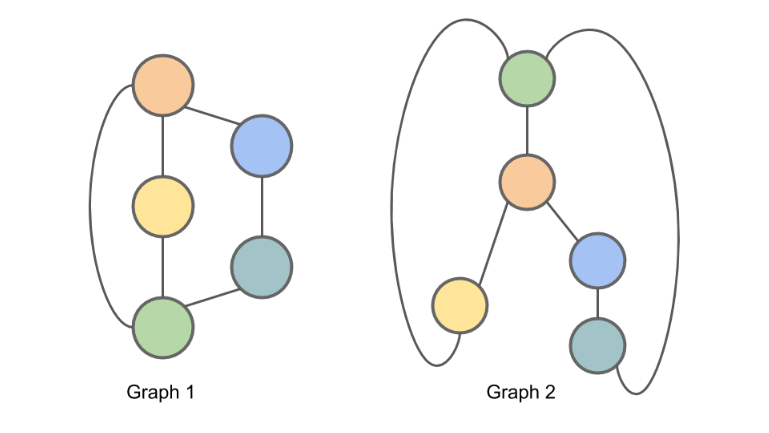
Basic idea: start with $c(v) = c^{(0)}(v)$, and
$c^{(t+1)}(v) = \text{hash}\left(c^{(t)}(v), \{\!\{c^{(t)}(w) : w \in N(v)\}\!\}\right)$[WL68]

Weisfeiler-Lehman Algorithm



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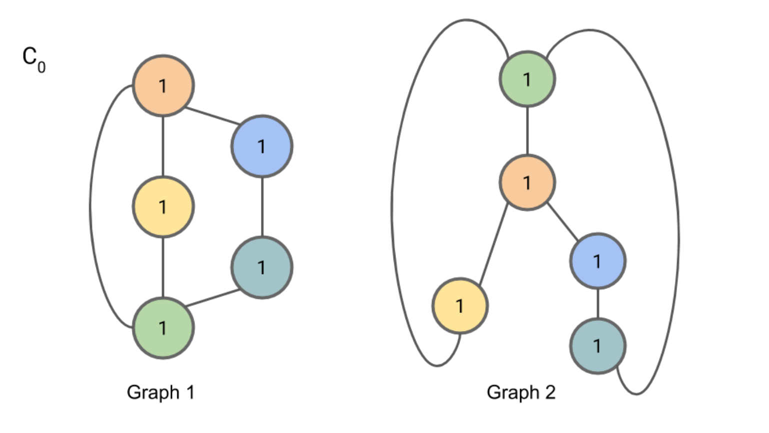

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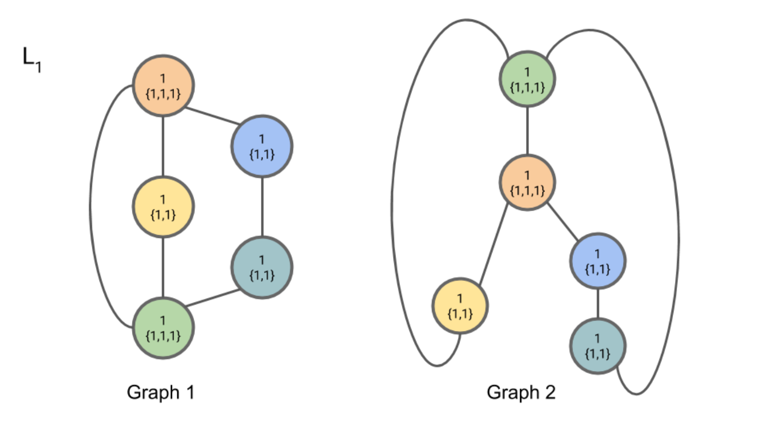

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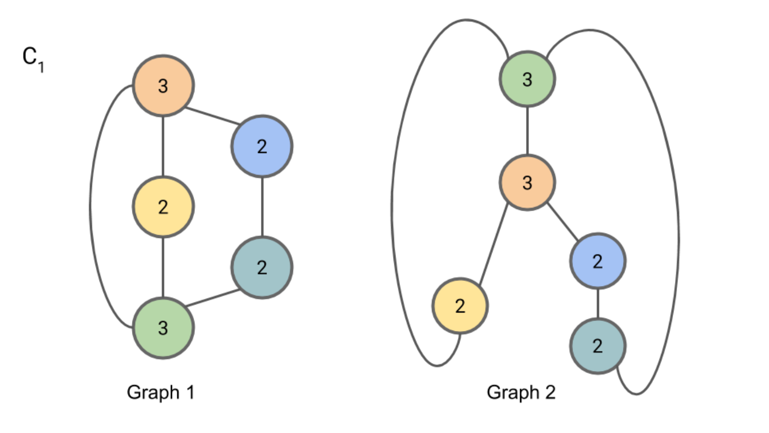

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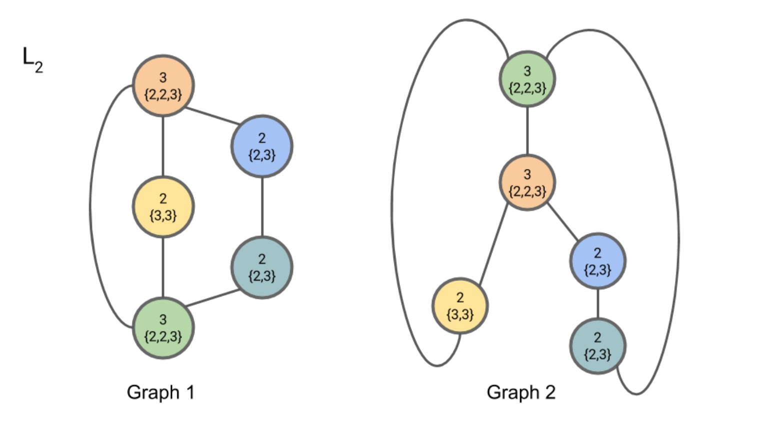

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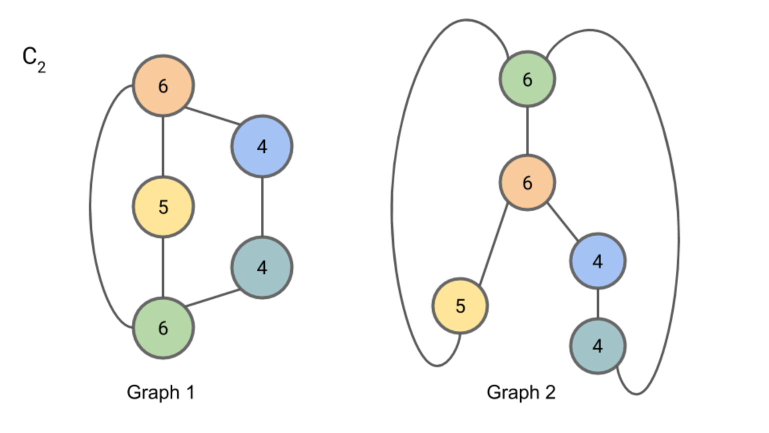

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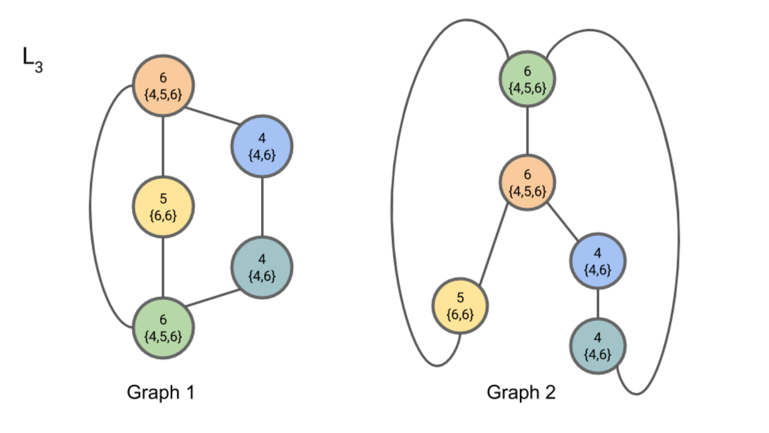

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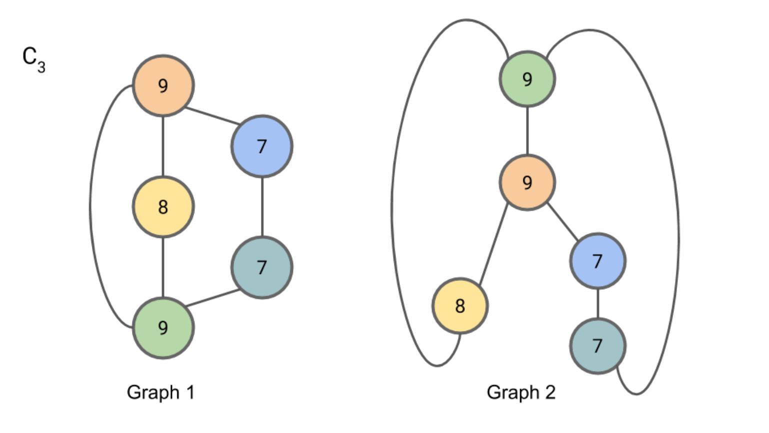

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Algorithm 1 Weisfeiler-Lehman (WL) or Naive vertex refinement

1: **Input**: (V, E, X_V) $\{\triangleright x_v \in \mathbb{Z}_2^d\}$
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: $\quad c^{(t+1)}(v) \longleftarrow \text{hash}\big(c^{(t)}(v), \{\!\{c^{(t)}(w) : w \in N(v)\}\!\}\big)$
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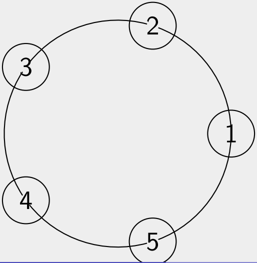

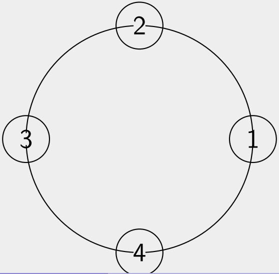

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AGGREGATE	COMBINE	Ref
$\text{MAX}\left(\left\{\sigma\left(W_1.x_u^{(k)}\right)\right\}, u \in N(v)\right)$	$W_2.\left[x_v^{(k)}, a_v^{(k+1)}\right]$	GraphSAGE
$W_1.\text{MEAN}\left(x_u^{(k)}, u \in N(v) \cup \{v\}\right)$	$\sigma\left(\left\{W_2.a_v^{(k+1)}\right\}\right)$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

Graph Neural Networks

or..

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

Graph Neural Networks

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Compare with

$$c^{(t+1)}(v) = \text{hash}\left(c^{(t)}(v), \{\{c^{(t)}(w) : w \in N(v)\}\}\right)$$

Graph Neural Networks

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Theorem

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

k-Weisfeiler-Lehman Algorithm

Algorithm 1 k-Weisfeiler-Lehman (k-WL)

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

Here, $hash\left(x_{\overrightarrow{v}}\right) = hash\left(x_{\overrightarrow{w}}\right)$ iff $x_{v_i} = x_{w_i}$ and if $(v_i, v_j) \in E$ iff $(w_i, w_j) \in E$ and $N_i\left(\overrightarrow{v}\right) = \{(v_1, \ldots, v_{i-1}, u, v_{i+1}, \ldots, v_k) : u \in V\}$

k-Weisfeiler-Lehman Algorithm

Algorithm 2 k-Weisfeiler-Lehman (k-WL)

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$N_i\left(\overrightarrow{v}\right) = \{(i, v_2 ..., v_k), (v_1, i, ..., v_k), ..., (v_1, ..., v_{k-1}, i) : i \in V\}$ for Folklore k-WL

k-Weisfeiler-Lehman Algorithm

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For directed graphs, use
$c^{t+1}(v) \longleftarrow \text{hash}\left(c^{(t)}(v), \{\!\{c^{(t)}(w) : w \in N_{in}(v)\}\!\}, \{\!\{c^{(t)}(w) : w \in N_{out}(v)\}\!\}\right)$
[MG21]

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\begin{aligned}
x_S^{(t)} &= \sigma\left(x_S^{(t-1)}.W_1^{(t)} + \sum_{u \in N_L(S) \cup N_G(S)} x_u^{(t-1)}.W_2^{(t)}\right) \text{ (global)} \\
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\end{aligned}
$$

where $S = (v_1, ..., v_k)$,
$N_L(S) = \left\{T \in V^k : |S \cap T| = k-1, (v, w) \in E \text{ for some unique } v, w \in S \setminus T\right\}$
$N(S) = \left\{T \in V^k : |S \cap T| = k-1\right\}$, $N_G(S) = N(S) \setminus N_L(S)$[MRF+19].

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- $(k+1)$-WL $\equiv$ k-FWL[HV21]
- For every k, there is an infinite family of graphs for which the k-WL test fails[CFI92]
- Note: DWL $\sqsubseteq$ WL, so GNN with directed edges are more powerful[RCDG+23]
  $a_v^{(k+1)} = \text{AGGREGATE}^{(k+1)}\left(\left\{x_u^{(k)}, x_v^{(k)} : (u,v) \in E\right\}\right)$

The case for higher order relations

Simplicial WL [BFW+21] uses

$$c^{t+1}(\sigma) \longleftarrow \mathrm{hash}\Big(c^{t}(\sigma), c^{t}_{\mathcal{B}}(\sigma), c^{t}_{\mathcal{C}}(\sigma), c^{t}_{\downarrow}(\sigma), c^{t}_{\uparrow}(\sigma)\Big)$$

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Conjecture

For each $n \leq k \leq |V(G)|$ and $a : V(G)^{n} \longrightarrow \mathbb{N}$ and $c : S_n \longrightarrow \mathbb{N}$ we have $c \sqsubseteq a|_{S_n}$, where S_n is the collection of directed n-simplices.

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- Therefore, DL $\sqsubseteq$ WL

Modelling higher relations

Kan extension of DG along $i : \Delta_{\leq 1} \longrightarrow \Delta$ produces the functor $Ran_{\imath}- := \imath_* : \mathcal{DG} \longrightarrow \mathcal{SS}ets$ and a natural bijection $\mathrm{Hom}_{\mathcal{S}Set}(X, \imath_*(G)) \cong \mathrm{Hom}_{\mathcal{G}}(\imath^*(X), G)$

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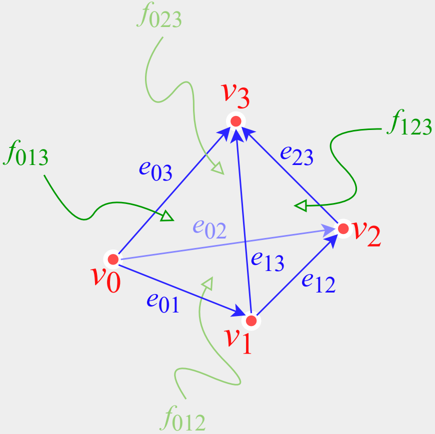

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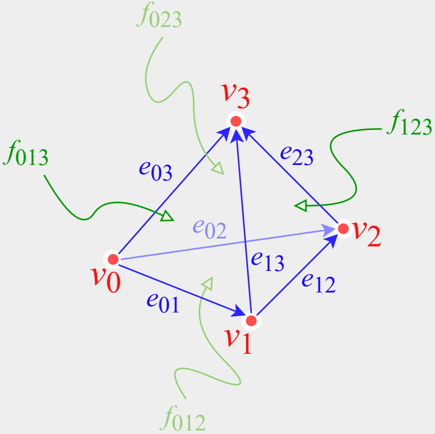

Clique complexes of graphs are given by Kan Extensions of UG along i

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Modelling higher relations

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- So, Simplicial Set WL$\sqsubseteq$Hypergraph WL

In summary:

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

Top Vertices

Recall simplicial set $\Delta[n]_\bullet$

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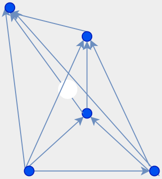

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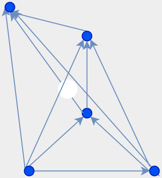

Algorithm 6 Creating 1-skeleton of the geometric realization of standard n-simplex

Input n
for i from 1 to n **do**
  for j from 1 to n **do**
    if $i < j$ **then**
      `src` $\leftarrow$ `src` $+ [i]$
      `dst` $\leftarrow$ `dst` $+ [j]$
      `edges` $\leftarrow$ `edges` $+ [(i, j)]$
    end if
  end for
end for
Output List of directed edges `edges`, source vertices `src` and target vertices

Top Vertices

Definition

A vertex $v \in G_0$ is said to be a **top vertex** of dimension k if there is a simplicial set x of dimension k such that $d_0^{(1)} d_0^{(2)} ... d_0^{(k-1)} d_0^{(k)} x = v$, where $d_0^{(k)} : X_k \longrightarrow X_{k-1}$ is the 0-th face map.

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Lemma

Let A be the adjacency matrix of G, and $\widetilde{A} = A - diag(A)$. If v is a top vertex for a k-simplex x, then the v-th column of $A \circledcirc \left(\widetilde{A} + \widetilde{A}^2 + ... + \widetilde{A}^k\right)$ is a decreasing sequence (possibly after a permutation), starting with $\sum_{n=0}^{k} \binom{k}{n}$.

Top Vertices

Lemma

Let $v \in G_0$*, and* A *be the adjacency matrix associated with the graph* G*. If*

$$\left(A + A^T\right)_{vv}^{k+1} \geq 4\sum_{n=0}^{k} \binom{k}{n}$$

and $\left|N_1^{in}(u) \cap N_1^{in}(v)\right| \geq k - 1$*, then the following are equivalent:*

1. $\exists u \in N_1^{in}(v)$ *such that* u *is a top vertex for a* $(k-1)$*-simplex*
2. v *is a top vertex for a* k*-simplex*

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Way around: $(A \bullet B)_{ij} = \bigvee_{k=1}^{n} a_{ik} \wedge b_{kj}$

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2. *v is a top vertex for a k-simplex*

Way around: $(A \bullet B)_{ij} = \bigvee_{k=1}^{n} a_{ik} \wedge b_{kj}$

Lemma

Let G be any directed graph. Then the i,j entry of $\widetilde{A} \odot \widetilde{A^{\bullet 2}} \odot \ldots \odot \widetilde{A^{\bullet k}}$, denoted by $\widetilde{a}_{ij}^{(k)}$, nonzero if and only if there is a path of length 1, length 2, ..., length k from vertex i to vertex j without repeating any vertices.

Here, $\widetilde{X} := X \oplus diag(X)$

Top Vertices

Lemma

Let $v \in G_0$. Then $\widetilde{a}_{iv}^{(2)}$ is nonzero if and only if v is a top 2 vertex.

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If $\widetilde{a}_{iu}^{(2)} \neq 0$, $\widetilde{a}_{iv}^{(3)} \neq 0$, $u \in \widetilde{N}_{in}^{1}(v)$ (i.e., u and v are top 2-vertices) and $\widetilde{N}_{out}^{1}(i) \cap \widetilde{N}_{in}^{1}(u) \cap \widetilde{N}_{in}^{1}(v)$ is nonempty, then v is a top 3-vertex

Top Vertices

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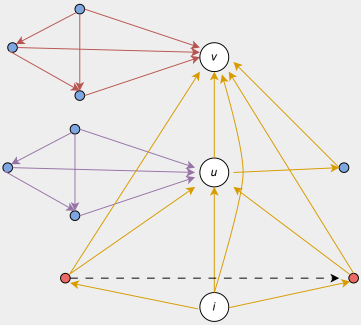
Lemma

For three vertices u, v, w with $u \in \widetilde{N}_{in}^{1}(v)$ and $w \in \widetilde{N}_{in}^{1}(v) \cap \widetilde{N}_{in}^{1}(u)$, if $\widetilde{a}_{iv}^{(4)}$ and $\widetilde{a}_{iu}^{(3)}$ and $\widetilde{a}_{iw}^{(2)}$ are nonzero, and if $\widetilde{N}_{out}^{1}(i) \cap \widetilde{N}_{in}^{1}(v) \cap \widetilde{N}_{in}^{1}(u)$ is nonempty, then $[i, x, w, u, v]$ is a 4 simplex for all $x \in \widetilde{N}_{out}^{1}(i) \cap \widetilde{N}_{in}^{1}(v) \cap \widetilde{N}_{in}^{1}(u) \cap \widetilde{N}_{in}^{1}(w)$

Pseudo Top Vertices

Definition

For $v \in G_0$, and any integer $k \geq 1$, u is said to be a k-pseudotop vertex if $\exists u \in \widetilde{N}^1_{in}(v)$ that is a $(k-1)$-semitop vertex such that $\left|\widetilde{N}^1_{out}(i) \cap \widetilde{N}^1_{in}(u) \cap \widetilde{N}^1_{in}(v)\right| > k-3$, where i is a vertex such that $\widetilde{a}^{(k-1)}_{iu}$ and $\widetilde{a}^{(k)}_{iv}$ are nonzero. For $k = 0$, all vertices are defined to be 0-semitop vertices. The integer k is said to be the dimension of the pseudotop vertex.



Pseudotop Vertex Neural Network

Algorithm 7 Required pre-processing for PTVNN

1: Find pseudotop vertices
2: Label every vertex v with its maximum dimension
3: Partition vertices based on dimension
4: Form partition vector $R(v) = ([v], [w_1], ..., [w_n])$, where $w_i \in N_{in}(v)$ {Refine partition}
5: If $R(v) = R(u)$, then $[u] = [v]$.
6: Repeat until refinement stabilizes

$$
\begin{aligned}
\mathbf{a}_v^{t+1} &= \text{AGG}\left(\mathbf{x}_v^t, \mathbf{x}_u^t : u \in N_{in}(v)\right) \\
\mathbf{x}_v^{t+1} &= \text{COMBINE}\left(\mathbf{x}_v^t, \mathbf{a}_v^{t+1}\right)
\end{aligned}
$$

Pseudotop Vertex Neural Network

Architecture 1

- Make one hot encoding of partition p after refinement
- If x_v is feature vector of v, then form $[x_v.p]$

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- Make one hot encoding of vertex dimension d
- Make one hot encoding of refinement index r
- If x_v is feature vector of v, then form $[x_v.d.r]$

Architecture 3

- Make multi hot encoding of vertex dimension d
- Make multi hot encoding of partition indices k
- If x_v is feature vector of v, then form $[x_v.k.d]$

Implementation

Dataset: Directed citation network[HFZ+20] with 40 subject areas.
Task: subject area classification.
Code: https://abdullahnaeemmalik.github.io/portfolio/ptvnn/

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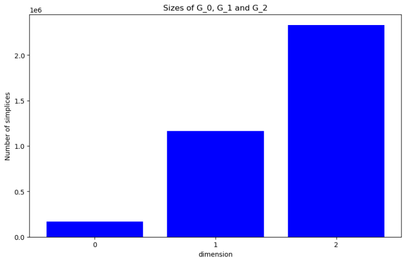
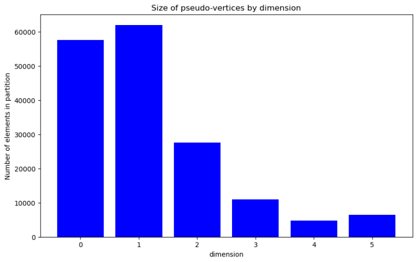
Number of nodes=169343. Number of edges=1166243. Number of 2-simplices=2332322





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