UNIVERSITÄT BONN

Wasserstein Weisfeiler-Lehman Graph Kernels

Matteo Togninalli, Felipe Llinares-López, Elisabetta Ghisu, Bastian Rieck, Karsten Borgwardt – ETH ZURICH

Fabrice Beaumont

Rheinische Friedrich-Wilhelms-Universität Bonn

01.07.2020

Motivation

TASK: Graph classification (via graph kernels as similarity measure)

Solution: $\mathfrak{R}$-Convolution kernels

Problem: Naive aggregation of substructures may disregard valuable information

Only a few approaches extendible for continuously attributed graphs

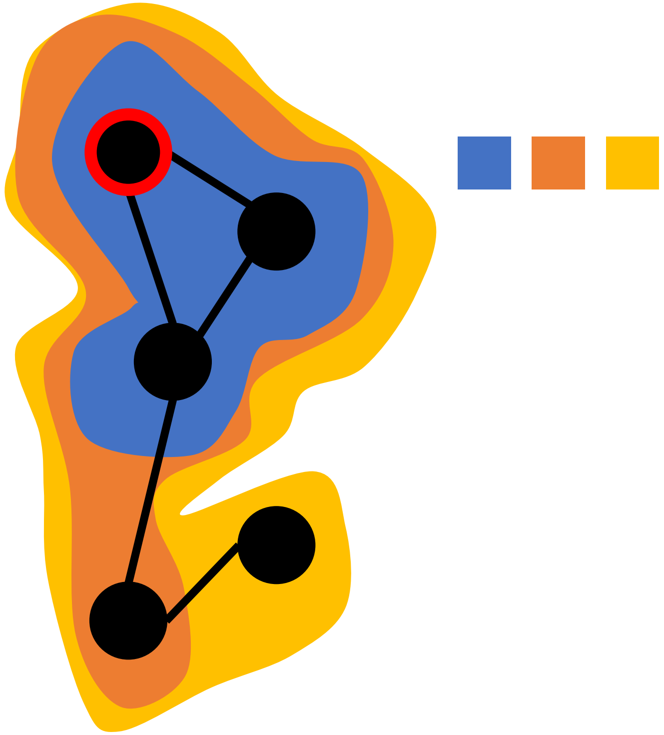
Method Overview

1. Transform each graph into a set of node embeddings
    1. Weisfeiler-Lehman node embedding scheme
    2. WL-features
2. Measure the Wasserstein distance between each pair of graphs
    1. Ground distance (similarity matrix)
    2. Wasserstein distance
3. Wasserstein Weisfeiler-Lehman kernel definition

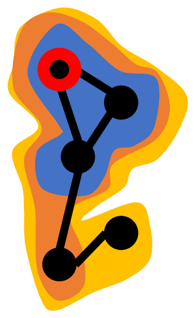
Optimal transport

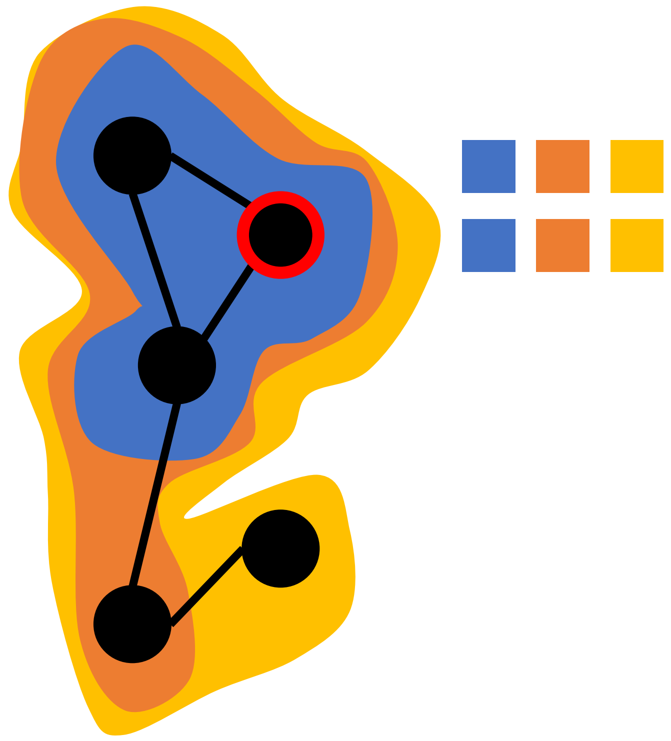
(Differentiate between a finite set of categorical **node labels** and real valued **node attributes**)

1.1 Weisfeiler-Lehman node embedding scheme
Idea

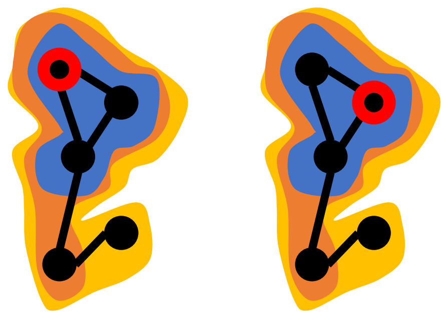


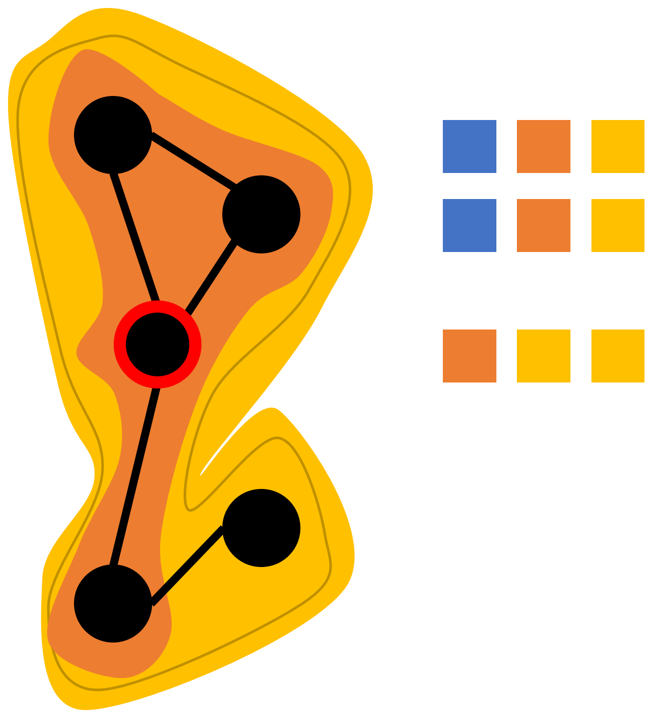
1.1 Weisfeiler-Lehman node embedding scheme
Idea



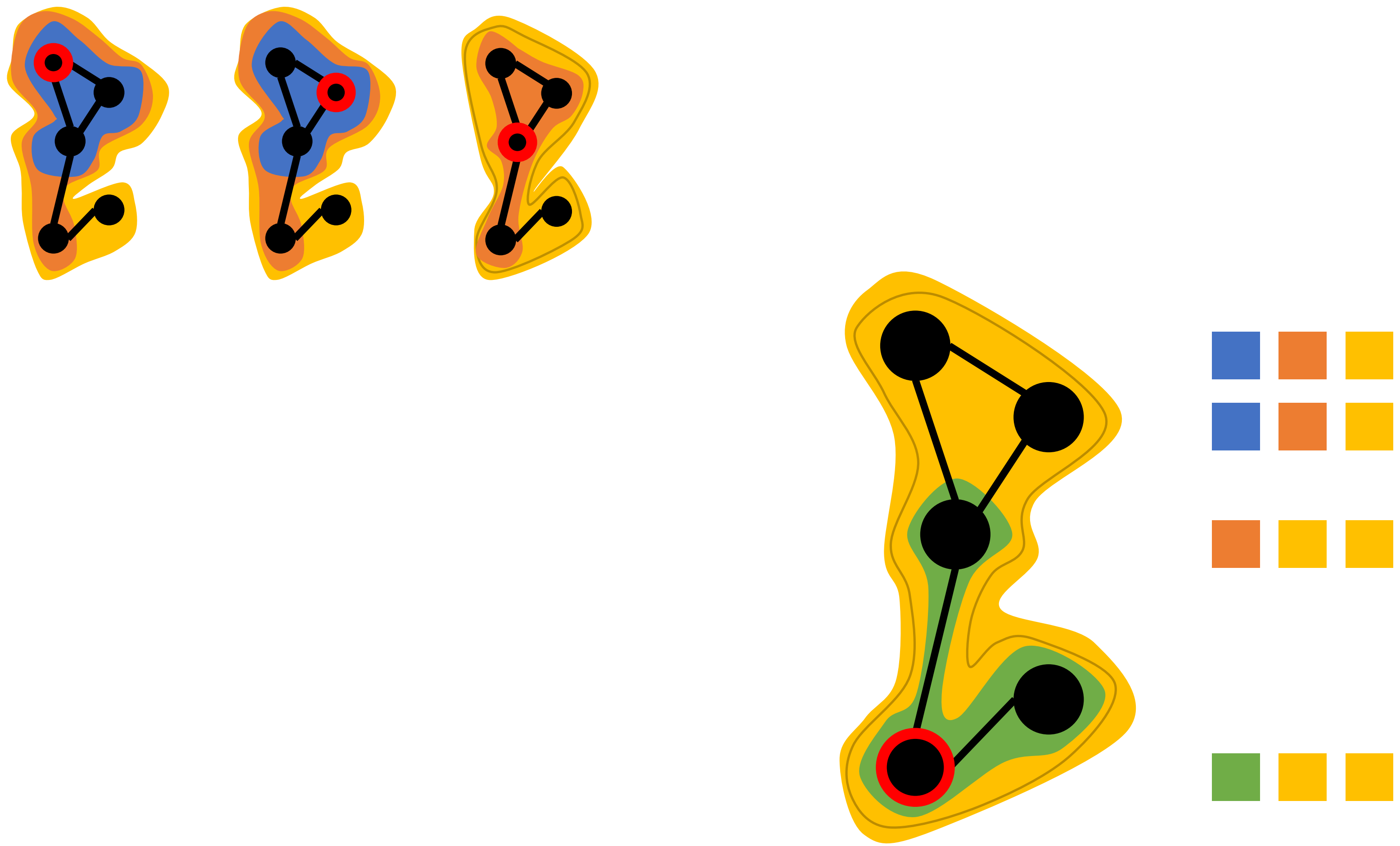


1.1 Weisfeiler-Lehman node embedding scheme
Idea

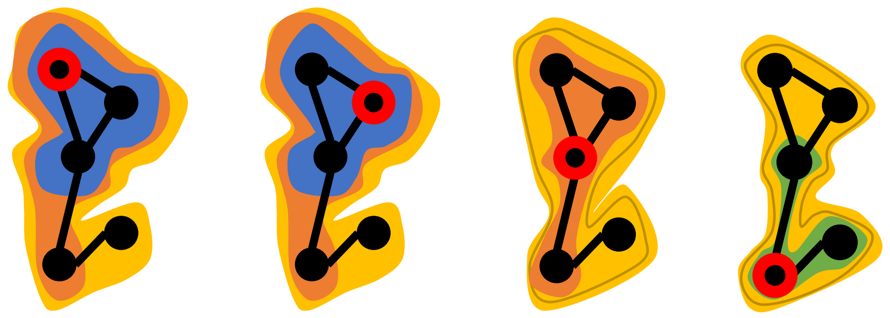


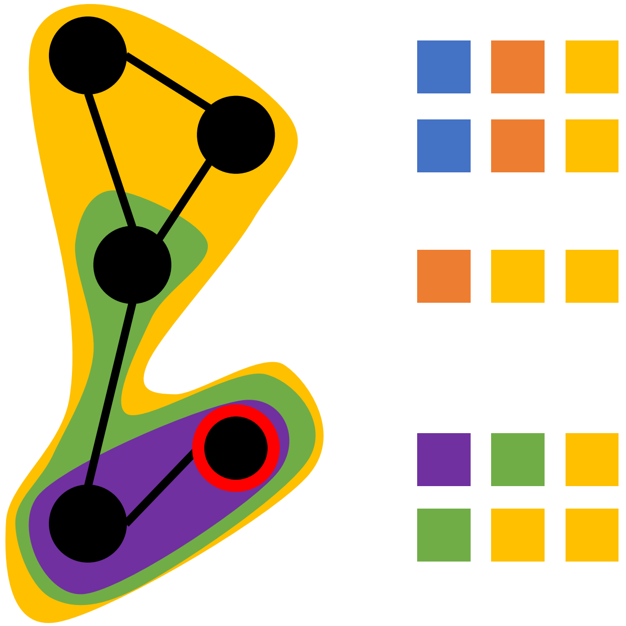


1.1 Weisfeiler-Lehman node embedding scheme
Idea

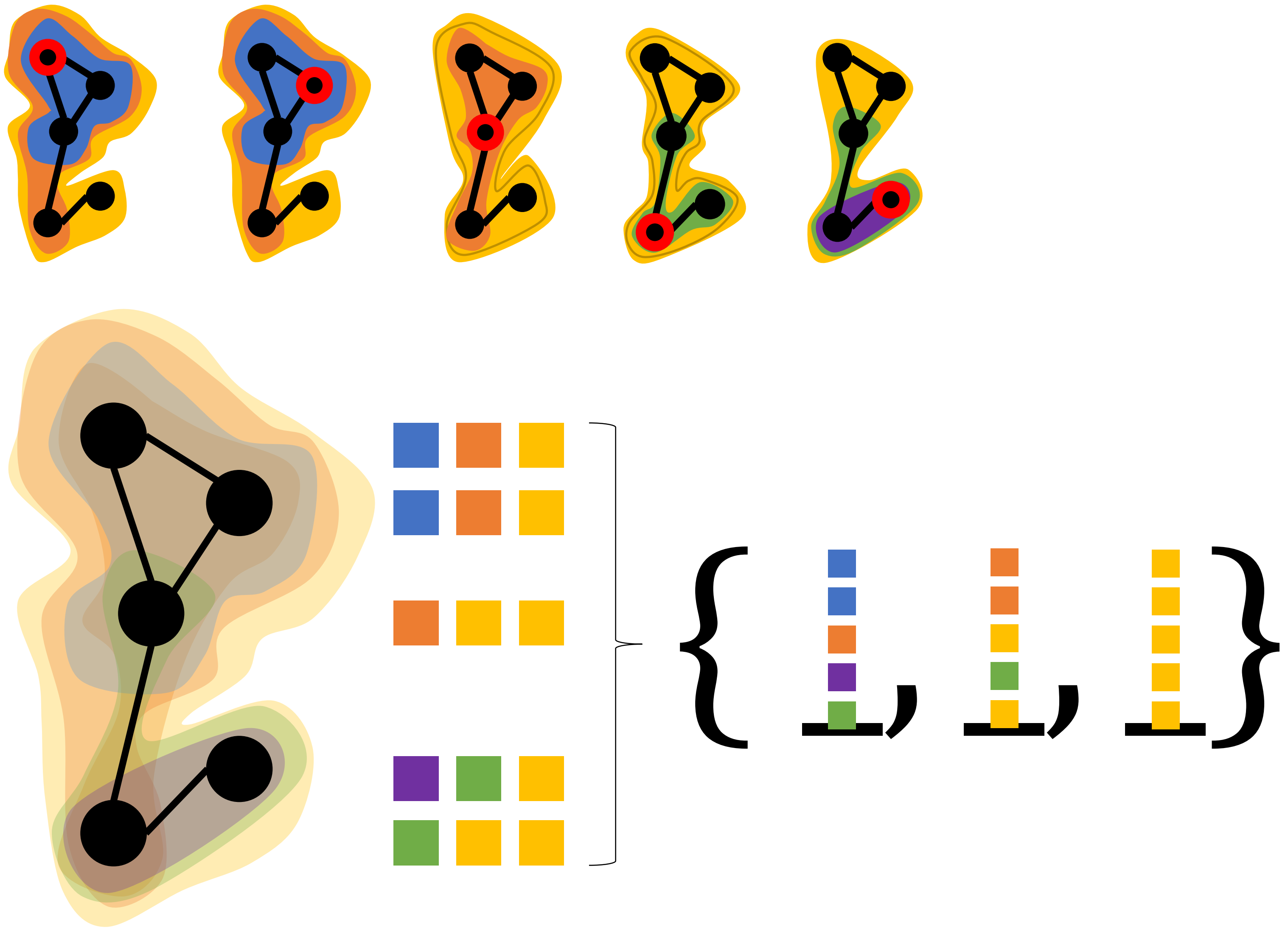


1.1 Weisfeiler-Lehman node embedding scheme
Idea

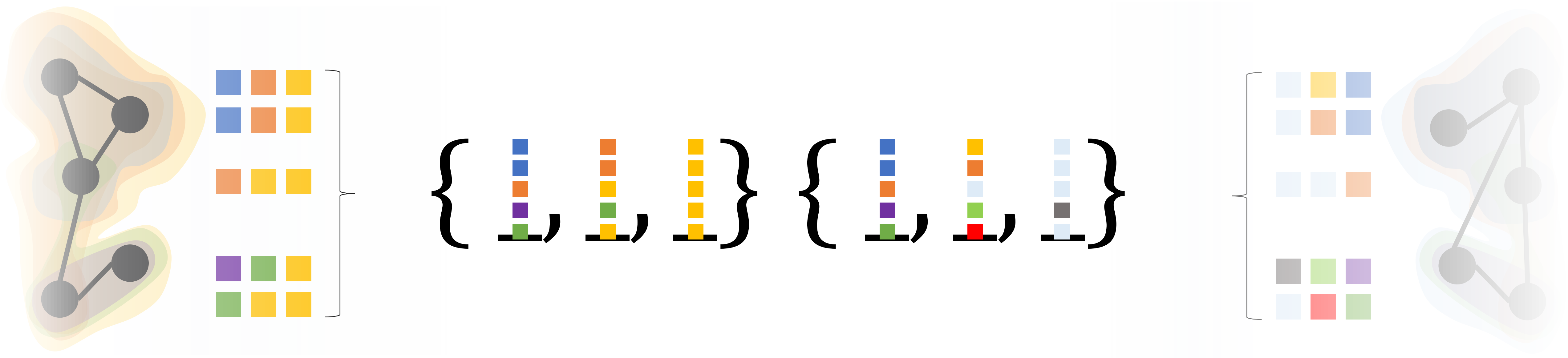




1.1 Weisfeiler-Lehman node embedding scheme
Idea



1.1 Weisfeiler-Lehman node embedding scheme
Idea



1.1 Weisfeiler-Lehman node embedding scheme Theory

UNIVERSITÄT BONN

m: dimensionality of the node labels

n_G: cardinality of the vertex set

$N(v)$: neighbourhood of v

$$N^h(v) = \{l^h(u_0), \dots, l^h(u_{\deg(v)-1})\}$$

NODE LABELS	
$l^{h+1}(v) = hash(l^h(v), N^h(v))$	

1.1 Weisfeiler-Lehman node embedding scheme
Theory

m: dimensionality of the node labels

n_G: cardinality of the vertex set

$N(v)$: neighbourhood of v

$$N^h(v) = \{l^h(u_0), \dots, l^h(u_{\deg(v)-1})\}$$

NODE LABELS	NODE ATTRIBUTES
$l^{h+1}(v) = hash(l^h(v), N^h(v))$	$a^{h+1}(v) = a^h(v) + \sum_{u \in N(v)} a^h(u)$

1.1 Weisfeiler-Lehman node embedding scheme Theory

m: dimensionality of the node labels

n_G: cardinality of the vertex set

$N(v)$: neighbourhood of v

$$N^h(v) = \{l^h(u_0), \dots, l^h(u_{\deg(v)-1})\}$$

NODE LABELS	NODE ATTRIBUTES
$l^{h+1}(v) = hash(l^h(v), N^h(v))$	$a^{h+1}(v) = a^h(v) + \sum_{u \in N(v)} w((u,v))a^h(u)$

1.1 Weisfeiler-Lehman node embedding scheme Theory

m: dimensionality of the node labels

n_G: cardinality of the vertex set

$N(v)$: neighbourhood of v

$$N^h(v) = \{l^h(u_0), \dots, l^h(u_{\deg(v)-1})\}$$

NODE LABELS	NODE ATTRIBUTES
$l^{h+1}(v) = hash(l^h(v), N^h(v))$	$a^{h+1}(v) = \frac{1}{2}\left(a^h(v) + \frac{1}{\deg(v)} \sum_{u \in N(v)} w((u,v))\, a^h(u)\right)$

1.1 Weisfeiler-Lehman node embedding scheme Theory

m: dimensionality of the node labels

n_G: cardinality of the vertex set

$N(v)$: neighbourhood of v

$$N^h(v) = \{l^h(u_0), \dots, l^h(u_{\deg(v)-1})\}$$

NODE LABELS	NODE ATTRIBUTES
$l^{h+1}(v) = hash(l^h(v), N^h(v))$	$a^{h+1}(v) = \frac{1}{2}\left(a^h(v) + \frac{1}{\deg(v)} \sum_{u \in N(v)} w((u,v))\, a^h(u)\right)$ $\in \mathbb{R}^m$

WL-features $$X_G^h = \left[x^h(v_1), \dots, x^h(v_{n_G})\right]^T \quad \in \mathbb{R}^{n_G \times m}$$

Node embedding $$f_{WL}^H : G \longrightarrow \left(X_G^0, \dots, X_G^H\right) \quad \in \mathbb{R}^{n_G \times m(H+1)}$$

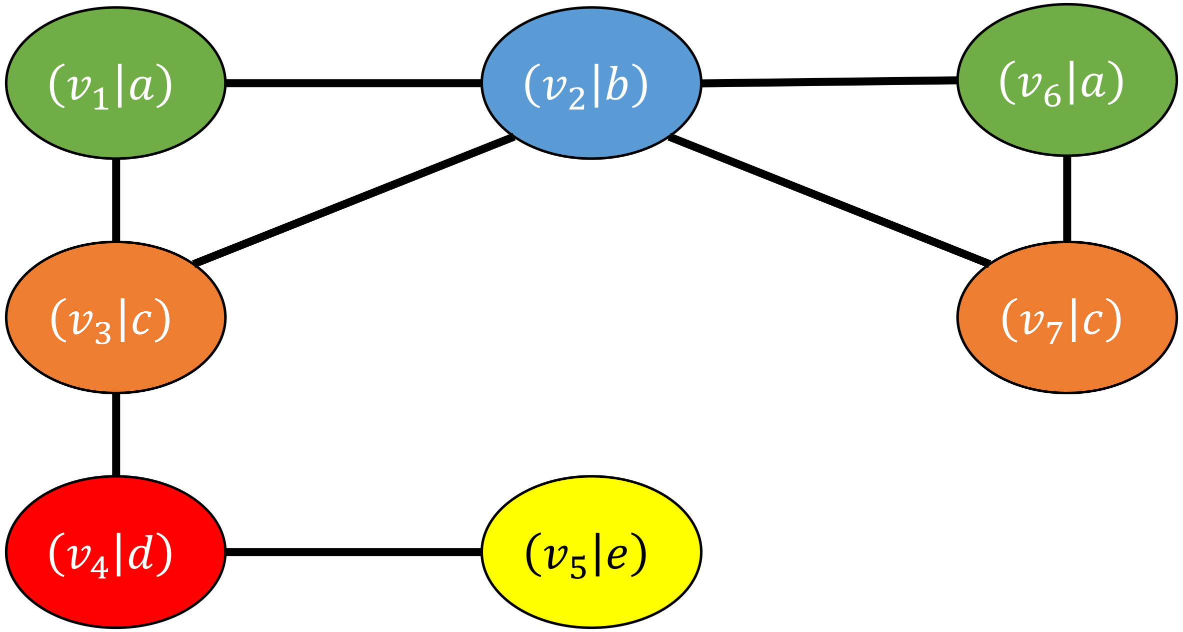
1.1 Weisfeiler-Lehman node embedding scheme
Example – Node labels

$m = 1$: dimensionality of the node labels

$n_G = 7$: cardinality of the vertex set

$N(v)$: neighbourhood of v

$$l^{h+1}(v) = hash(l^h(v), N^h(v))$$



1.1 Weisfeiler-Lehman node embedding scheme
Example – Node labels

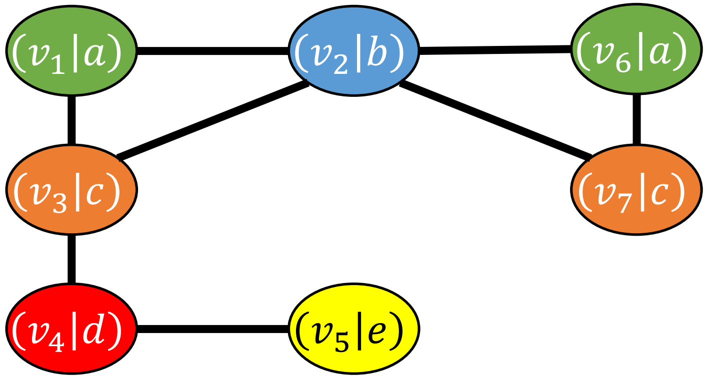
UNIVERSITÄT BONN

$m = 1$: dimensionality of the node labels

$n_G = 7$: cardinality of the vertex set

$N(v)$: neighbourhood of v

$$l^{h+1}(v) = hash(l^h(v), N^h(v))$$



i	$l^0(v_i)$	$l^1(v_i)$	$l^2(v_i)$	…	$l^H(v_i)$
1	a			…	…
2	b			…	…
3	c			…	…
4	d			…	…
5	e			…	…
6	a			…	…
7	c			…	…

1.1 Weisfeiler-Lehman node embedding scheme
Example – Node labels

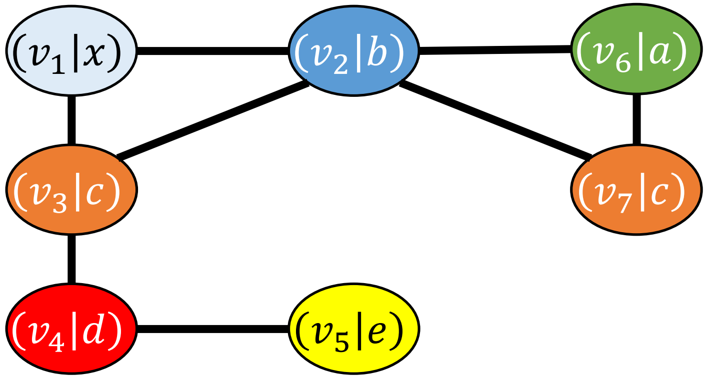
UNIVERSITÄT BONN

$m = 1$: dimensionality of the node labels

$n_G = 7$: cardinality of the vertex set

$N(v)$: neighbourhood of v

$$l^{h+1}(v) = hash(l^h(v), N^h(v))$$



i	$l^0(v_i)$	$l^1(v_i)$	$l^2(v_i)$	…	$l^H(v_i)$
1	a	hash$(a, \{b, c\}) = x$		…	…
2	b			…	…
3	c			…	…
4	d			…	…
5	e			…	…
6	a			…	…
7	c			…	…

1.1 Weisfeiler-Lehman node embedding scheme
Example – Node labels

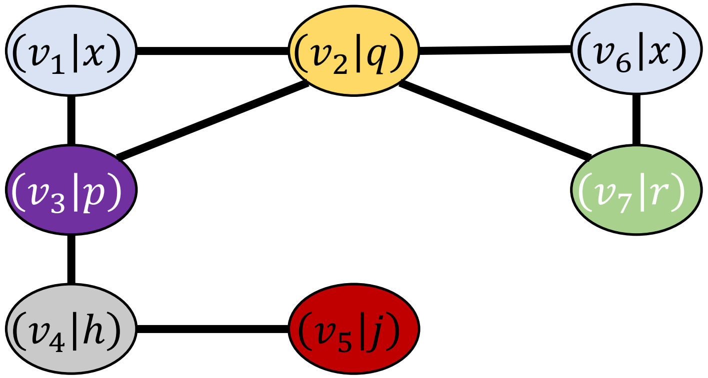
UNIVERSITÄT BONN

$m = 1$: dimensionality of the node labels

$n_G = 7$: cardinality of the vertex set

$N(v)$: neighbourhood of v

$$l^{h+1}(v) = hash(l^h(v), N^h(v))$$



i	$l^0(v_i)$	$l^1(v_i)$	$l^2(v_i)$	…	$l^H(v_i)$
1	a	hash$(a, \{b, c\}) = x$		…	…
2	b	hash$(b, \{a, c\}) = q$		…	…
3	c	hash$(c, \{a, b, d\}) = p$		…	…
4	d	hash$(d, \{c, e\}) = h$		…	…
5	e	hash$(e, \{d\}) = j$		…	…
6	a	hash$(a, \{b, c\}) = x$		…	…
7	c	hash$(c, \{a, b\}) = r$		…	…

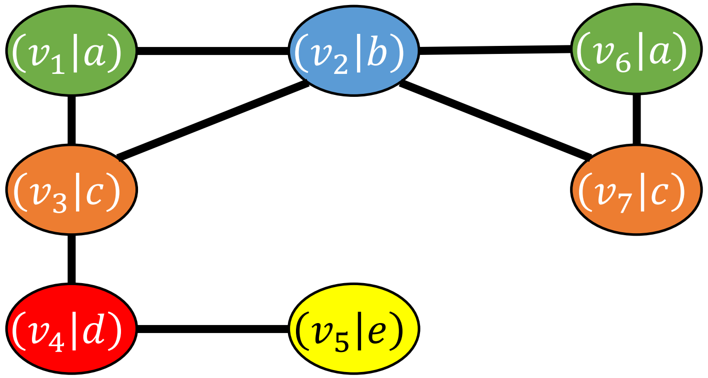
1.1 Weisfeiler-Lehman node embedding scheme
Example – Node labels

$m = 1$: dimensionality of the node labels

$n_G = 7$: cardinality of the vertex set

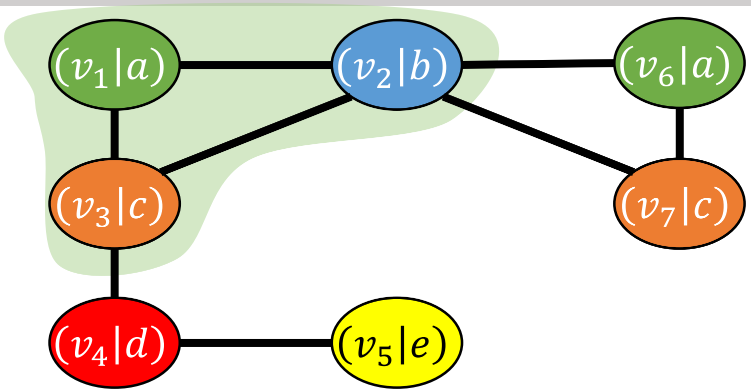
$N(v)$: neighbourhood of v

$$l^{h+1}(v) = hash(l^h(v), N^h(v))$$



i	$l^0(v_i)$	$l^1(v_i)$	$l^2(v_i)$	...	$l^H(v_i)$
1	a	hash$(a, \{b, c\}) = x$	hash$(x, \{q, p\}) = k$	...	...
2	b	hash$(b, \{a, c\}) = q$	hash$(q, \{x, p\}) = o$	...	...
3	c	hash$(c, \{a, b, d\}) = p$	hash$(p, \{x, q, h\}) = r$	...	...
4	d	hash$(d, \{c, e\}) = h$	hash$(h, \{p, j\}) = w$	...	...
5	e	hash$(e, \{d\}) = j$	hash$(j, \{h\}) = f$	...	...
6	a	hash$(a, \{b, c\}) = x$	hash$(x, \{q, r\}) = g$	...	...
7	c	hash$(c, \{a, b\}) = r$	hash$(r, \{x, q\}) = s$	...	...

1.1 Weisfeiler-Lehman node embedding scheme Example – Node labels



$m = 1$: dimensionality of the node labels

$n_G = 7$: cardinality of the vertex set

$N(v)$: neighbourhood of v

$$l^{h+1}(v) = hash(l^h(v), N^h(v))$$

i	$l^0(v_i)$	$l^1(v_i)$	$l^2(v_i)$	...	$l^H(v_i)$
1	a	hash$(a, \{b, c\}) = x$	hash$(x, \{q, p\}) = k$	...	...
2	b	hash$(b, \{a, c\}) = q$	hash$(q, \{x, p\}) = o$	...	...
3	c	hash$(c, \{a, b, d\}) = p$	hash$(p, \{x, q, h\}) = r$	...	...
4	d	hash$(d, \{c, e\}) = h$	hash$(h, \{p, j\}) = w$	...	...
5	e	hash$(e, \{d\}) = j$	hash$(j, \{h\}) = f$	...	...
6	a	hash$(a, \{b, c\}) = x$	hash$(x, \{q, r\}) = g$	...	...
7	c	hash$(c, \{a, b\}) = r$	hash$(r, \{x, q\}) = s$	...	...

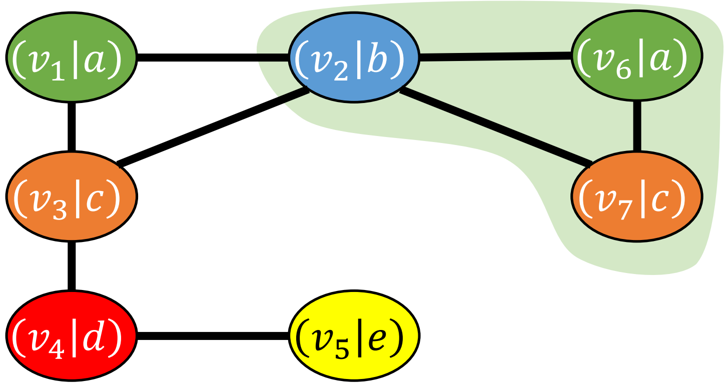
1.1 Weisfeiler-Lehman node embedding scheme
Example – Node labels

$m = 1$: dimensionality of the node labels

$n_G = 7$: cardinality of the vertex set

$N(v)$: neighbourhood of v

$$l^{h+1}(v) = hash(l^h(v), N^h(v))$$



i	$l^0(v_i)$	$l^1(v_i)$	$l^2(v_i)$	...	$l^H(v_i)$
1	a	hash$(a, \{b, c\}) = x$	hash$(x, \{q, p\}) = k$	...	...
2	b	hash$(b, \{a, c\}) = q$	hash$(q, \{x, p\}) = o$	...	...
3	c	hash$(c, \{a, b, d\}) = p$	hash$(p, \{x, q, h\}) = r$	...	...
4	d	hash$(d, \{c, e\}) = h$	hash$(h, \{p, j\}) = w$	...	...
5	e	hash$(e, \{d\}) = j$	hash$(j, \{h\}) = f$	...	...
6	a	hash$(a, \{b, c\}) = x$	hash$(x, \{q, r\}) = g$	...	...
7	c	hash$(c, \{a, b\}) = r$	hash$(r, \{x, q\}) = s$	...	...

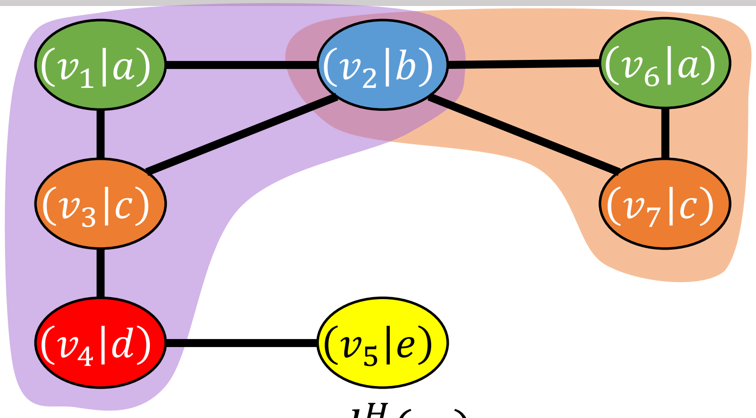
1.1 Weisfeiler-Lehman node embedding scheme
Example – Node labels

$m = 1$: dimensionality of the node labels

$n_G = 7$: cardinality of the vertex set

$N(v)$: neighbourhood of v

$$l^{h+1}(v) = hash(l^h(v), N^h(v))$$



i	$l^0(v_i)$	$l^1(v_i)$	$l^2(v_i)$	…	$l^H(v_i)$
1	a	hash$(a, \{b, c\}) = x$	hash$(x, \{q, \boldsymbol{p}\}) = \boldsymbol{k}$	…	…
2	b	hash$(b, \{a, c\}) = q$	hash$(q, \{x, p\}) = o$	…	…
3	c	hash$(c, \{a, b, d\}) = p$	hash$(p, \{x, q, h\}) = r$	…	…
4	d	hash$(d, \{c, e\}) = h$	hash$(h, \{p, j\}) = w$	…	…
5	e	hash$(e, \{d\}) = j$	hash$(j, \{h\}) = f$	…	…
6	a	hash$(a, \{b, c\}) = x$	hash$(x, \{q, \boldsymbol{r}\}) = \boldsymbol{g}$	…	…
7	c	hash$(c, \{a, b\}) = r$	hash$(r, \{x, q\}) = s$	…	…

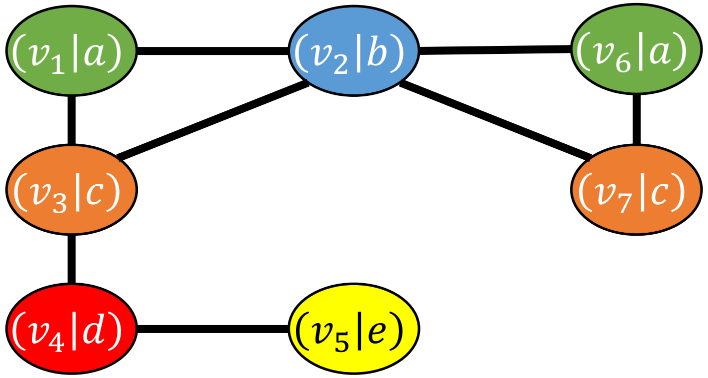
1.1 Weisfeiler-Lehman node embedding scheme
Example – Node labels

$m = 1$: dimensionality of the node labels

$n_G = 7$: cardinality of the vertex set

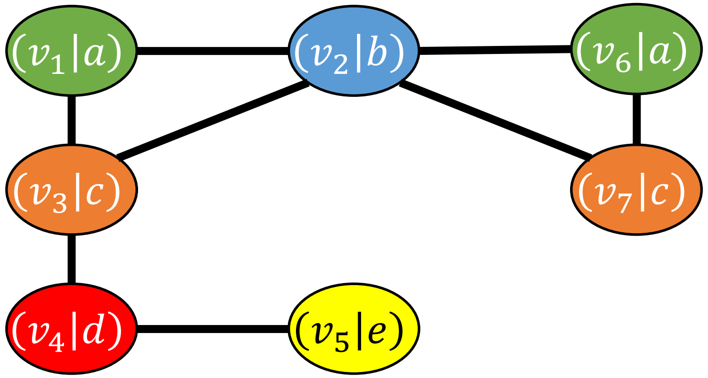
$N(v)$: neighbourhood of v

$$l^{h+1}(v) = hash(l^h(v), N^h(v))$$



i	$l^0(v_i)$	$l^1(v_i)$	$l^2(v_i)$	...	$l^H(v_i)$
1	a	hash$(a, \{b, c\}) = x$	hash$(x, \{q, p\}) = k$	...	...
2	b	hash$(b, \{a, c\}) = q$	hash$(q, \{x, p\}) = o$	...	...
3	c	hash$(c, \{a, b, d\}) = p$	hash$(p, \{x, q, h\}) = r$	...	...
4	d	hash$(d, \{c, e\}) = h$	hash$(h, \{p, j\}) = w$	...	...
5	e	hash$(e, \{d\}) = j$	hash$(j, \{h\}) = f$	...	...
6	a	hash$(a, \{b, c\}) = x$	hash$(x, \{q, r\}) = g$	...	...
7	c	hash$(c, \{a, b\}) = r$	hash$(r, \{x, q\}) = s$	...	...
	$\boldsymbol{X_G^0}$	$\boldsymbol{X_G^1}$	$\boldsymbol{X_G^2}$	...	$\boldsymbol{X_G^H}$

1.1 Weisfeiler-Lehman node embedding scheme
Example – Node labels



$m = 1$: dimensionality of the node labels

$n_G = 7$: cardinality of the vertex set

$N(v)$: neighbourhood of v

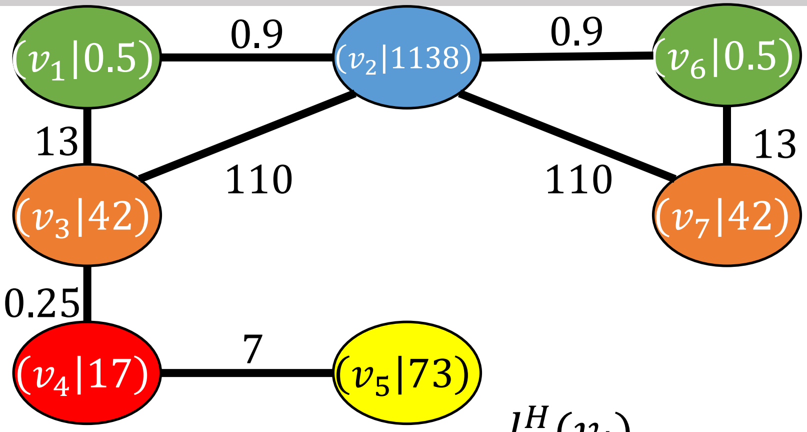
$$l^{h+1}(v) = hash(l^h(v), N^h(v))$$

i	$l^0(v_i)$	$l^1(v_i)$	$l^2(v_i)$	...	$l^H(v_i)$
1	a	hash$(a, \{b, c\}) = x$	hash$(x, \{q, p\}) = k$	...	...
2	b	hash$(b, \{a, c\}) = q$	hash$(q, \{x, p\}) = o$	...	...
3	c	hash$(c, \{a, b, d\}) = p$	hash$(p, \{x, q, h\}) = r$	...	...
4	d	hash$(d, \{c, e\}) = h$	hash$(h, \{p, j\}) = w$	...	...
5	e	hash$(e, \{d\}) = j$	hash$(j, \{h\}) = f$	...	...
6	a	hash$(a, \{b, c\}) = x$	hash$(x, \{q, r\}) = g$	...	...
7	c	hash$(c, \{a, b\}) = r$	hash$(r, \{x, q\}) = s$	...	...

$f_{WL}^H : G \longrightarrow (\; \boldsymbol{X}_G^0 \quad \boldsymbol{X}_G^1 \quad \boldsymbol{X}_G^2 \quad \ldots \quad \boldsymbol{X}_G^H \;)$

1.1 Weisfeiler-Lehman node embedding scheme Example – Attribute labels

$$a^{h+1}(v) = \frac{1}{2}\left(a^h(v) + \frac{1}{\deg(v)} \sum_{u \in N(v)} w((u,v))\, a^h(u) \right)$$

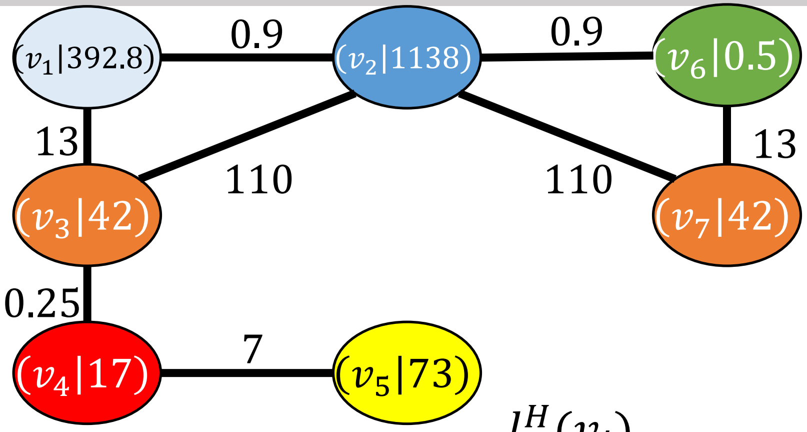


i	$l^0(v_i)$	$l^1(v_i)$	...	$l^H(v_i)$
1	0.5		...	...
2	42		...	...
3	1138		...	...
4	17		...	...
5	73		...	...
6	0.5		...	...
7	42		...	...

1.1 Weisfeiler-Lehman node embedding scheme Example – Attribute labels

UNIVERSITÄT BONN

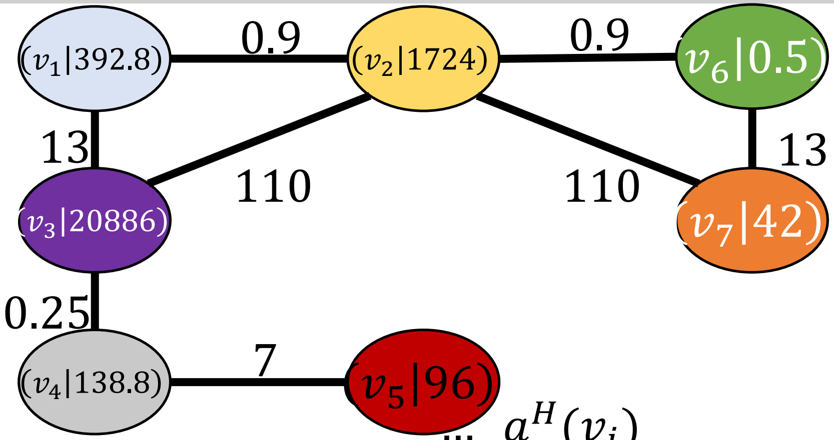
$$a^{h+1}(v) = \frac{1}{2}\left(a^h(v) + \frac{1}{\deg(v)} \sum_{u \in N(v)} w((u,v))\, a^h(u) \right)$$



i	$l^0(v_i)$	$l^1(v_i)$	...	$l^H(v_i)$
1	0.5	$^1/_2\left(0.5 + {^1/_2}\,[0.9 * 1138 + 13 * 42]\right) = 392.8$	...	...
2	42		...	...
3	1138		...	...
4	17		...	...
5	73		...	...
6	0.5		...	...
7	42		...	...

1.1 Weisfeiler-Lehman node embedding scheme Example – Attribute labels

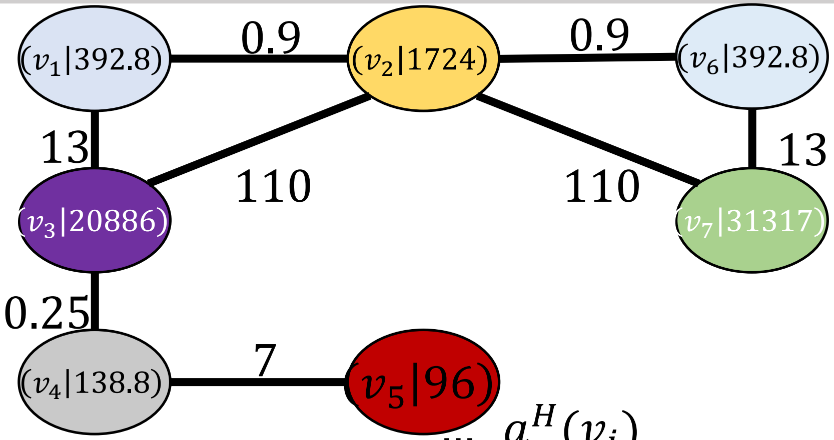
$$a^{h+1}(v) = \frac{1}{2}\left(a^h(v) + \frac{1}{\deg(v)} \sum_{u \in N(v)} w((u,v))\, a^h(u) \right)$$



i	$a^0(v_i)$	$a^1(v_i)$	…	$a^H(v_i)$
1	0.5	${}^1/_2\left(0.5 + {}^1/_2\,[0.9 * 1138 + 13 * 42]\right) = 392.8$	…	…
2	42	${}^1/_2\left(42 + {}^1/_3\,[13 * 0.5 + 110 * 1138 + 0.25 * 17]\right) = 20886.125$	…	…
3	1138	${}^1/_2\left(1138 + {}^1/_4\,[0.9 * 0.5 + 110 * 42 + 0.9 * 0.5 + 110 * 42]\right) = 1724.1125$	…	…
4	17	${}^1/_2\left(17 + {}^1/_2\,[0.25 * 42 + 7 * 73]\right) = 138.875$	…	…
5	73	${}^1/_2\left(73 + {}^1/_1\,[7 * 17]\right) = 96$	…	…
6	0.5		…	…
7	42		…	…

1.1 Weisfeiler-Lehman node embedding scheme
Example – Attribute labels

$$a^{h+1}(v) = \frac{1}{2}\left(a^h(v) + \frac{1}{\deg(v)} \sum_{u \in N(v)} w((u,v))\, a^h(u)\right)$$

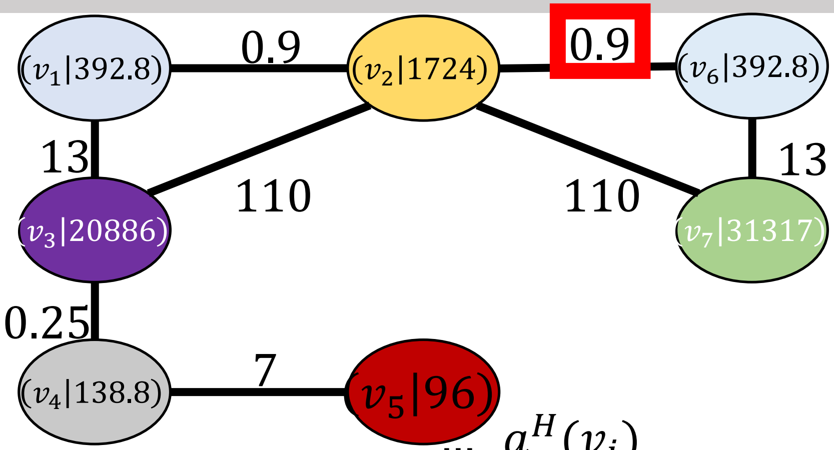


i	$a^0(v_i)$	$a^1(v_i)$	…	$a^H(v_i)$
1	0.5	$^1/_2\left(0.5 + {^1/_2}\,[0.9 * 1138 + 13 * 42]\right) = 392.8$	…	…
2	42	$^1/_2\left(42 + {^1/_3}\,[13 * 0.5 + 110 * 1138 + 0.25 * 17]\right) = 20886.125$	…	…
3	1138	$^1/_2\left(1138 + {^1/_4}\,[0.9 * 0.5 + 110 * 42 + 0.9 * 0.5 + 110 * 42]\right) = 1724.1125$	…	…
4	17	$^1/_2\left(17 + {^1/_2}\,[0.25 * 42 + 7 * 73]\right) = 138.875$	…	…
5	73	$^1/_2\left(73 + {^1/_1}\,[7 * 17]\right) = 96$	…	…
6	0.5	$^1/_2\left(0.5 + {^1/_2}\,[0.9 * 1138 + 13 * 42]\right) = 392.8$	…	…
7	42	$^1/_2\left(42 + {^1/_2}\,[13 * 0.5 + 110 * 1138]\right) = 31317.625$	…	…

1.1 Weisfeiler-Lehman node embedding scheme Example – Attribute labels

UNIVERSITÄT BONN

$$a^{h+1}(v) = \frac{1}{2}\left(a^h(v) + \frac{1}{\deg(v)} \sum_{u \in N(v)} w((u,v))\, a^h(u)\right)$$



i	$a^0(v_i)$	$a^1(v_i)$	…	$a^H(v_i)$
1	0.5	$^1/_2\,(0.5 + {^1/_2}\,[0.9 * 1138 + 13 * 42]) = 392.8$	…	…
2	42	$^1/_2\,(42 + {^1/_3}\,[13 * 0.5 + 110 * 1138 + 0.25 * 17]) = 20886.125$	…	…
3	1138	$^1/_2\,(1138 + {^1/_4}\,[0.9 * 0.5 + 110 * 42 + \boxed{0.9} * 0.5 + 110 * 42]) = 1724.1125$	…	…
4	17	$^1/_2\,(17 + {^1/_2}\,[0.25 * 42 + 7 * 73]) = 138.875$	…	…
5	73	$^1/_2\,(73 + {^1/_1}\,[7 * 17]) = 96$	…	…
6	0.5	$^1/_2\,(0.5 + {^1/_2}\,[\boxed{0.9} * 1138 + 13 * 42]) = 392.8$	…	…
7	42	$^1/_2\,(42 + {^1/_2}\,[13 * 0.5 + 110 * 1138]) = 31317.625$	…	…

2.1 Ground disance between nodes

UNIVERSITÄT BONN

$$\rho(x,y) = \begin{cases} 1 \text{ if } x \neq y \\ 0 \text{ if } x = y \end{cases}$$

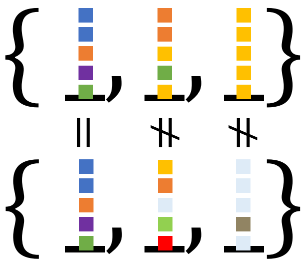
NODE LABELS	NODE ATTRIBUTES
Normalised Hamming distance: $$d_{Ham}(v,v') = \frac{1}{H+1}\sum_{i=1}^{H+1} \rho(v_i, v'_i)$$	Euclidean distance: $$d_E(v,v') = \lVert v - v' \rVert_2$$

$\neq$ 1
$\neq$ 2
$=$
$\neq$ $3 \Longrightarrow d_{Ham} = 3$
$=$

2.1 Ground disance between nodes

$$\rho(x, y) = \begin{cases} 1 \text{ if } x \neq y \\ 0 \text{ if } x = y \end{cases}$$

NODE LABELS	NODE ATTRIBUTES
Normalised Hamming distance: $$d_{Ham}(v, v') = \frac{1}{H+1} \sum_{i=1}^{H+1} \rho(v_i, v'_i)$$	Euclidean distance: $$d_E(v, v') = \lVert v - v' \rVert_2$$



1 2

$\Longrightarrow d_{Ham} = 2$

2.2 Wasserstein distance - L^p

$p \in [1, \infty)$: parameter for the $\boldsymbol{L^p}$ Wasserstein distance

σ, μ: probability distributions on a metric space $\boldsymbol{M}$

$d: \mathbb{R}^m x \mathbb{R}^m \to \mathbb{R}^m$: ground distance (on M)

$\Gamma(\sigma, \mu)$: set of all transportaion plans over MxM (with marginals σ and μ on the first and second factor)

$$W_p(\sigma, \mu) := \left(\lim_{\gamma \in \Gamma(\sigma,\mu)} \int_{MxM} d(x, y)^p \, d\gamma(x, y) \right)^{\frac{1}{p}}$$

2.2 Graph Wasserstein distance

UNIVERSITÄT BONN

$p \in [1, \infty)$: parameter for the $\boldsymbol{L^p}$ Wasserstein distance

$X \in \mathbb{R}^{n \times m}$

$X' \in \mathbb{R}^{n' \times m}$: set of vectors

$M = [d(x,y)]_{x \in X, y \in X'}$: distance matrix on a ground distance

$\Gamma(X, X')$: set of all transportaion plans

$\langle ., . \rangle$: Frobenius dot product

$$W_1(X, X') := \min_{P \in \Gamma(X, X')} \langle P, M \rangle$$

$$G, G' \quad \rightarrowtail f_{WL}^H : G \to \mathbb{R}^{n_G \times m(H+1)} \quad \rightarrowtail \quad D_W^f(G, G') := W_1(f(G), f(G')) = \min_{P \in \Gamma(f(G), f(G'))} \langle P, M \rangle$$

2.2 Graph Wasserstein distance

UNIVERSITÄT BONN

$p \in [1, \infty)$: parameter for the $\boldsymbol{L^p}$ Wasserstein distance

$X \in \mathbb{R}^{n \times m}$

$X' \in \mathbb{R}^{n' \times m}$: set of vectors

$M = [d(x,y)]_{x \in X, y \in X'}$: distance matrix on a ground distance

$\Gamma(X, X')$: set of all transportaion plans

$\langle .,. \rangle$: Frobenius dot product

$$W_1(X, X') := \min_{P \in \Gamma(X, X')} \langle P, M \rangle$$

$$G, G' \quad \rightarrowtail \quad f_{WL}^H : G \to \mathbb{R}^{n_G \times m(H+1)} \quad \rightarrowtail \quad D_W^f(G, G') := W_1(f(G), f(G')) = \min_{P \in \Gamma(f(G), f(G'))} \langle P, M \rangle \quad \rightarrowtail \quad K_{WWL} = e^{-\lambda D_W^{f_{WL}}(G, G')}$$

3 Kernel definition

Experimental evaluation

NODE LABELS	NODE ATTRIBUTES
• **Competitive** with best graph kernel	• **Outperforms** all state-of-the art graph kernels

TODO: summarize tables in pile chart with slack

Sumary

TODO: the whole method only in 3-4 graphics
(graphics from above)

Thank you

for your attention!