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Wasserstein Weisfeiler-Lehman Graph Kernels

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

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Rheinische Friedrich-Wilhelms-Universität Bonn

01.07.2020

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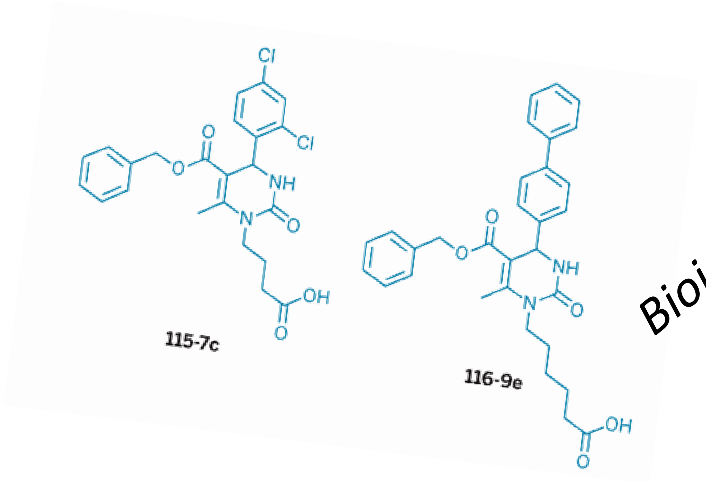
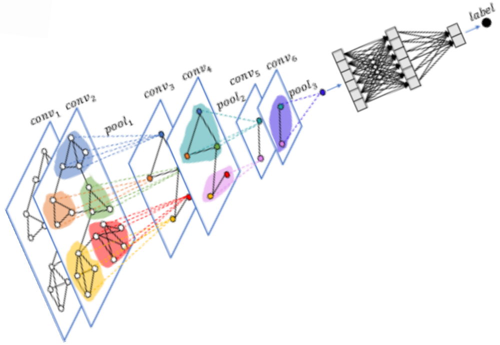
Motivation

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

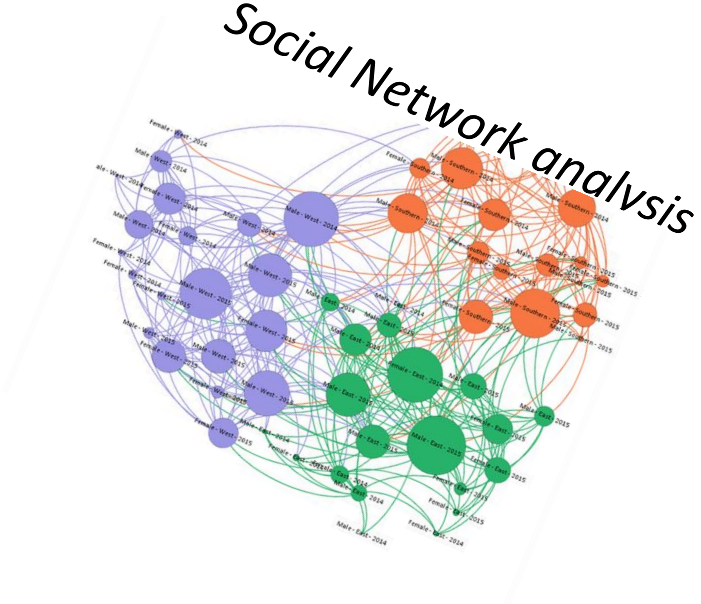


Bioinformatics

Computer vision



Social Network analysis



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

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

Problem: **1.** Naive **aggregation** of **substructures** may disregard valuable information

2. Only a few approaches extendible for **continuously labelled** graphs

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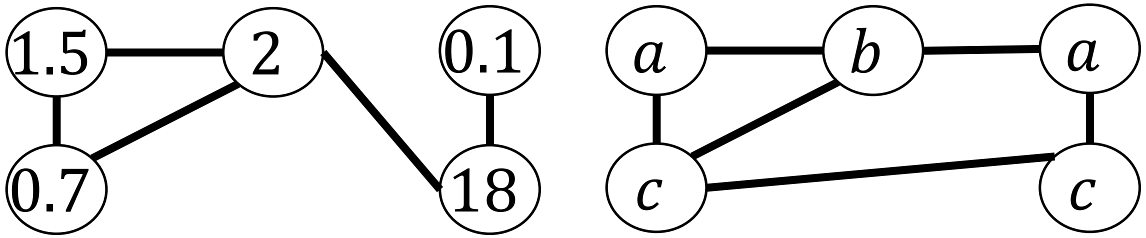
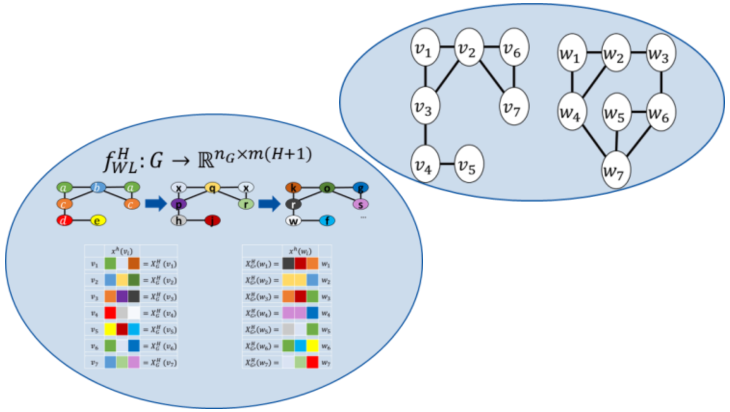


Method Overview



1. Transform each graph into a set of node embeddings
   Weisfeiler-Lehman node embedding scheme
   1. Idea / example
   2. Theory
   3. Example

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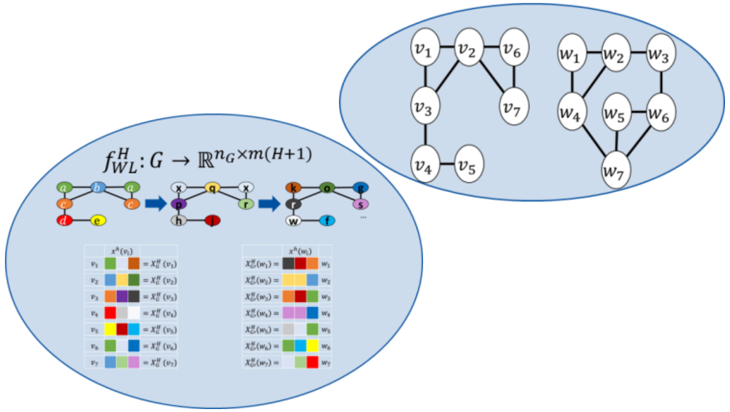
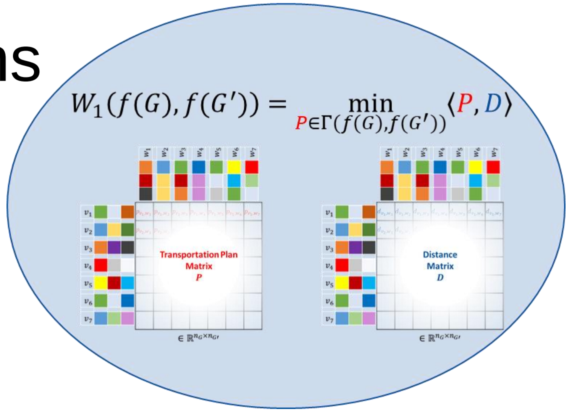


2. Measure the **Wasserstein distance** between each pair of graphs
   1. Transportation plan
   2. Distance measure
   3. Wasserstein distance



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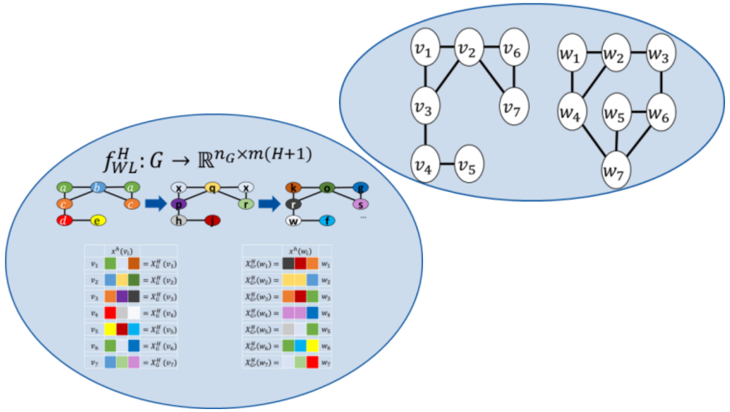

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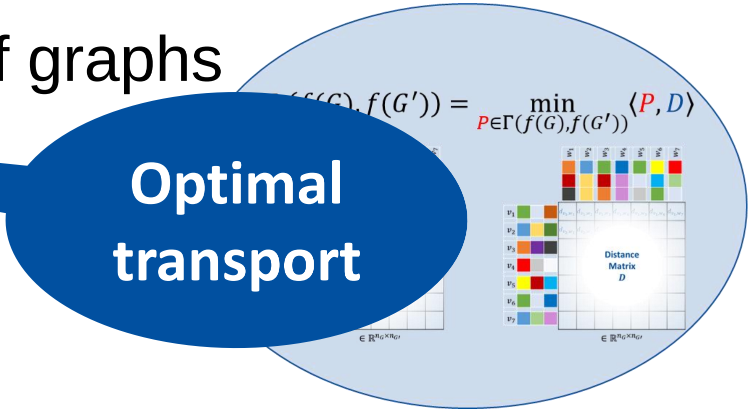

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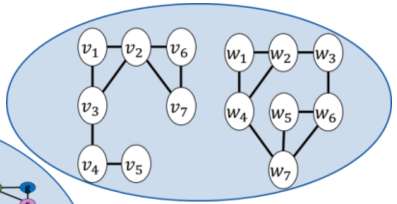

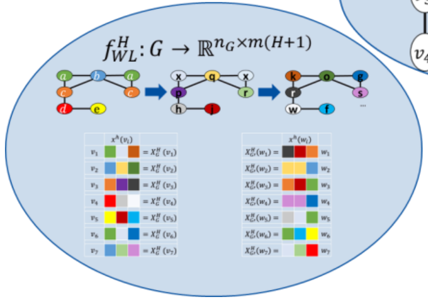

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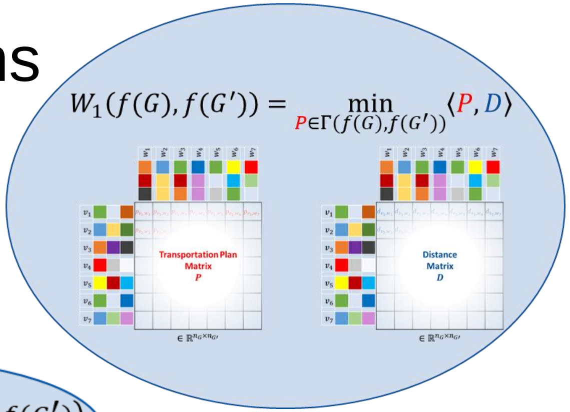

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$$K_{WWL} = e^{-\lambda W_1(f(G), f(G'))}$$

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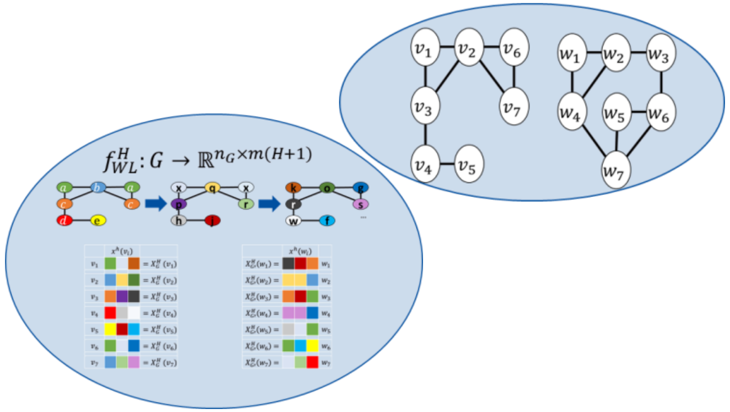

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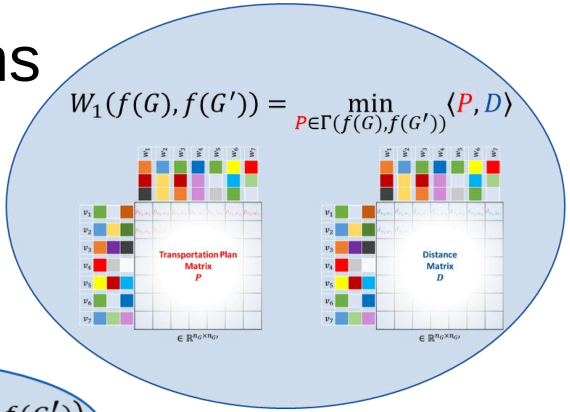

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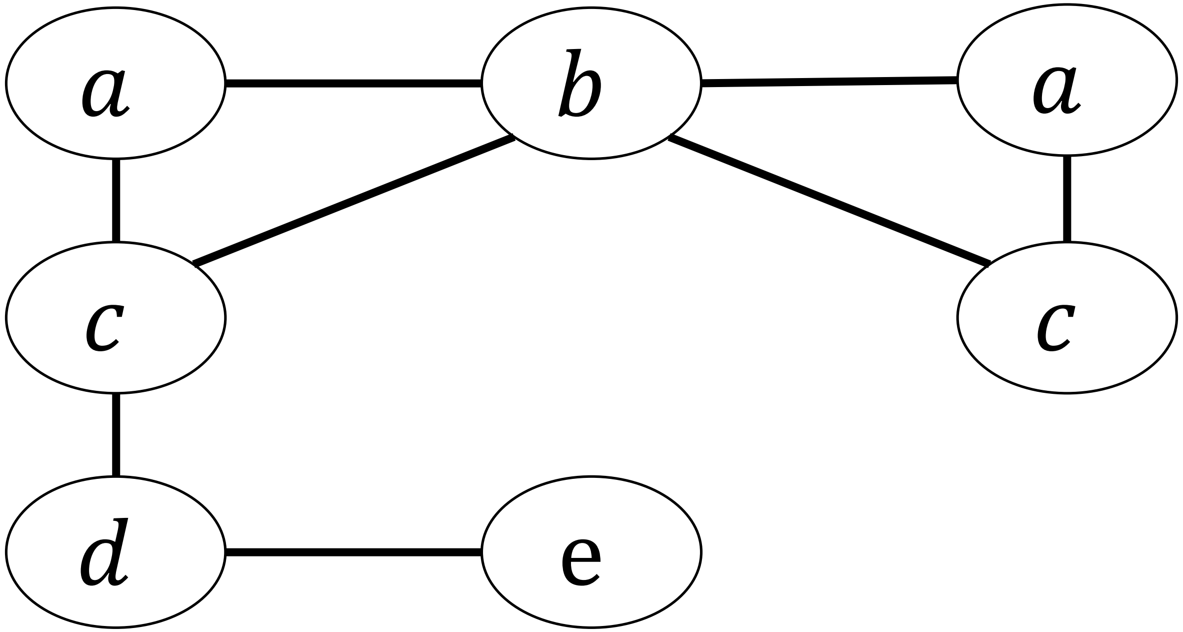
$$K_{WWL} = e^{-\lambda W_1(f(G), f(G'))}$$

(Differentiate between a finite set of **discrete** node labels and **continuously** valued node labels)

1.1 Weisfeiler-Lehman node embedding scheme
Idea



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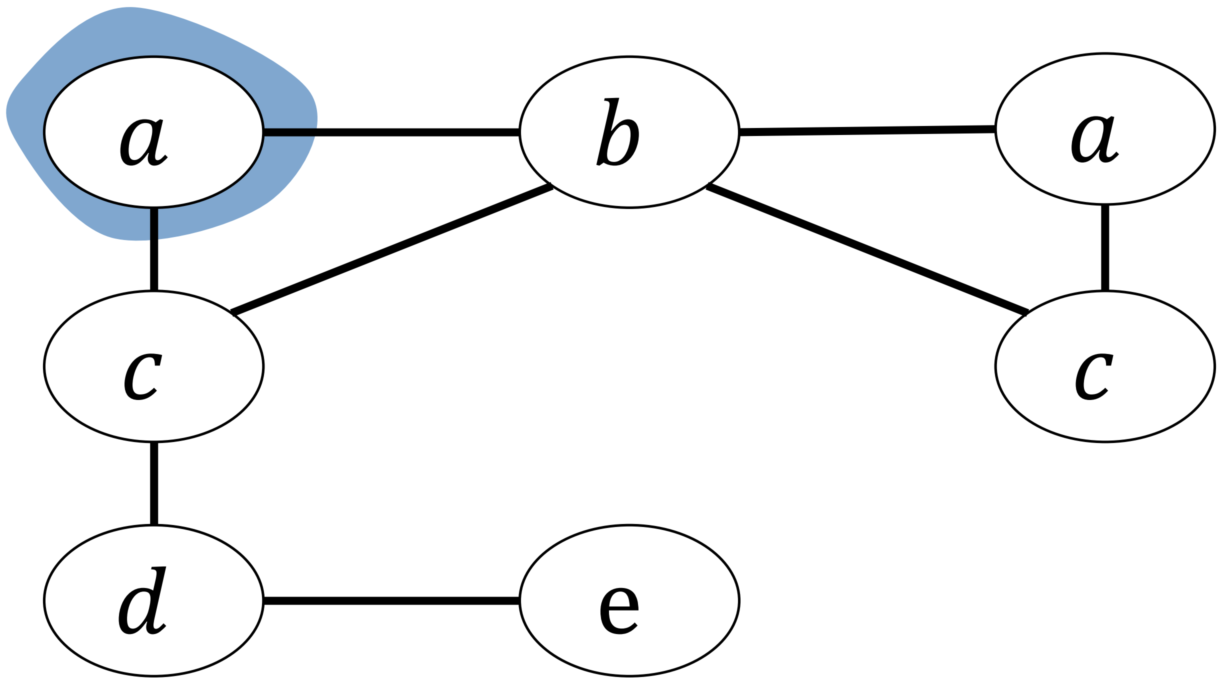

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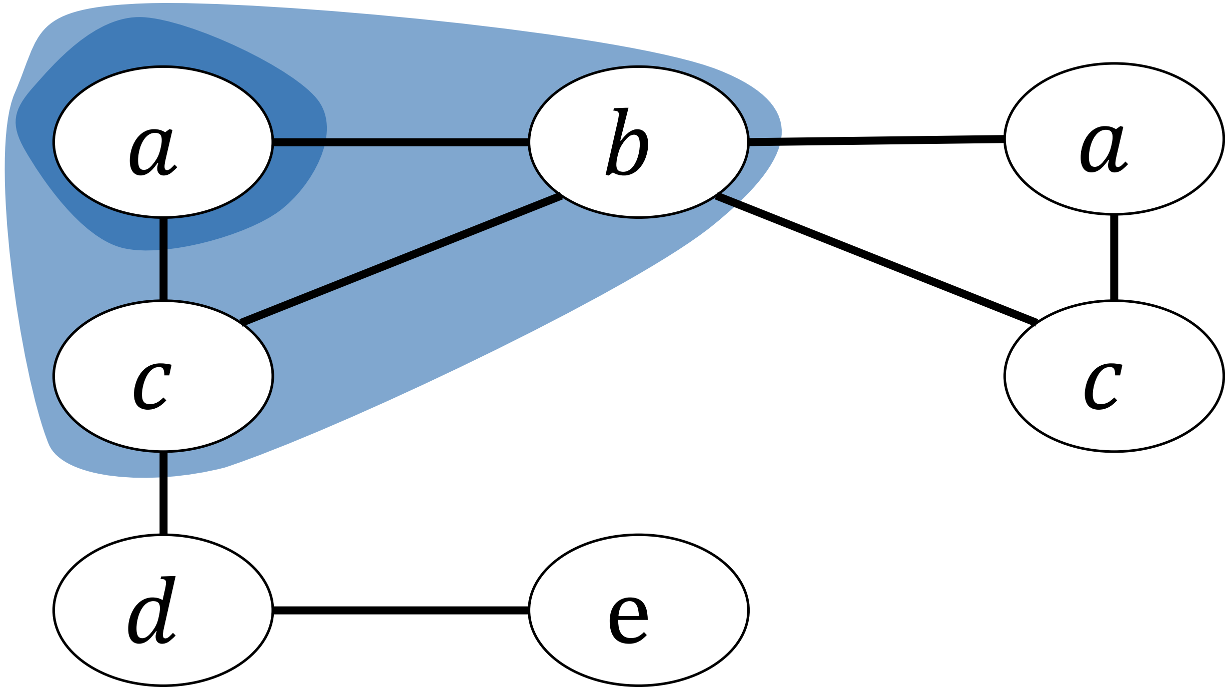

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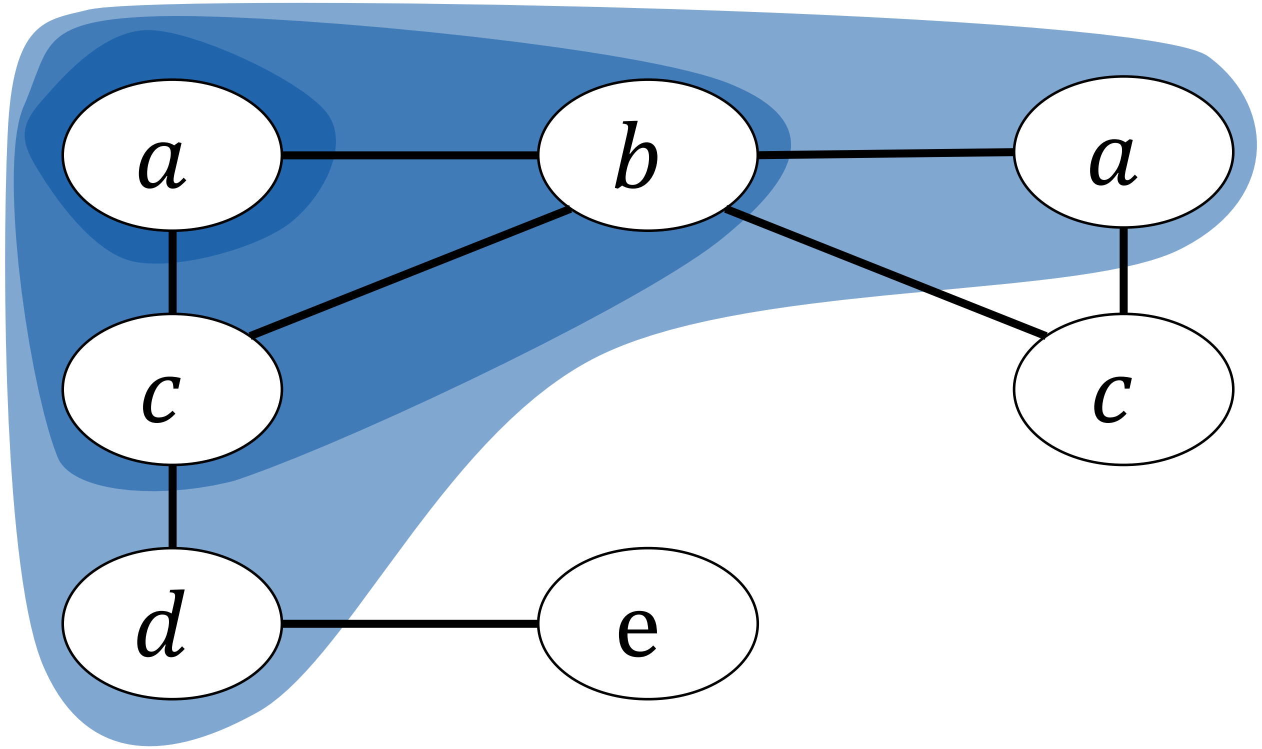

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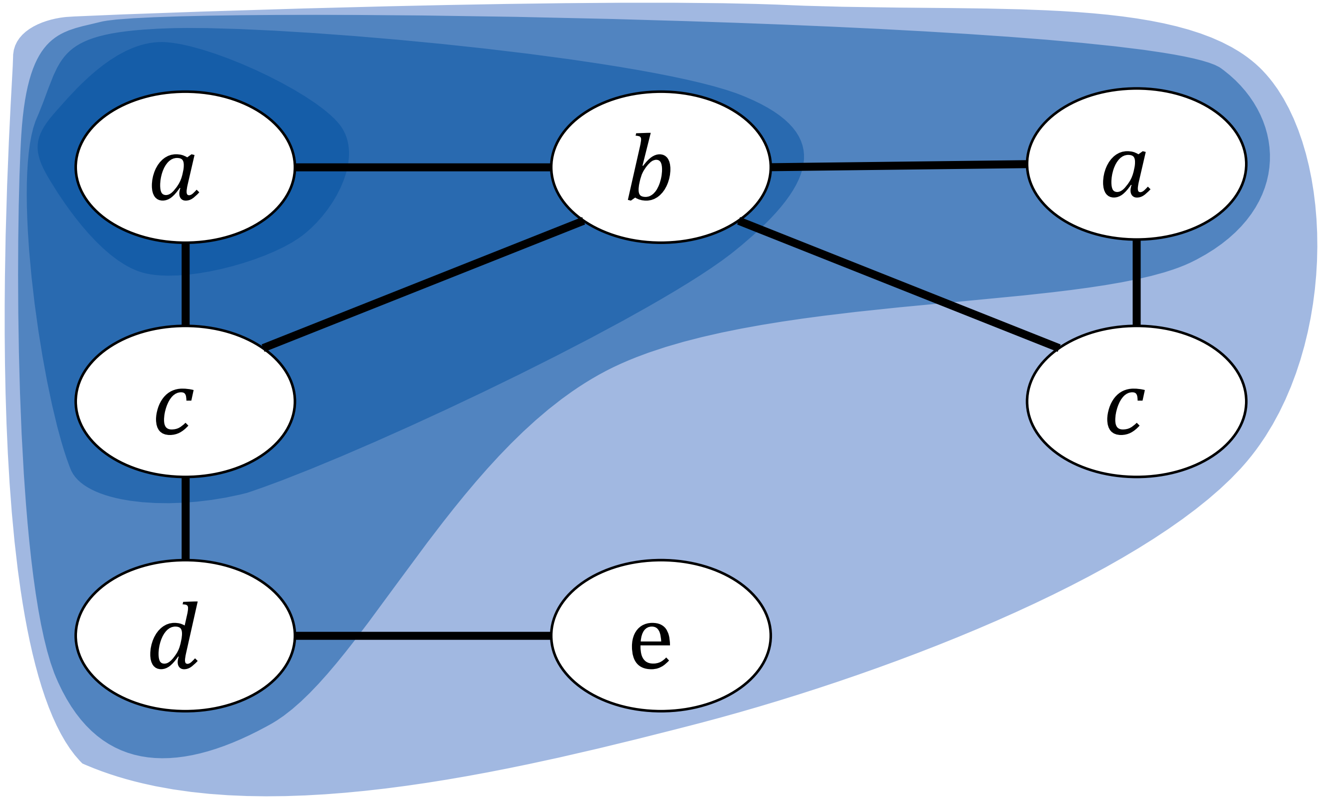

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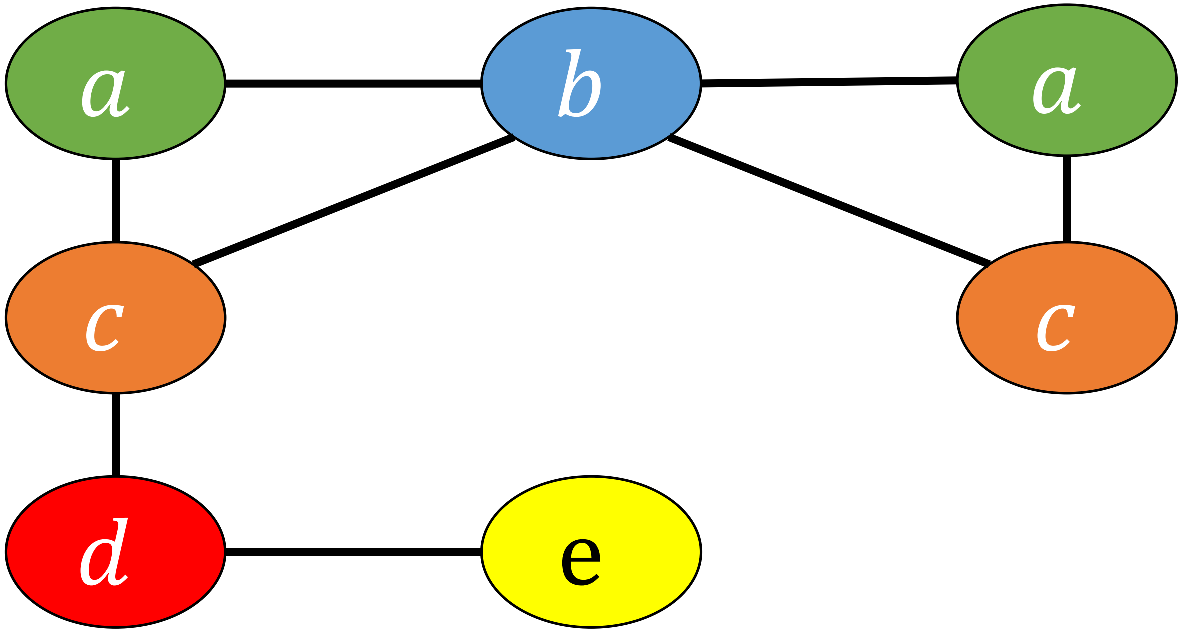

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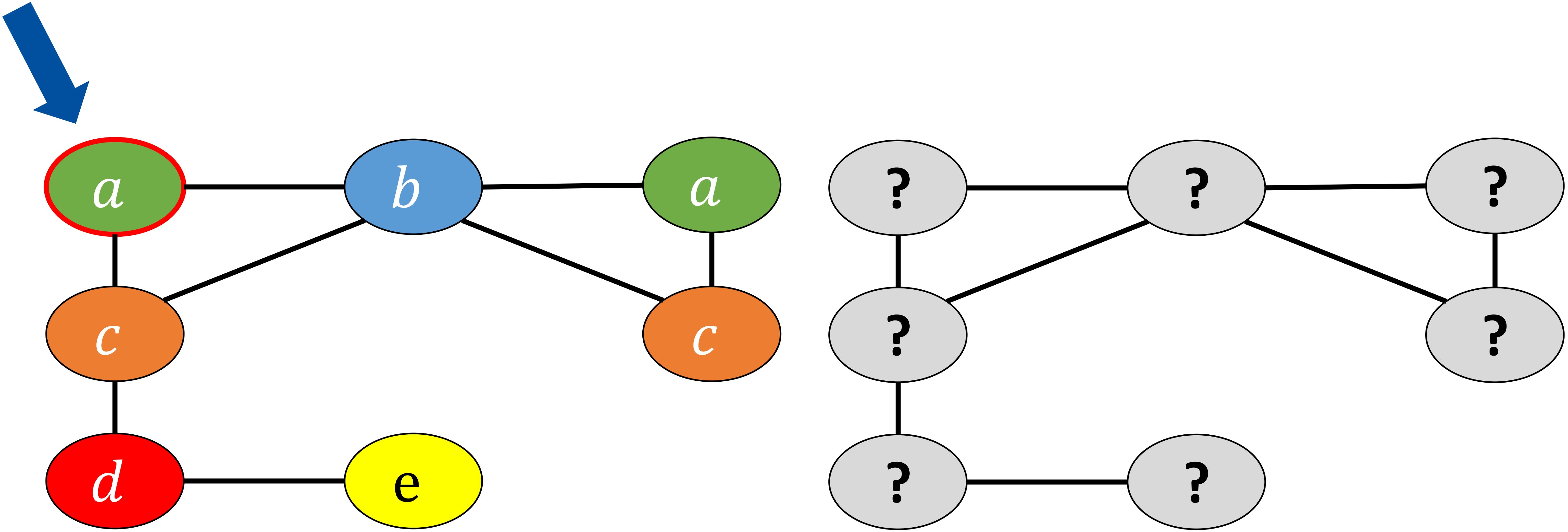

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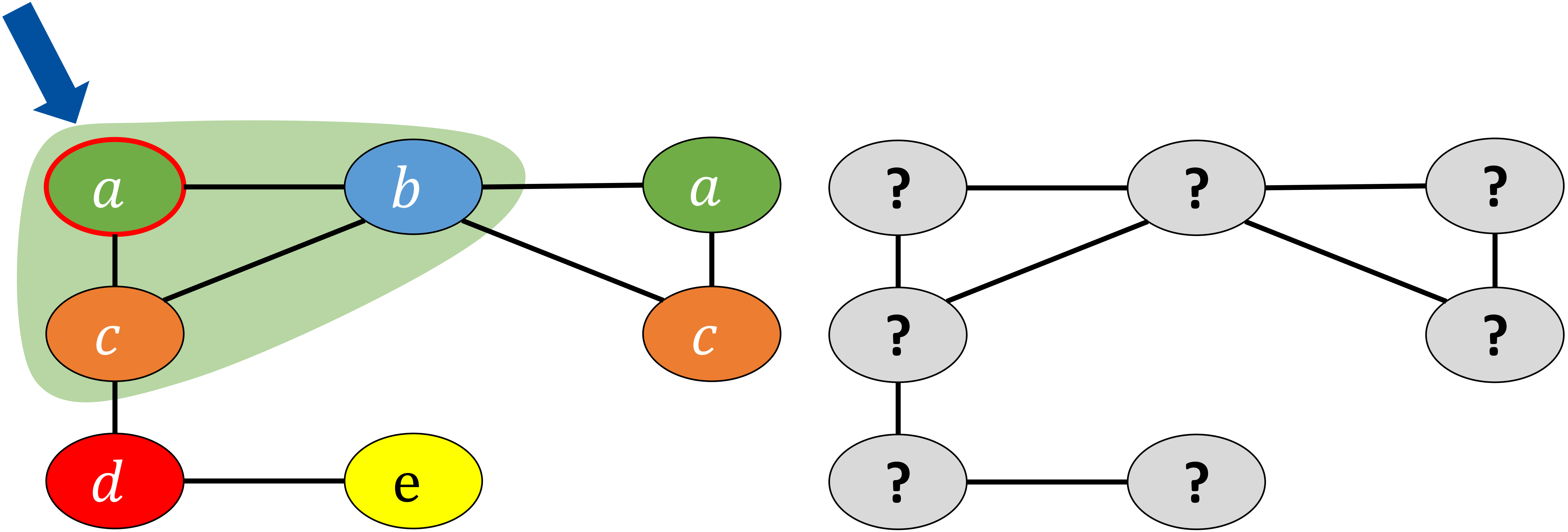

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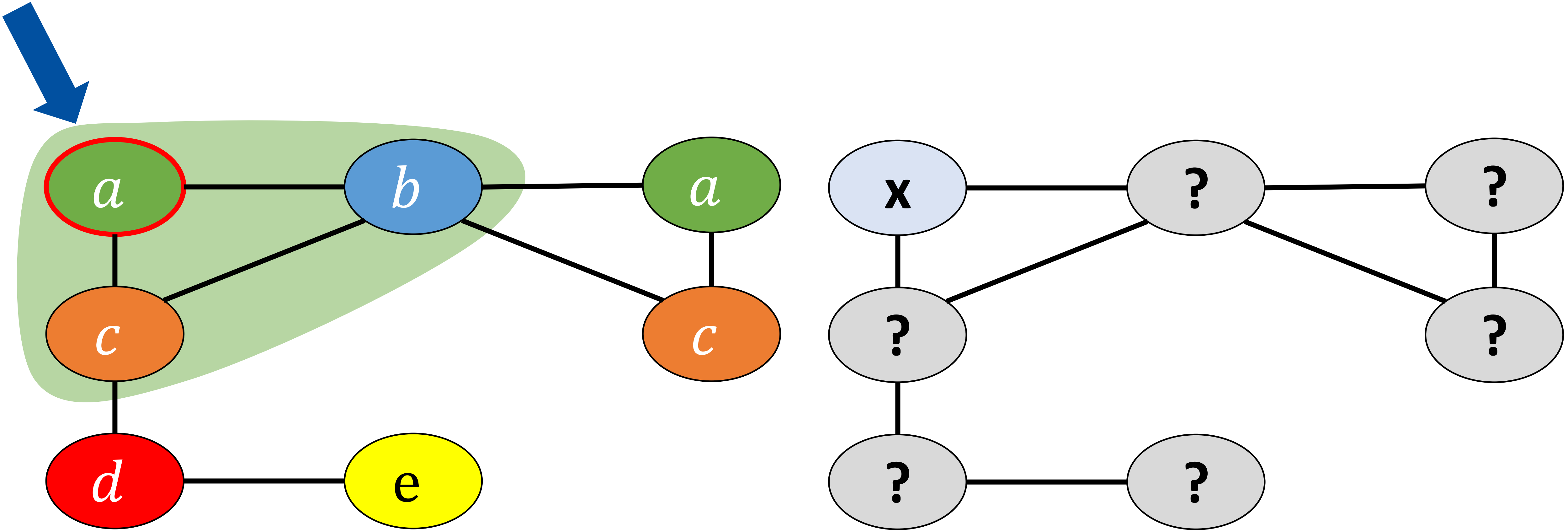

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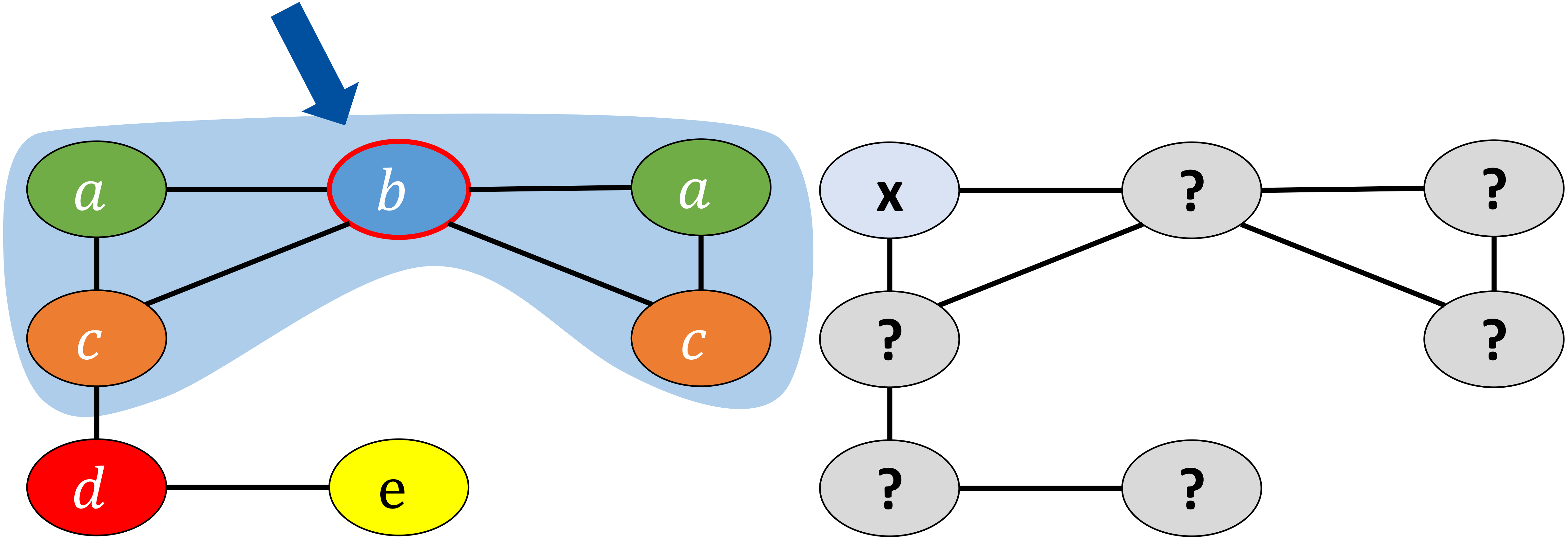

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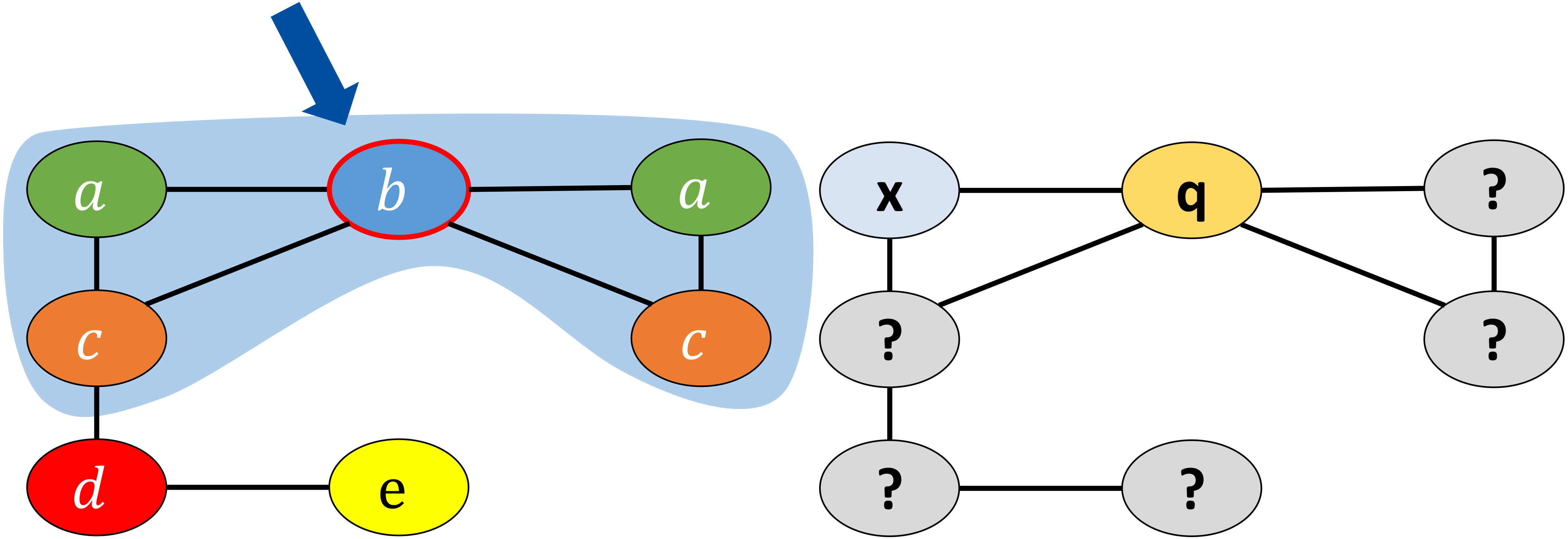

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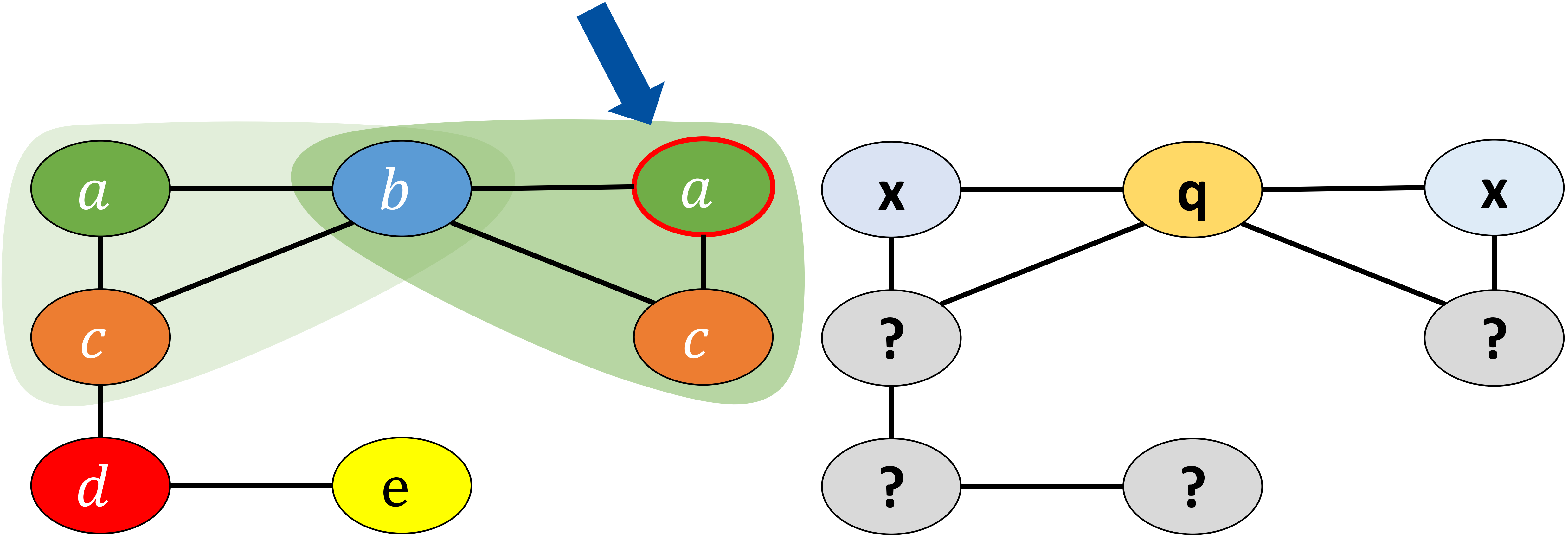

1.1 Weisfeiler-Lehman node embedding scheme Definition

m: dimensionality of the node labels

n_G: cardinality of the node set

$N(v)$: neighbourhood of v

DISCRETE node labels	CONTINUOUS node labels
$x^{h+1}(v) = hash(x^h(v), N^h(v))$	

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DISCRETE node labels	CONTINUOUS node labels
$x^{h+1}(v) = hash(x^h(v), N^h(v))$	$x^{h+1}(v) = \frac{1}{2}\left(x^h(v) + \frac{1}{\deg(v)} \sum_{u \in N(v)} w((u,v))\, x^h(u)\right)$

$(h+1)$-Neighbourhood embedding of v

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Node embedding of v_1

$$X_G^H(v_1) = [x^0(v_1), \dots, x^H(v_1)] \quad \in \mathbb{R}^{m(H+1)}$$

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Node embedding of v_1 $\quad X_G^H(v_1) = [x^0(v_1), \dots, x^H(v_1)] \quad \in \mathbb{R}^{m(H+1)}$

Graph embedding $\quad f^H: G \longrightarrow \left(X_G^H(v_1), \dots, X_G^H(v_{n_G})\right)^T \quad \in \mathbb{R}^{n_G \times m(H+1)}$

1.1 Weisfeiler-Lehman node embedding scheme
Example – Node labels

$m = 1$: dimensionality of the node labels

$n_G = 7$: cardinality of the node set

$N(v)$: neighbourhood of v

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

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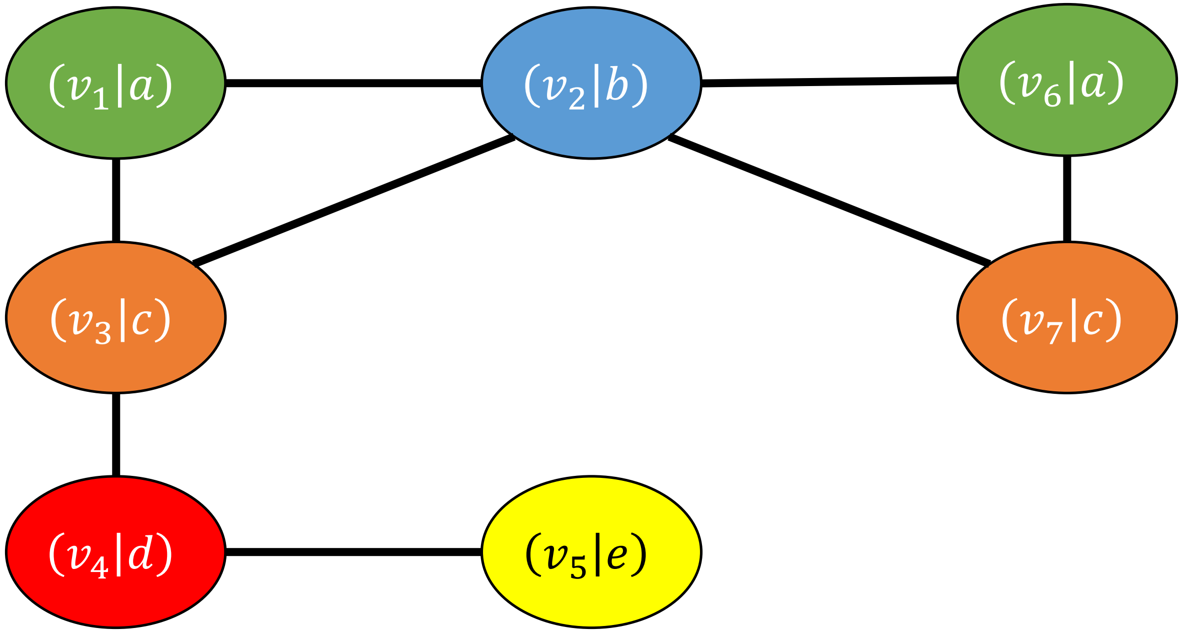

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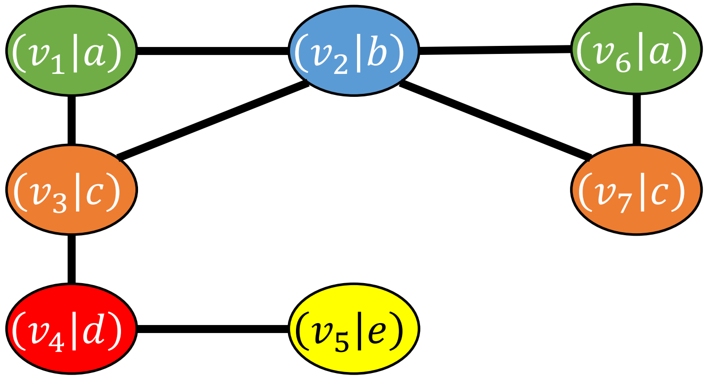

i	$x^0(v_i)$	$x^1(v_i)$	$x^2(v_i)$	…	$x^H(v_i)$
1	a			…	…
2	b			…	…
3	c			…	…
4	d			…	…
5	e			…	…
6	a			…	…
7	c			…	…

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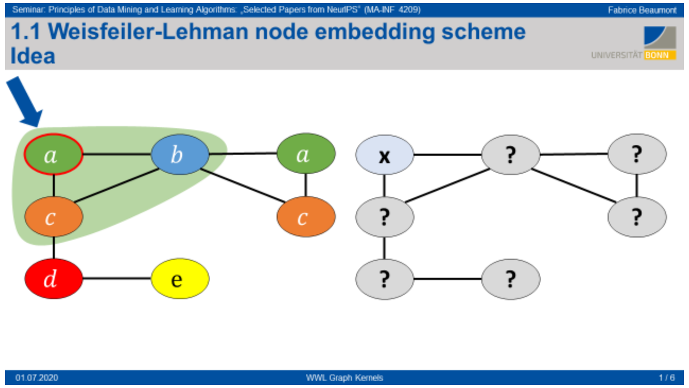

i	$x^0(v_i)$	$x^1(v_i)$	$x^2(v_i)$	…	$x^H(v_i)$
1	a	$\text{hash}(a, \{b, c\}) = x$		…	…
2	b			…	…
3	c			…	…
4	d			…	…
5	e			…	…
6	a			…	…
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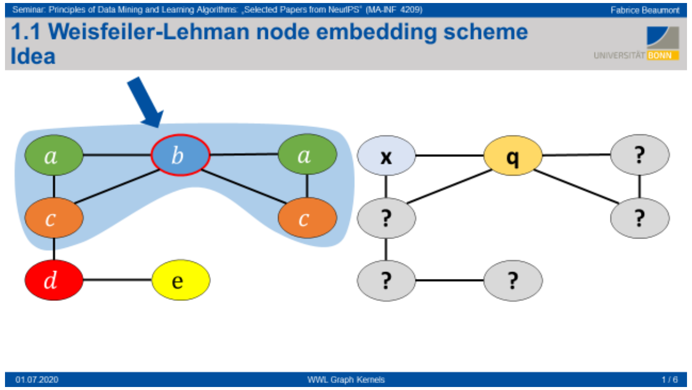

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1	a	hash$(a, \{b, c\}) = x$		…	…
2	b	hash$(b, \{a, c\}) = q$		…	…
3	c			…	…
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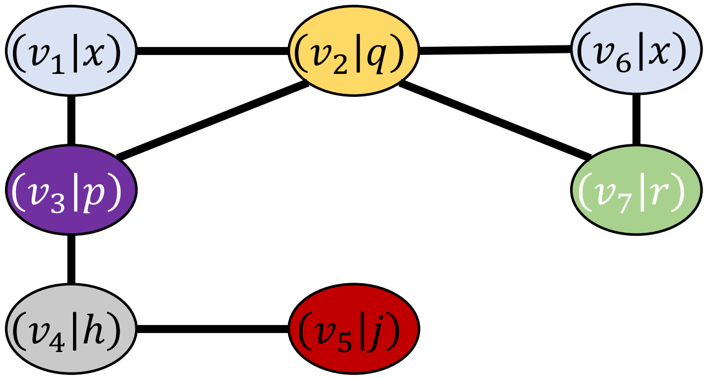

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1	a	hash$(a, \{b, c\}) = x$		…	…
2	b	hash$(b, \{a, c\}) = q$		…	…
3	c	hash$(c, \{a, b, d\}) = p$		…	…
4	d	hash$(d, \{c, e\}) = h$		…	…
5	e	hash$(e, \{d\}) = j$		…	…
6	a	hash$(a, \{b, c\}) = x$		…	…
7	c	hash$(c, \{a, b\}) = r$		…	…

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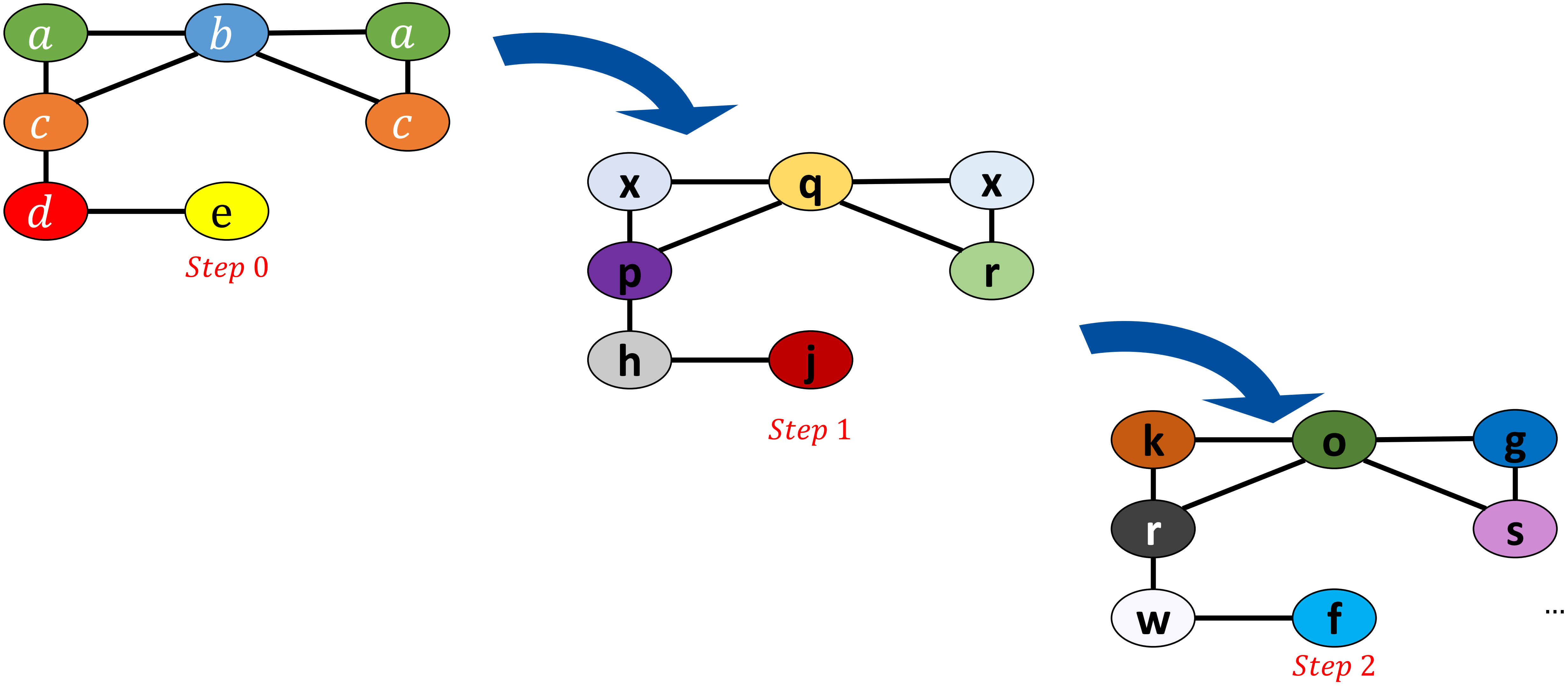

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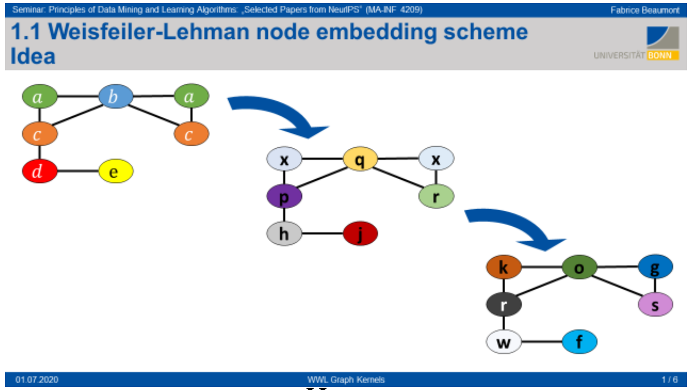

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$$x^{h+1}(v) = hash(x^h(v), N^h(v))$$

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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$(r, \{x, q\}) = s$	…	…

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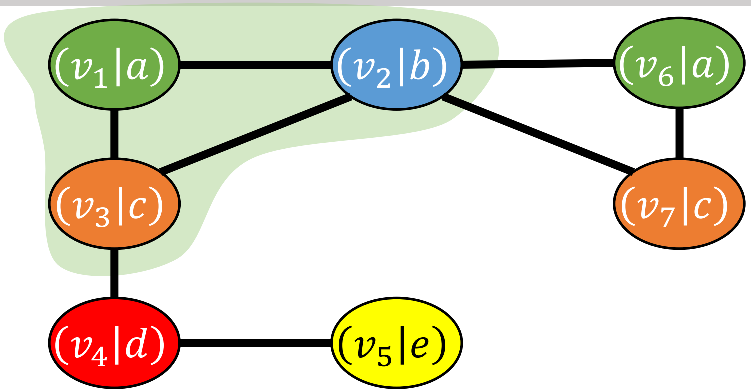

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5	e	$\text{hash}(e, \{d\}) = j$	$\text{hash}(j, \{h\}) = f$	...	...
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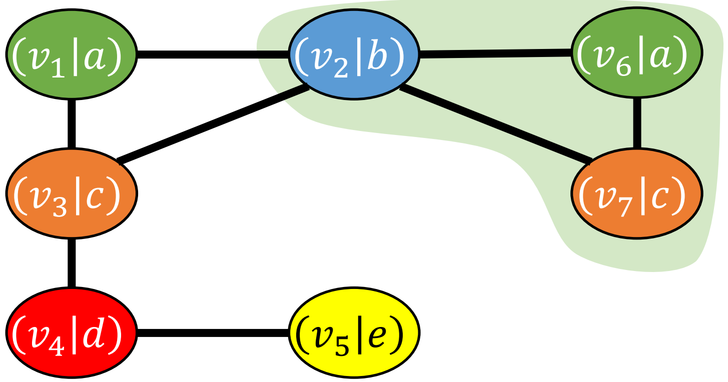

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5	e	$\text{hash}(e, \{d\}) = j$	$\text{hash}(j, \{h\}) = f$	…	…
6	a	$\text{hash}(a, \{b, c\}) = x$	$\text{hash}(x, \{q, r\}) = g$	…	…
7	c	$\text{hash}(c, \{a, b\}) = r$	$\text{hash}(r, \{x, q\}) = s$	…	…

1.1 Weisfeiler-Lehman node embedding scheme Example – Node labels

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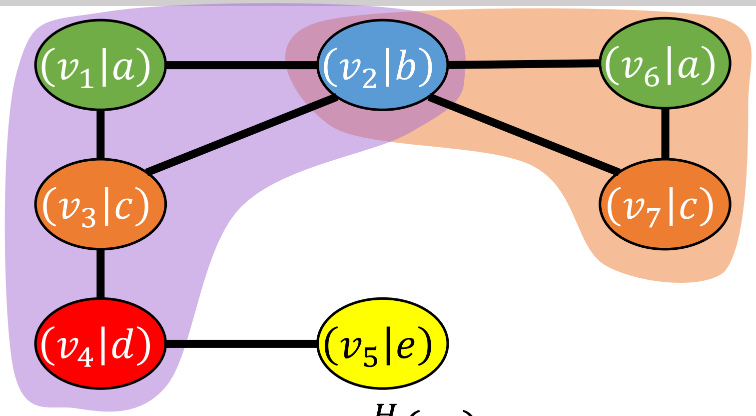
$m = 1$: dimensionality of the node labels

$n_G = 7$: cardinality of the node set

$N(v)$: neighbourhood of v

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



i	$x^0(v_i)$	$x^1(v_i)$	$x^2(v_i)$	…	$x^H(v_i)$
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

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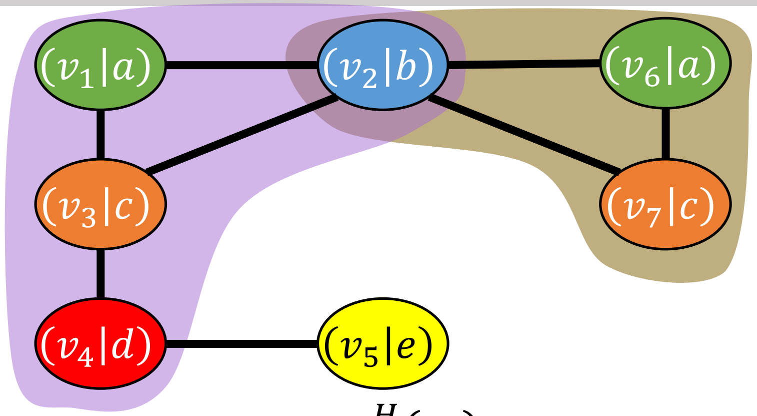

i	$x^0(v_i)$	$x^1(v_i)$	$x^2(v_i)$	…	$x^H(v_i)$
1	a	hash$(a, \{b, c\}) = x$	hash$(x, \{q, \mathbf{p}\}) = \boldsymbol{k}$	…	…
2	b	hash$(b, \{a, c\}) = q$	hash$(q, \{x, p\}) = o$	…	…
3	c	hash$(c, \{a, b, d\}) = p$	hash$(p, \{x, q, h\}) = r$	…	…
4	d	hash$(d, \{c, e\}) = h$	hash$(h, \{p, j\}) = w$	…	…
5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

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

i	$x^0(v_i)$	$x^1(v_i)$	$x^2(v_i)$	…	$x^H(v_i)$	
1	a	$\text{hash}(a, \{b, c\}) = x$	$\text{hash}(x, \{q, p\}) = k$	…	…	$X_G^H(v_1)$
2	b	$\text{hash}(b, \{a, c\}) = q$	$\text{hash}(q, \{x, p\}) = o$	…	…	$X_G^H(v_2)$
3	c	$\text{hash}(c, \{a, b, d\}) = p$	$\text{hash}(p, \{x, q, h\}) = r$	…	…	$X_G^H(v_3)$
4	d	$\text{hash}(d, \{c, e\}) = h$	$\text{hash}(h, \{p, j\}) = w$	…	…	$X_G^H(v_4)$
5	e	$\text{hash}(e, \{d\}) = j$	$\text{hash}(j, \{h\}) = f$	…	…	$X_G^H(v_5)$
6	a	$\text{hash}(a, \{b, c\}) = x$	$\text{hash}(x, \{q, r\}) = g$	…	…	$X_G^H(v_6)$
7	c	$\text{hash}(c, \{a, b\}) = r$	$\text{hash}(r, \{x, q\}) = s$	…	…	$X_G^H(v_7)$

1.1 Weisfeiler-Lehman node embedding scheme Example – Node labels

$m = 1$: dimensionality of the node labels

$n_G = 7$: cardinality of the node set

$N(v)$: neighbourhood of v

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

Graph embedding $\boldsymbol{f^H}(G)$

2^{nd}-Neighbourhood embedding of v

i	$x^0(v_i)$	$x^1(v_i)$	$x^2(v_i)$	…	$x^H(v_i)$	
1	a	hash$(a, \{b, c\}) = x$	hash$(x, \{q, p\}) = k$	…	…	$X_G^H(v_1)$
2	b	hash$(b, \{a, c\}) = q$	hash$(q, \{x, p\}) = o$	…	…	$X_G^H(v_2)$
3	c	hash$(c, \{a, b, d\}) = p$	hash$(p, \{x, q, h\}) = r$	…	…	$X_G^H(v_3)$
4	d	hash$(d, \{c, e\}) = h$	hash$(h, \{p, j\}) = w$	…	…	$X_G^H(v_4)$
5	e	hash$(e, \{d\}) = j$	hash$(j, \{h\}) = f$	…	…	$X_G^H(v_5)$
6	a	hash$(a, \{b, c\}) = x$	hash$(x, \{q, r\}) = g$	…	…	$X_G^H(v_6)$
7	c	hash$(c, \{a, b\}) = r$	hash$(r, \{x, q\}) = s$	…	…	$X_G^H(v_7)$

Node embedding of v_7

Method Overview

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1. Transform each graph into a set of node embeddings

   Weisfeiler-Lehman node embedding scheme

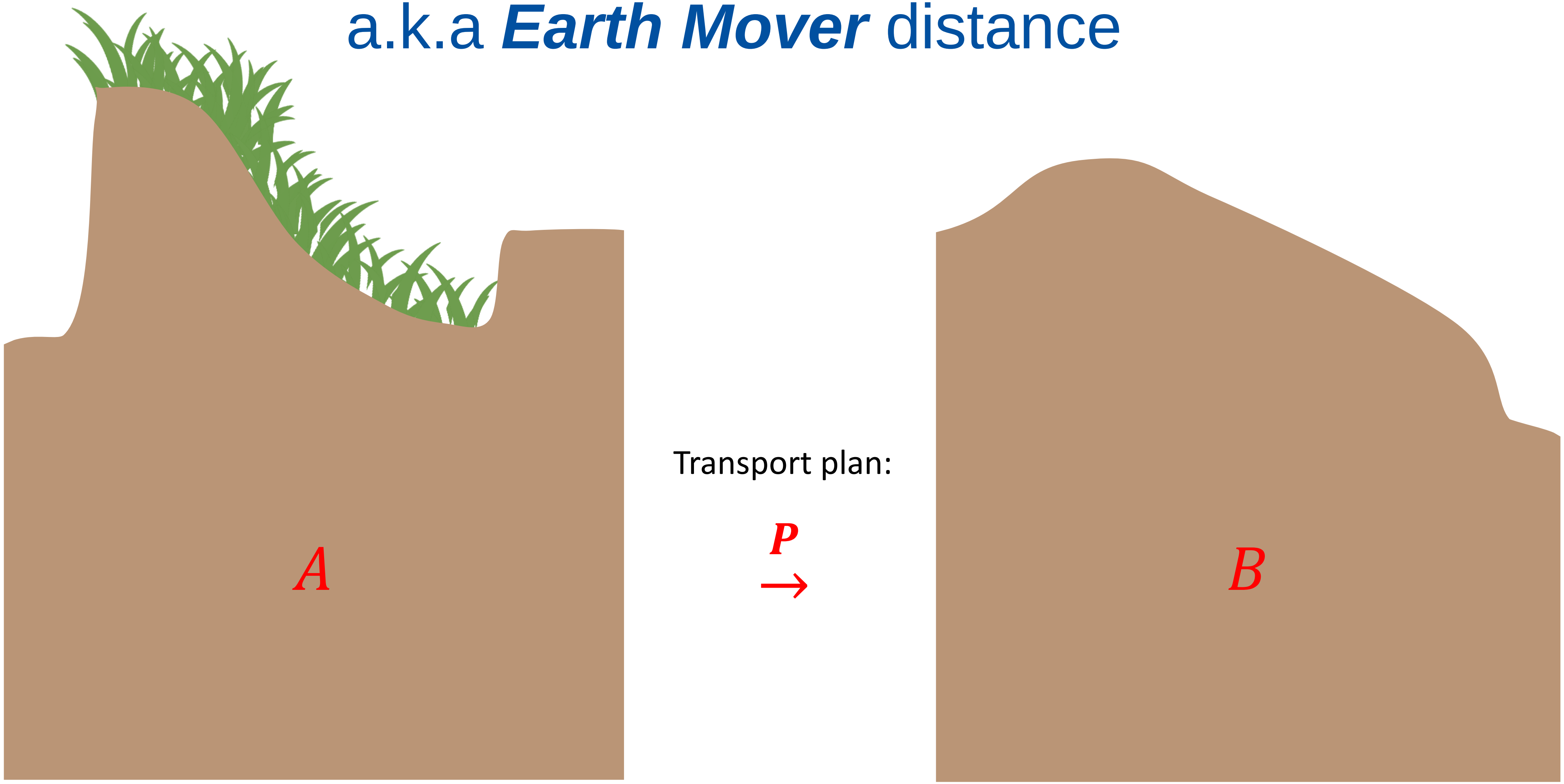
   1. Idea / example
   2. Theory
   3. Example

Method Overview

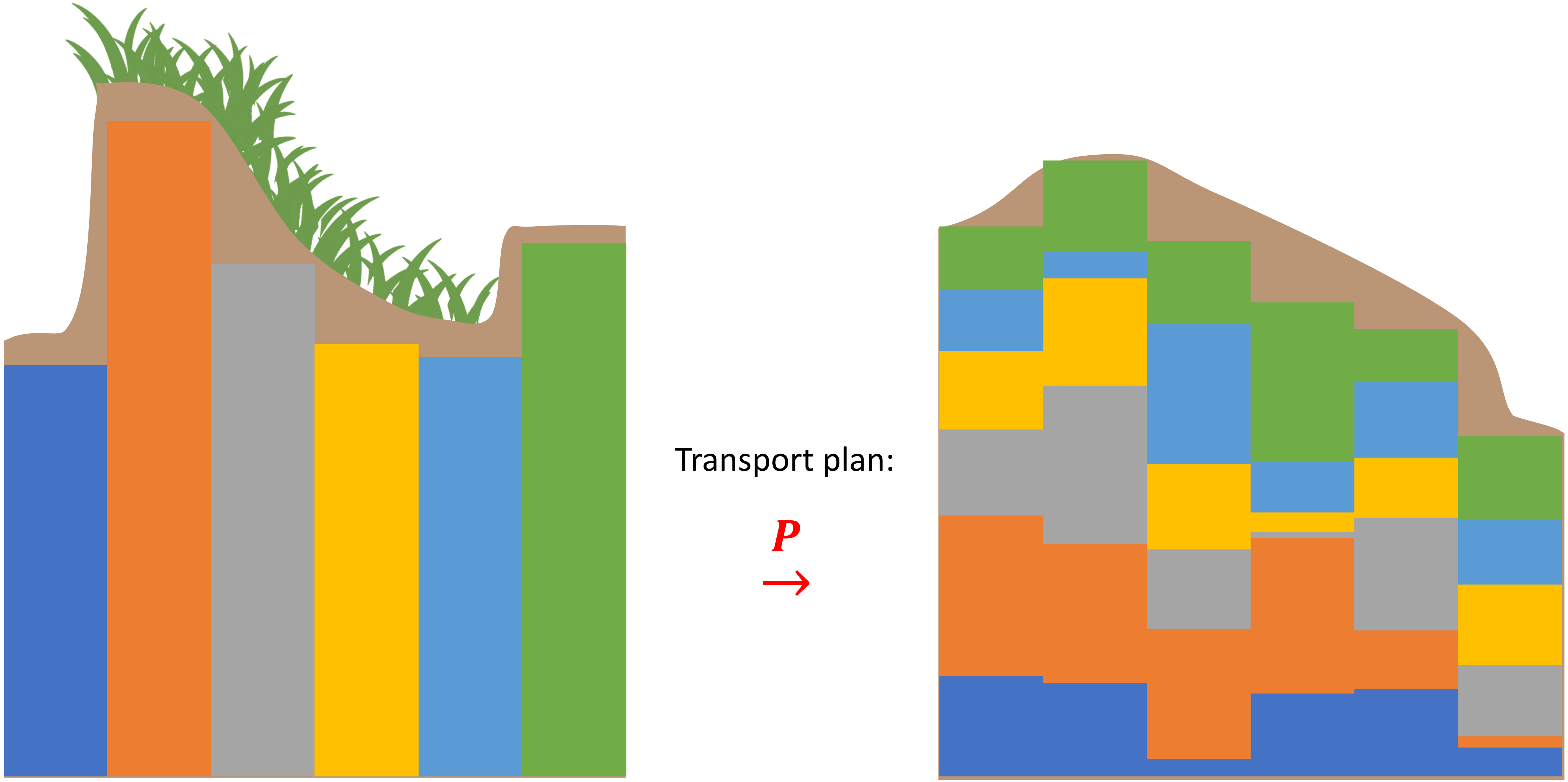
1. Transform each graph into a set of node embeddings
   Weisfeiler-Lehman node embedding scheme
    1. Idea / example
    2. Theory
    3. Example
2. Measure the **Wasserstein distance** between each pair of graphs
    1. Transportation plan
    2. Distance measure
    3. Wasserstein distance

2.2 Graph Wasserstein distance
Motivation

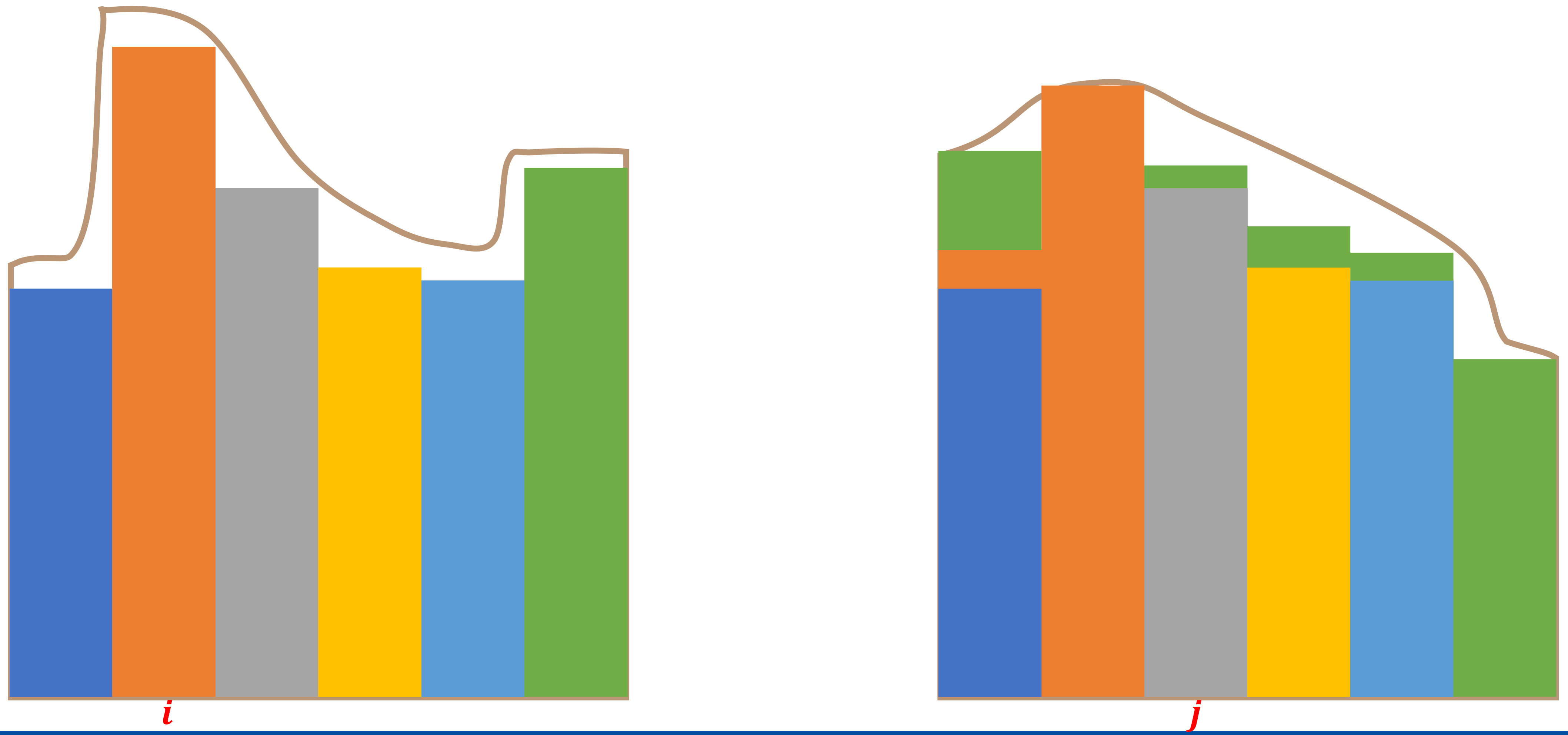
a.k.a ***Earth Mover*** distance



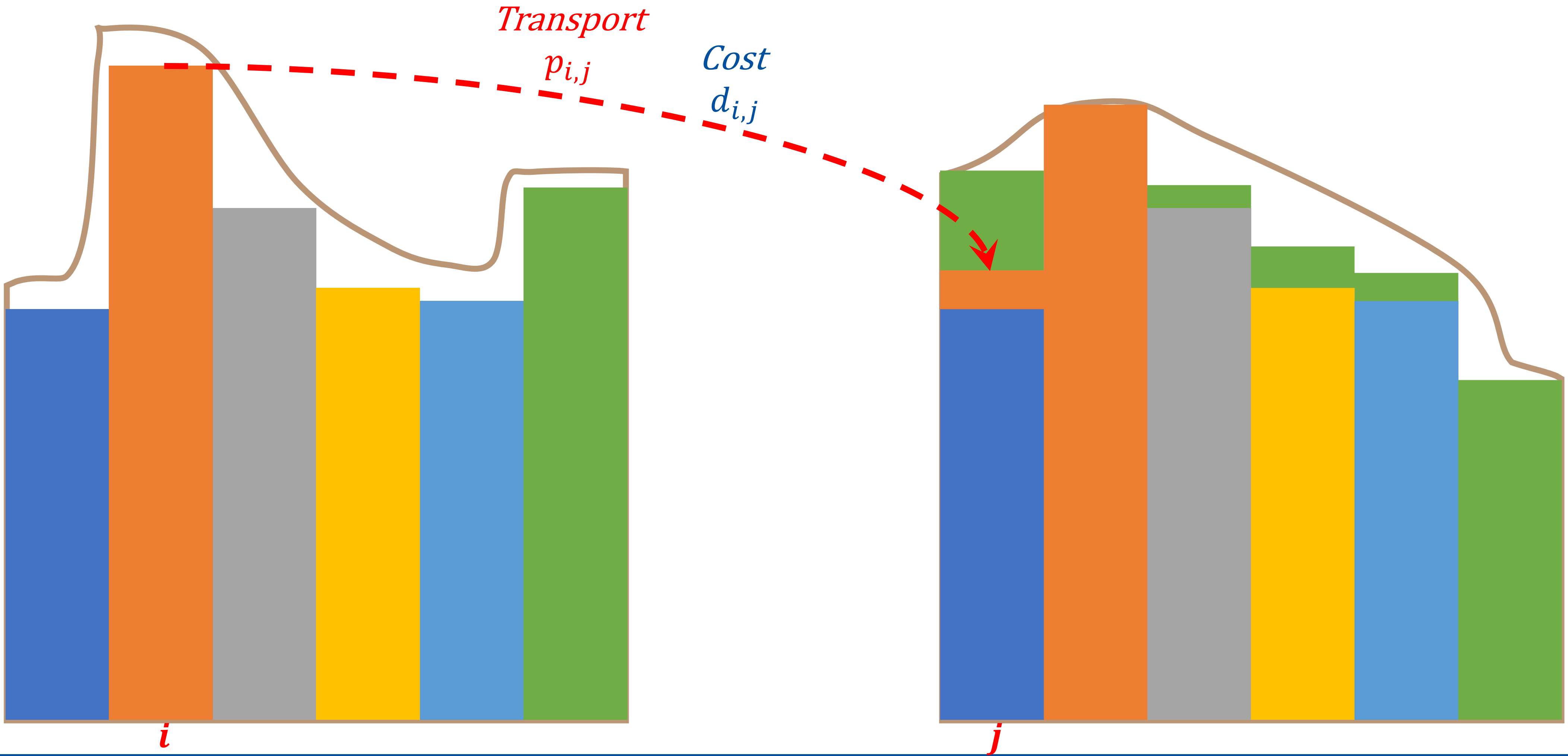
2.2 Graph Wasserstein distance
Motivation



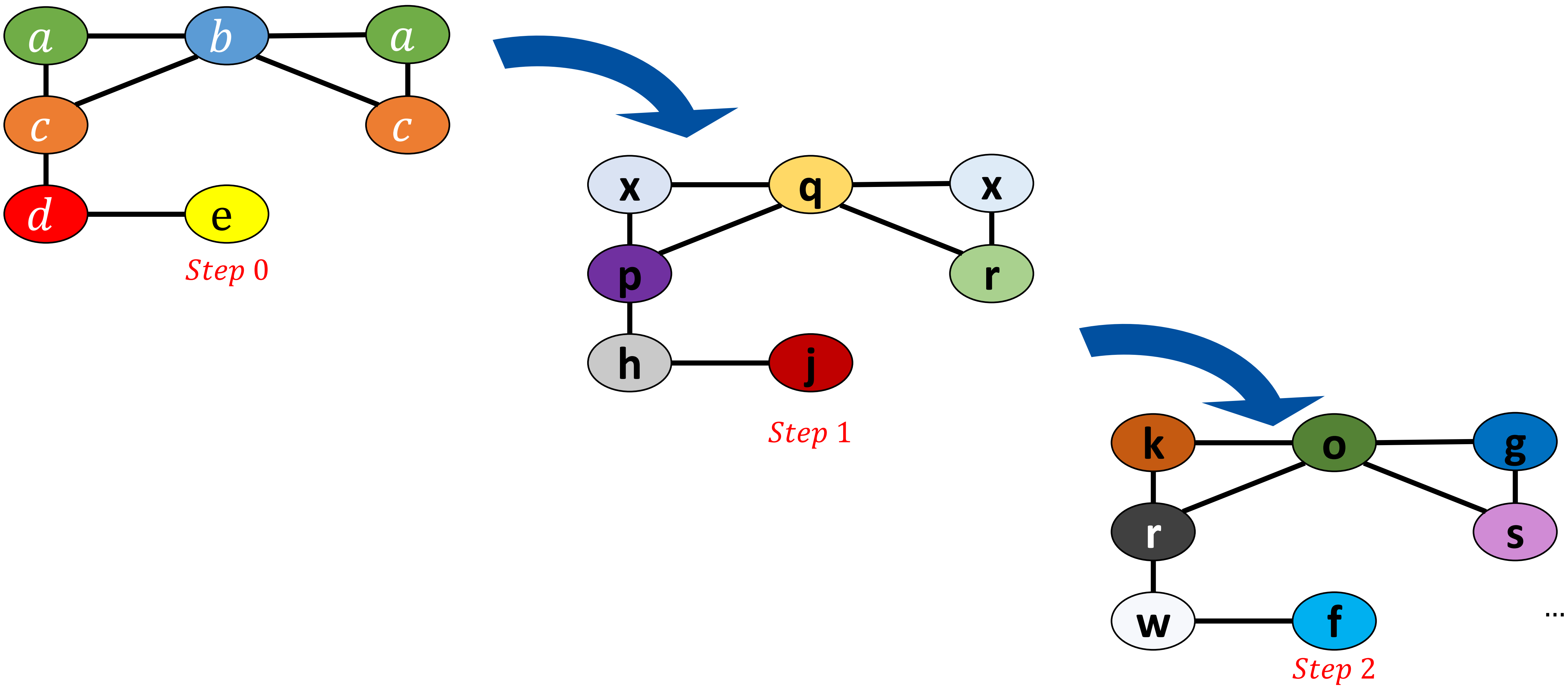
2.2 Graph Wasserstein distance
Motivation



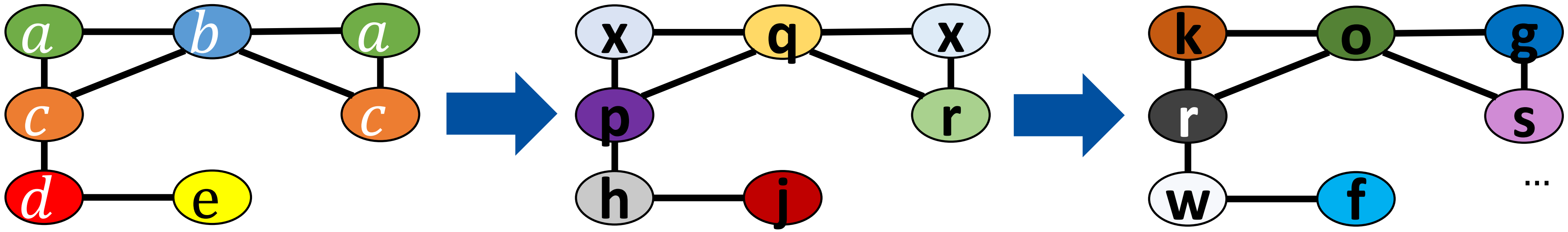
2.2 Graph Wasserstein distance
Motivation

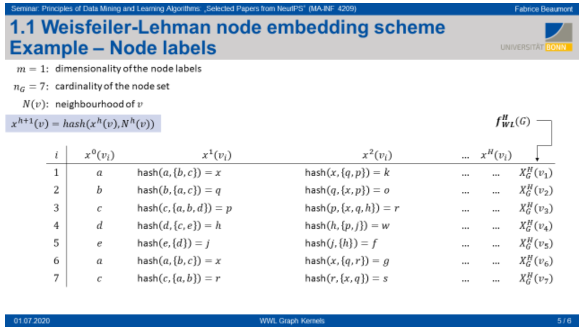


2.2 Graph Wasserstein distance
Idea



2.2 Graph Wasserstein distance
Idea




Seminar: Principles of Data Mining and Learning Algorithms: „Selected Papers from NeurIPS“ (MA-INF 4209) Fabrice Beaumont

1.1 Weisfeiler-Lehman node embedding scheme
Example – Node labels

$m = 1$: dimensionality of the node labels

$n_G = 7$: cardinality of the node set

$N(v)$: neighbourhood of v

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

$f^H_{WL}(G)$

i	$x^0(v_i)$	$x^1(v_i)$	$x^2(v_i)$	...	$x^H(v_i)$	
1	a	$\text{hash}(a, \{b, c\}) = x$	$\text{hash}(x, \{q, p\}) = k$	...	...	$X_G^H(v_1)$
2	b	$\text{hash}(b, \{a, c\}) = q$	$\text{hash}(q, \{x, p\}) = o$	...	...	$X_G^H(v_2)$
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5	e	$\text{hash}(e, \{d\}) = j$	$\text{hash}(j, \{h\}) = f$	...	...	$X_G^H(v_5)$
6	a	$\text{hash}(a, \{b, c\}) = x$	$\text{hash}(x, \{q, r\}) = g$	...	...	$X_G^H(v_6)$
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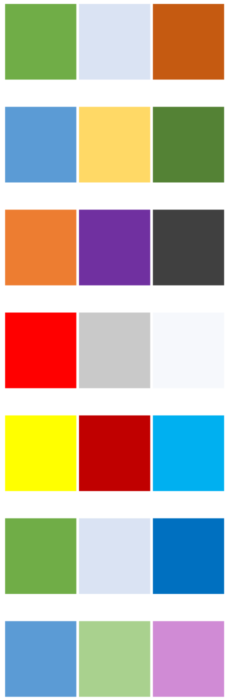
01.07.2020 WWL Graph Kernels 5 / 6

$(H = 2)$

$x^h(v_i)$



$v_1 \; = X_G^H\,(v_1)$

$v_2 \; = X_G^H\,(v_2)$

$v_3 \; = X_G^H\,(v_3)$

$v_4 \; = X_G^H\,(v_4)$

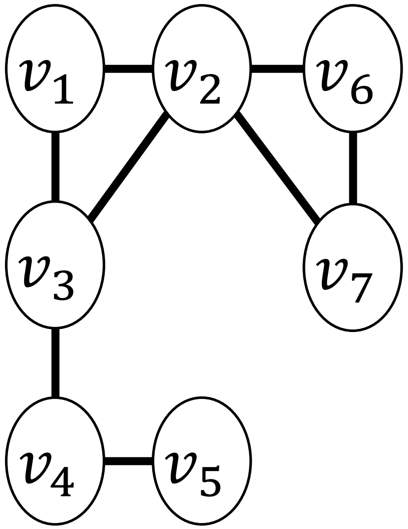
$v_5 \; = X_G^H\,(v_5)$

$v_6 \; = X_G^H\,(v_6)$

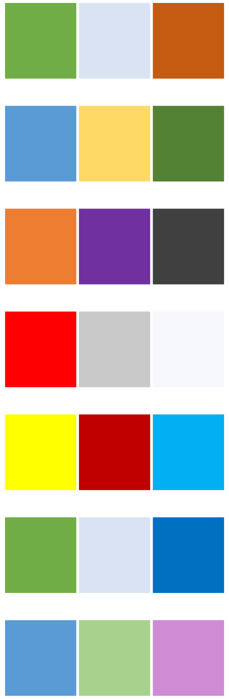
$v_7 \; = X_G^H\,(v_7)$

2.2 Graph Wasserstein distance
Idea

G



$x^h(v_i)$



$v_1 \quad = X_G^H\ (v_1)$

$v_2 \quad = X_G^H\ (v_2)$

$v_3 \quad = X_G^H\ (v_3)$

$v_4 \quad = X_G^H\ (v_4)$

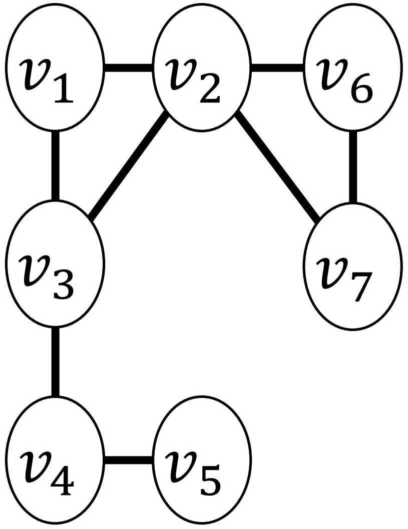
$v_5 \quad = X_G^H\ (v_5)$

$v_6 \quad = X_G^H\ (v_6)$

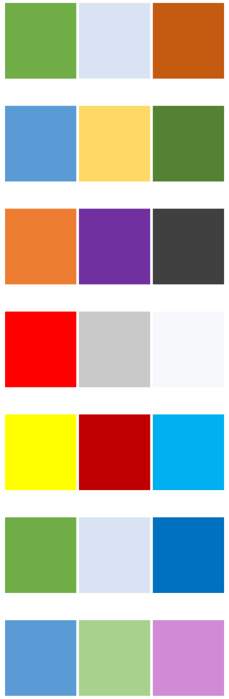
$v_7 \quad = X_G^H\ (v_7)$

2.2 Graph Wasserstein distance
Idea

G



$x^h(v_i)$



$v_1 \quad = X_G^H(v_1)$

$v_2 \quad = X_G^H(v_2)$

$v_3 \quad = X_G^H(v_3)$

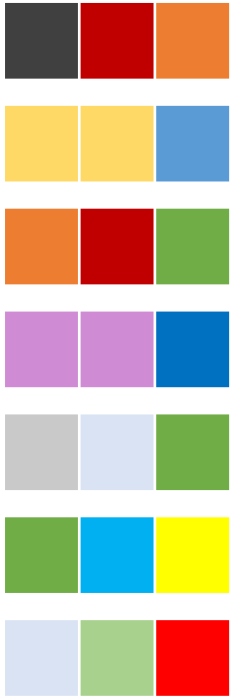
$v_4 \quad = X_G^H(v_4)$

$v_5 \quad = X_G^H(v_5)$

$v_6 \quad = X_G^H(v_6)$

$v_7 \quad = X_G^H(v_7)$

$x^h(w_i)$



$X_{G'}^H(w_1) = \quad w_1$

$X_{G'}^H(w_2) = \quad w_2$

$X_{G'}^H(w_3) = \quad w_3$

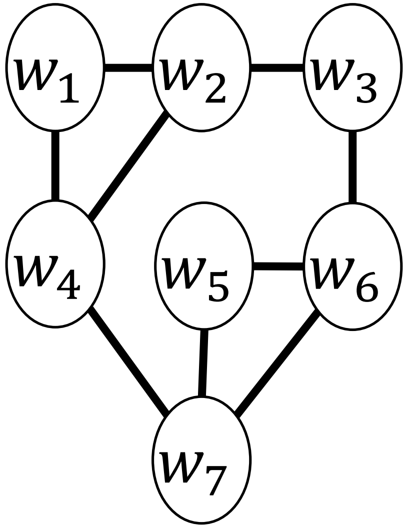
$X_{G'}^H(w_4) = \quad w_4$

$X_{G'}^H(w_5) = \quad w_5$

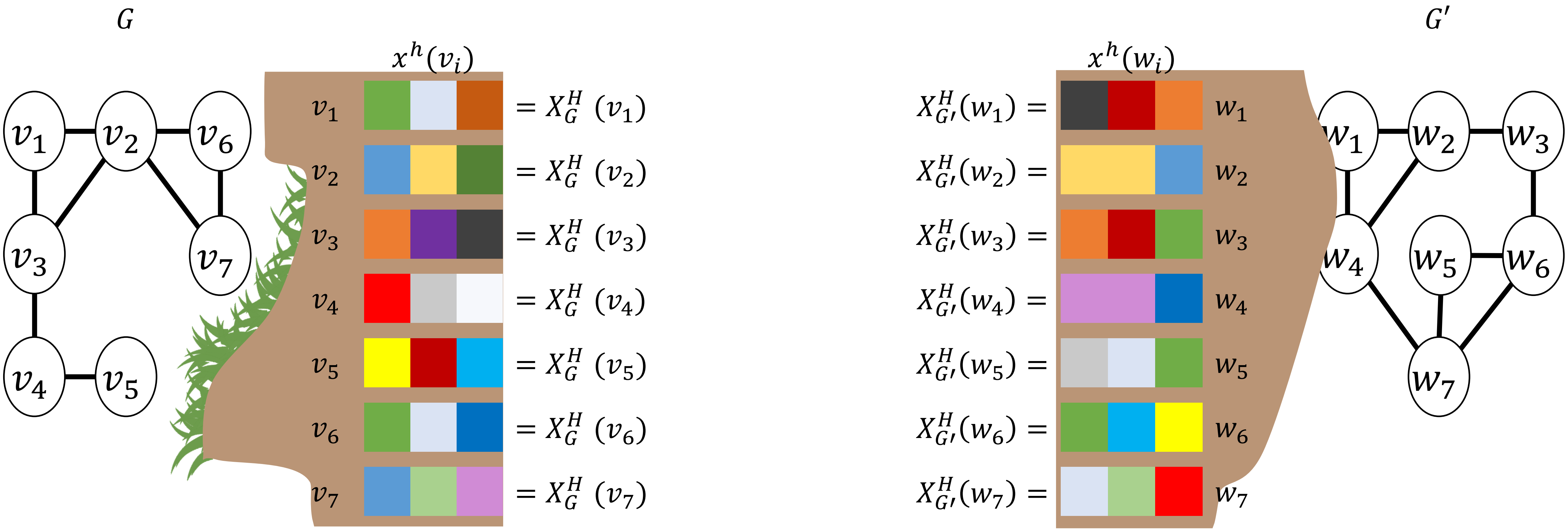
$X_{G'}^H(w_6) = \quad w_6$

$X_{G'}^H(w_7) = \quad w_7$

G'

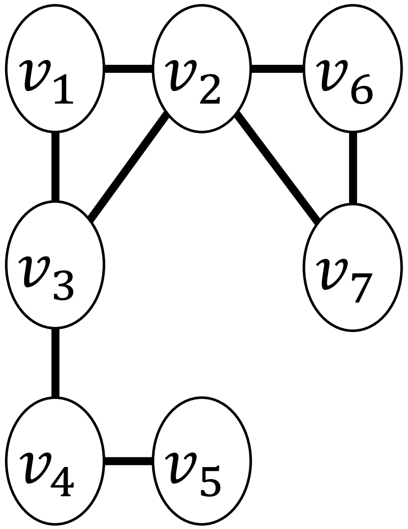


2.2 Graph Wasserstein distance
Idea

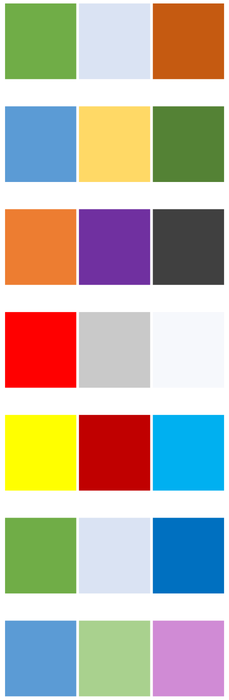


2.2 Graph Wasserstein distance
Transportation plan

G



$x^h(v_i)$



$v_1 = X_G^H(v_1)$

$v_2 = X_G^H(v_2)$

$v_3 = X_G^H(v_3)$

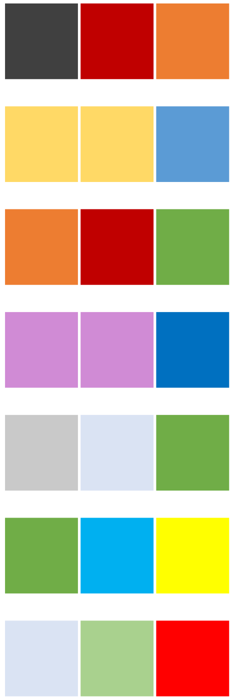
$v_4 = X_G^H(v_4)$

$v_5 = X_G^H(v_5)$

$v_6 = X_G^H(v_6)$

$v_7 = X_G^H(v_7)$

$x^h(w_i)$



$X_{G'}^H(w_1) = \; w_1$

$X_{G'}^H(w_2) = \; w_2$

$X_{G'}^H(w_3) = \; w_3$

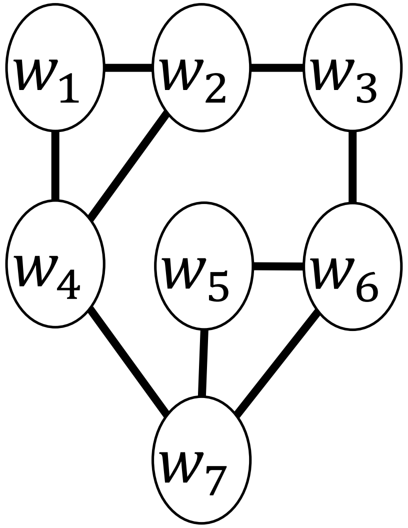
$X_{G'}^H(w_4) = \; w_4$

$X_{G'}^H(w_5) = \; w_5$

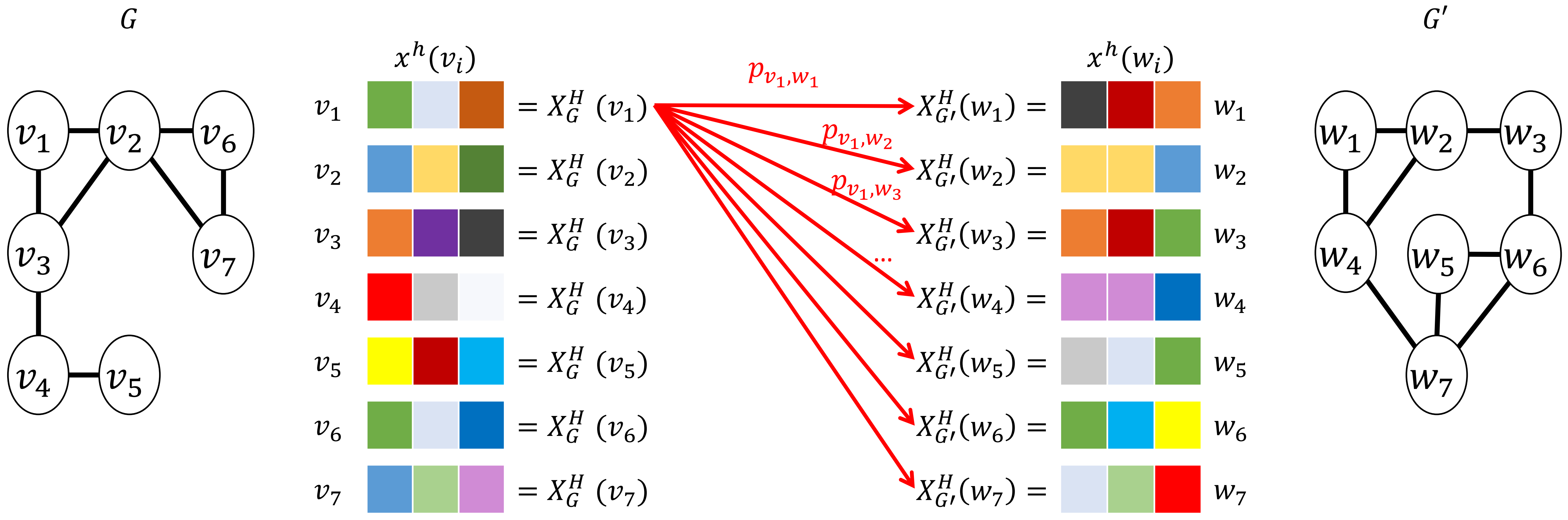
$X_{G'}^H(w_6) = \; w_6$

$X_{G'}^H(w_7) = \; w_7$

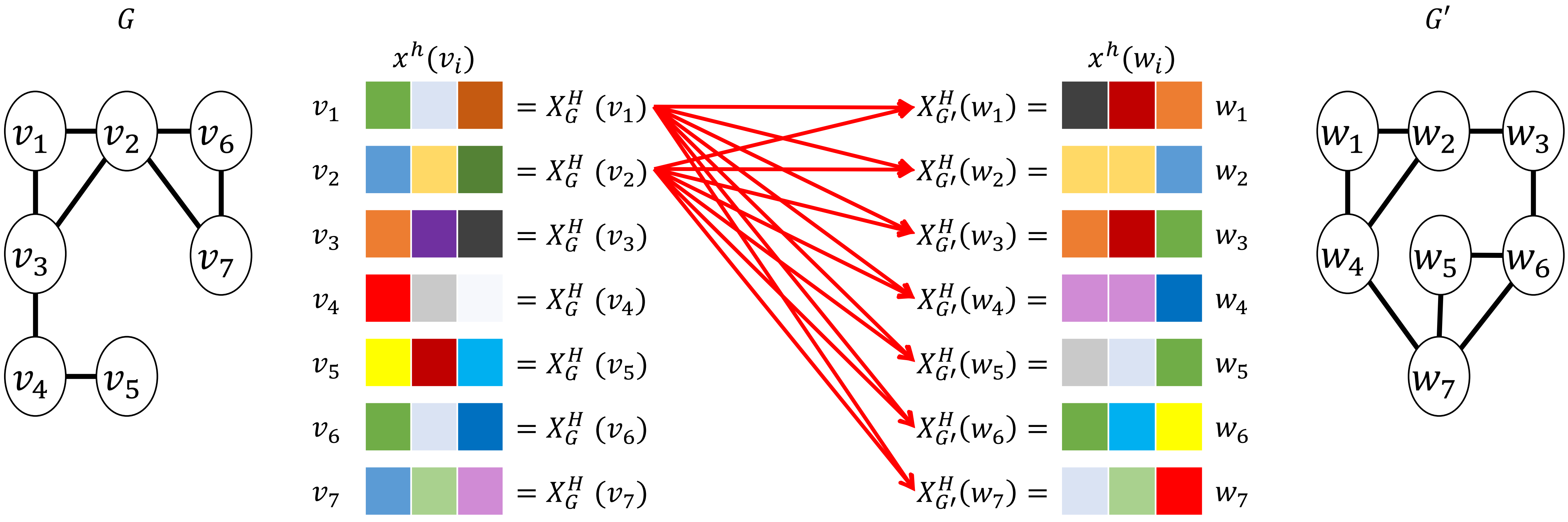
G'



2.2 Graph Wasserstein distance
Transportation plan



2.2 Graph Wasserstein distance
Transportation plan



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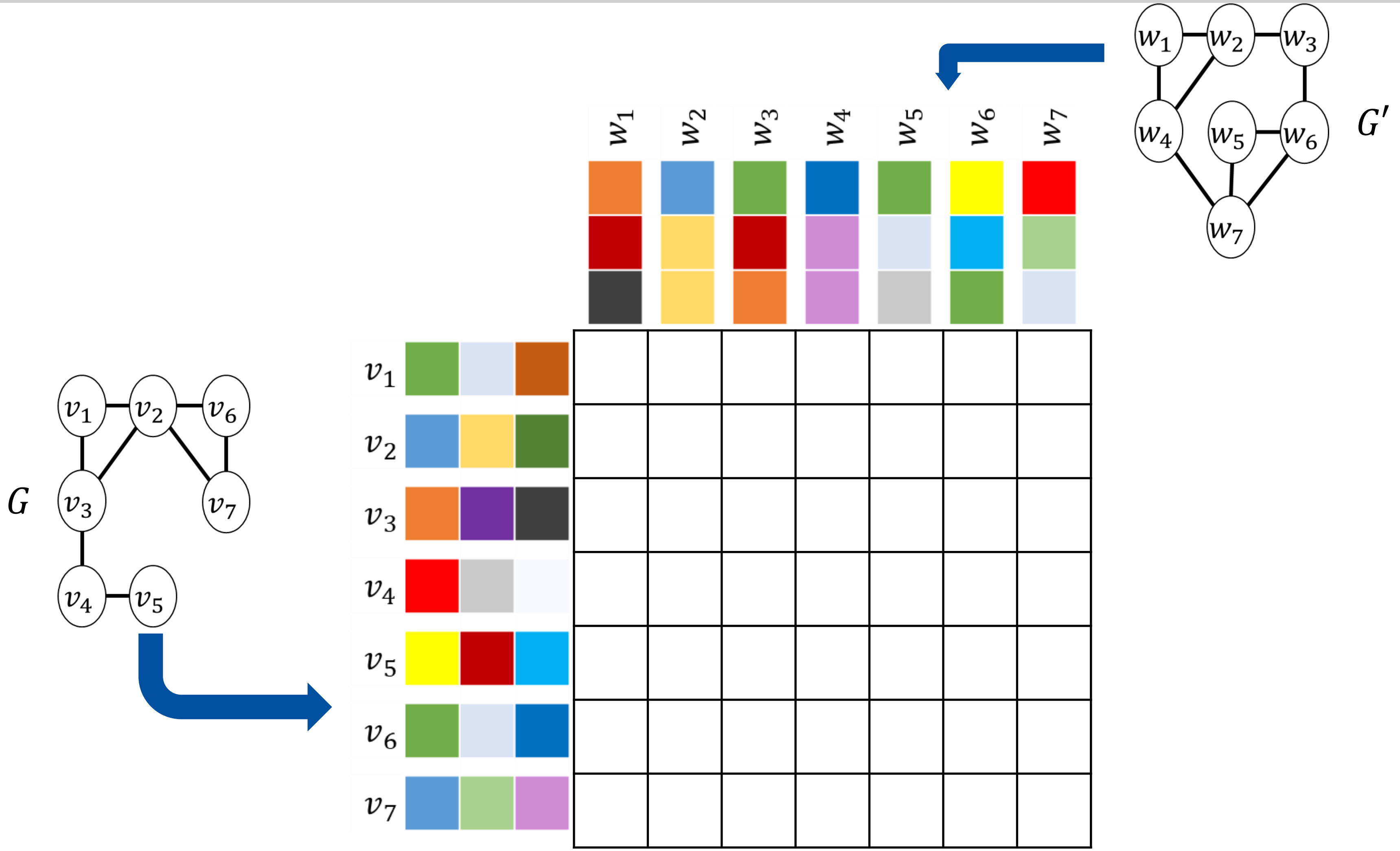
Transportation plan



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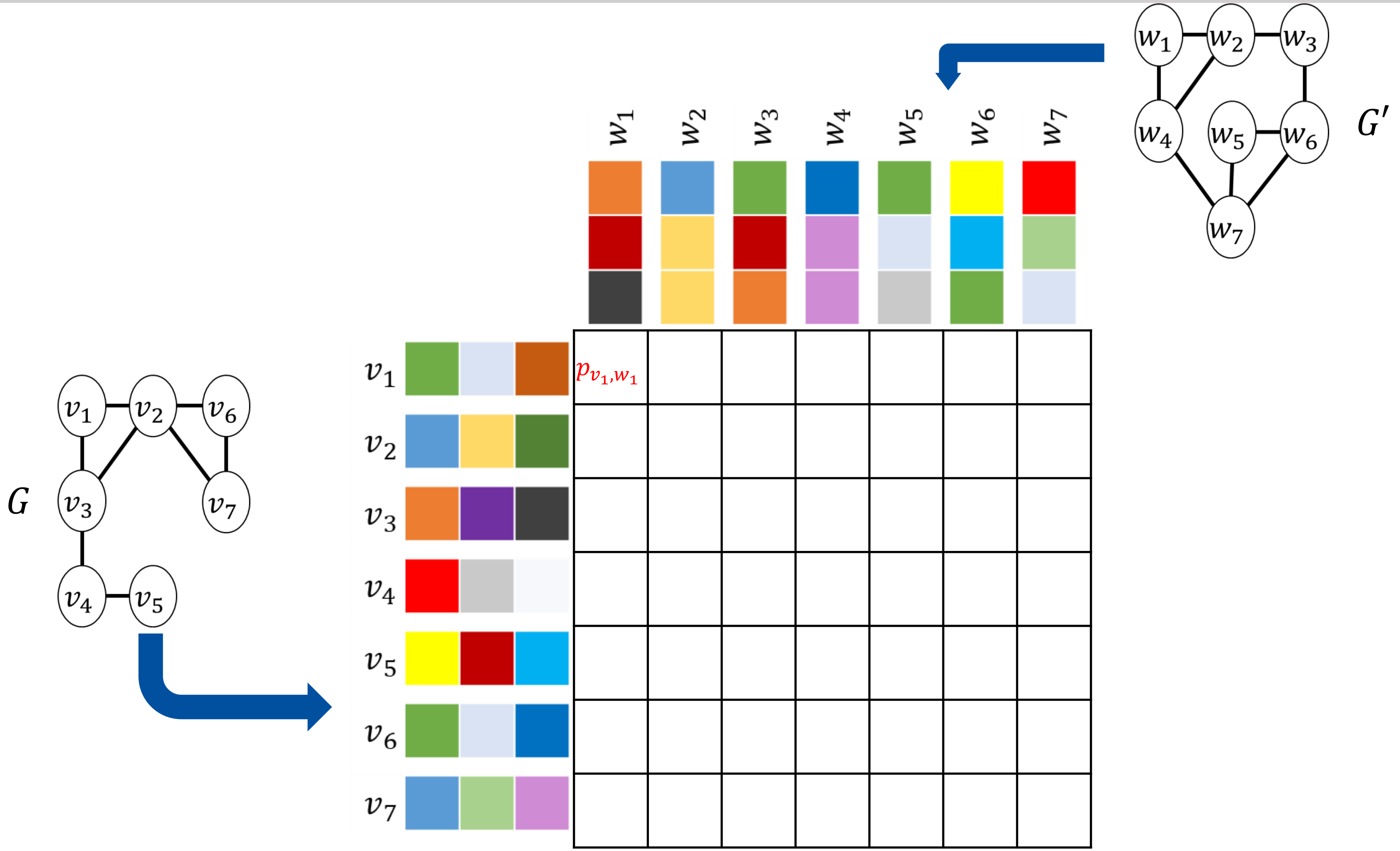

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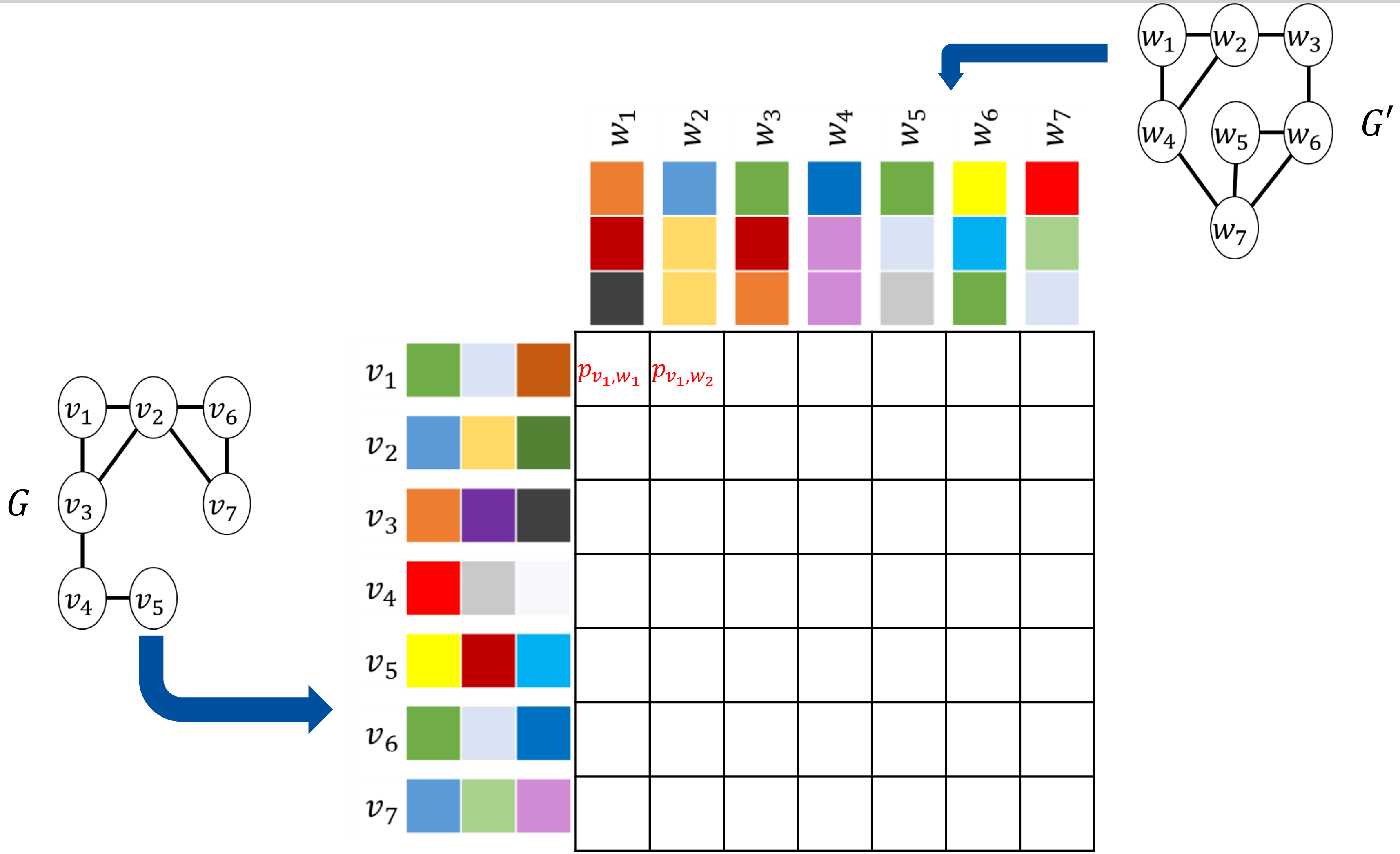
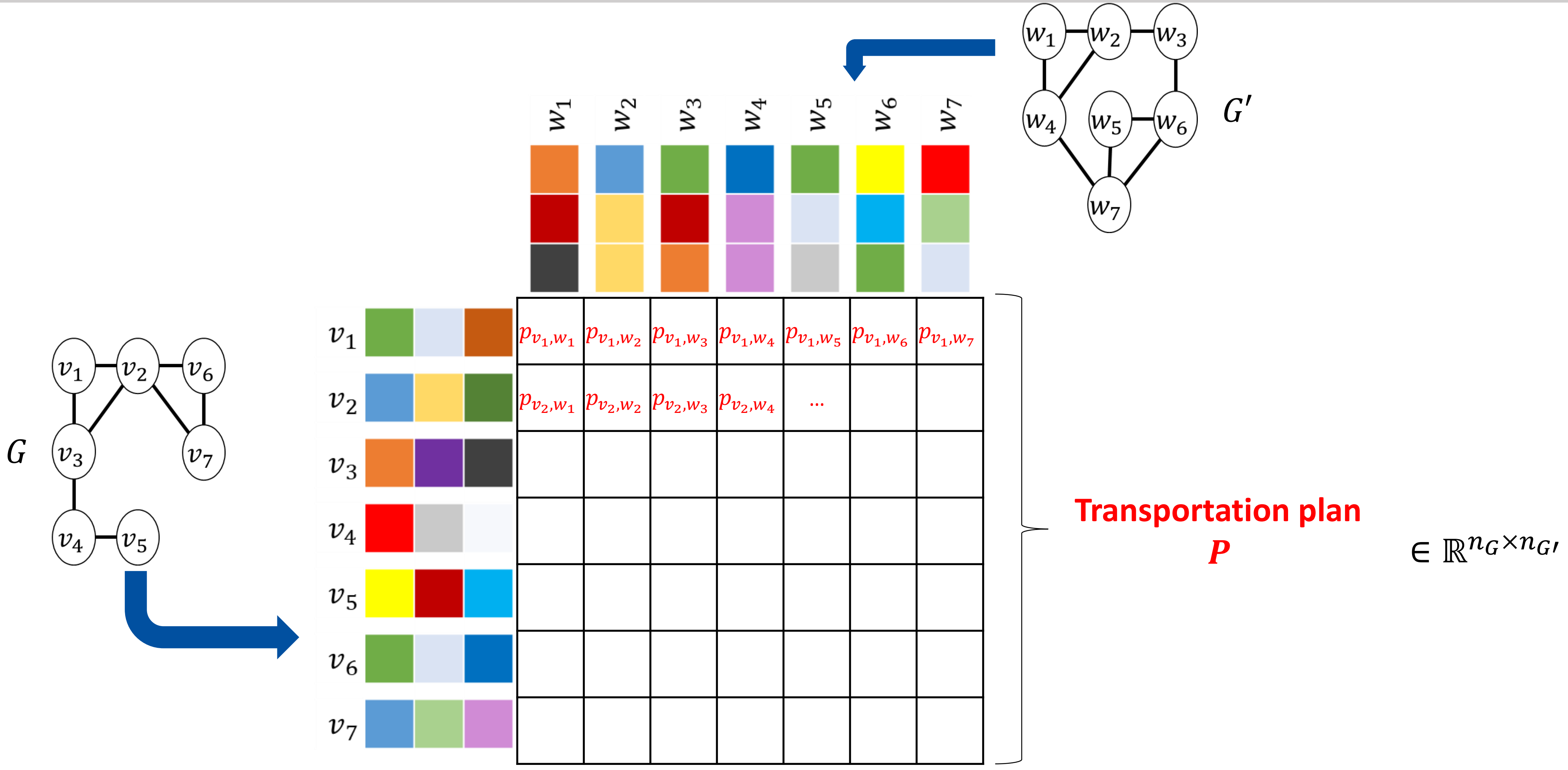
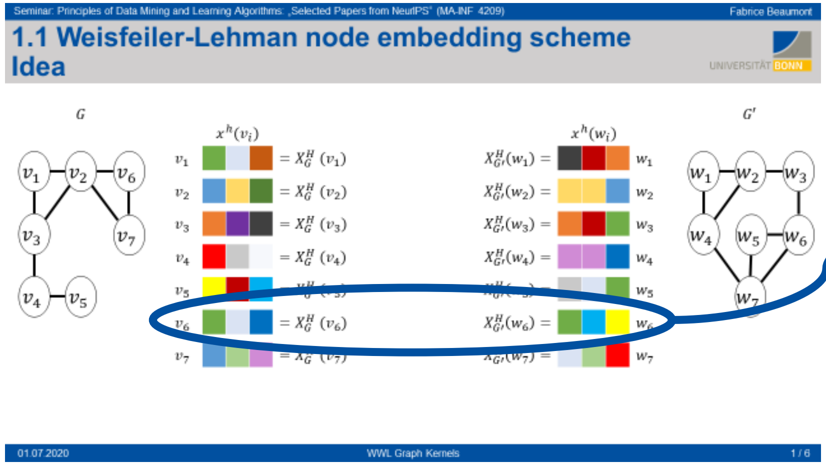
Transportation plan

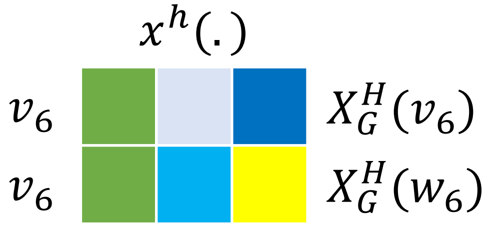


2.2 Graph Wasserstein distance
Transportation plan

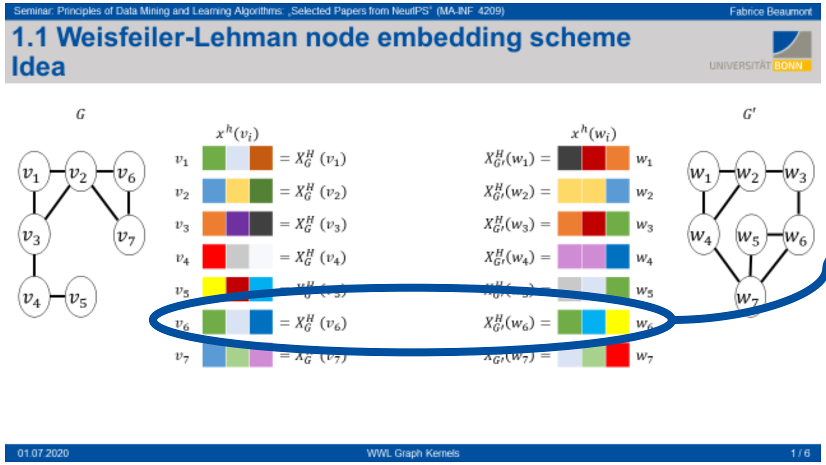


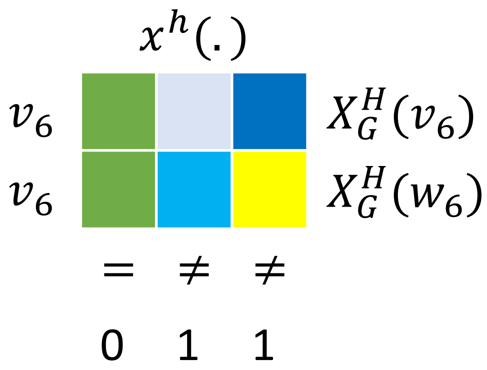
2.2 Graph Wasserstein distance
Distance measure





2.2 Graph Wasserstein distance
Distance measure





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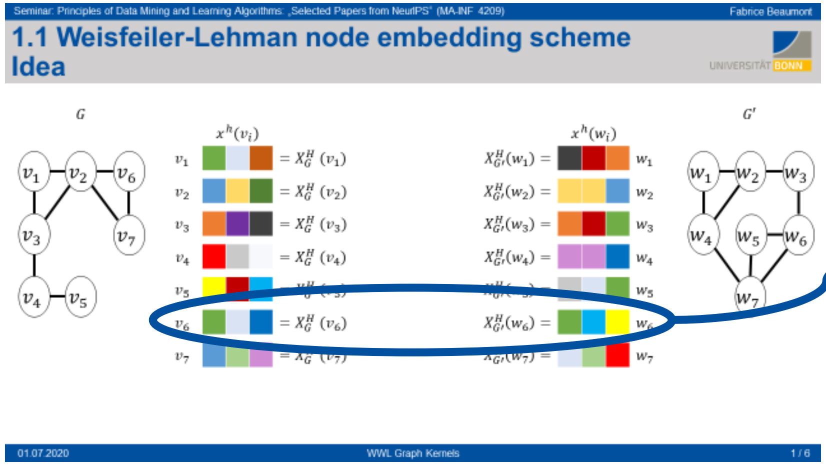
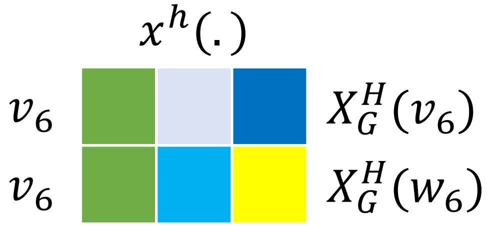
Distance measure



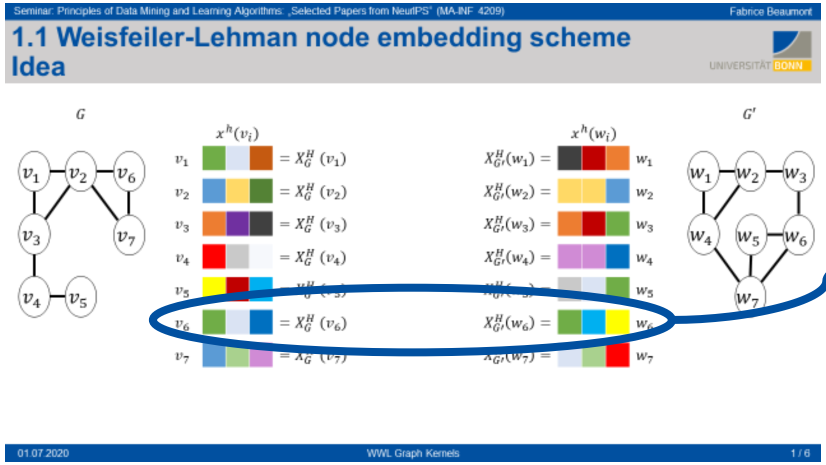


$=\quad \neq \quad \neq$

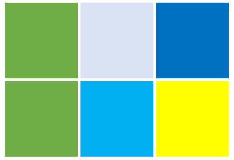
0 1 1

$$\Rightarrow d_{Ham} = \frac{1}{3}2$$

2.2 Graph Wasserstein distance
Distance measure



$x^h(.)$



$$= \quad \neq \quad \neq$$

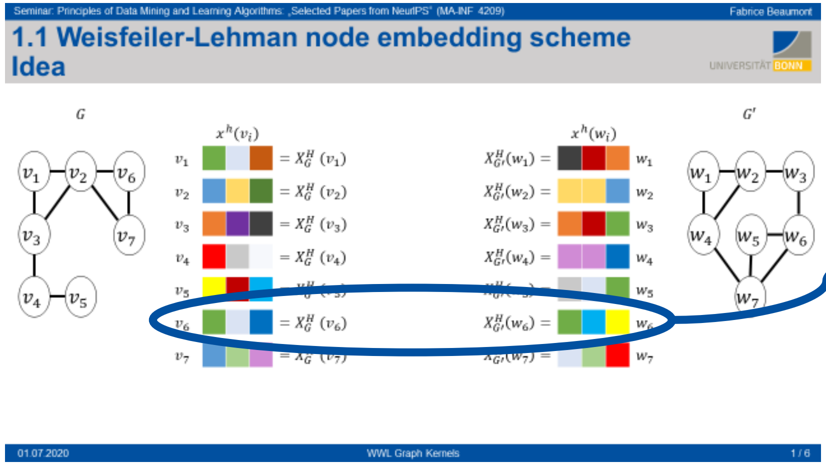
$$0 \quad 1 \quad 1$$

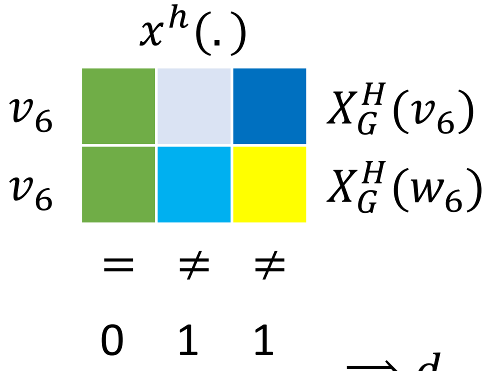
$$\Longrightarrow d_{Ham} = \frac{1}{3} 2$$

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

$$d_{Ham}\left(X_G^H(v_6), X_G^H(w_6)\right) = \frac{1}{H+1} \sum_{h=0}^{H} \rho(x^h(v_6), x^h(w_6))$$

2.2 Graph Wasserstein distance
Distance measure





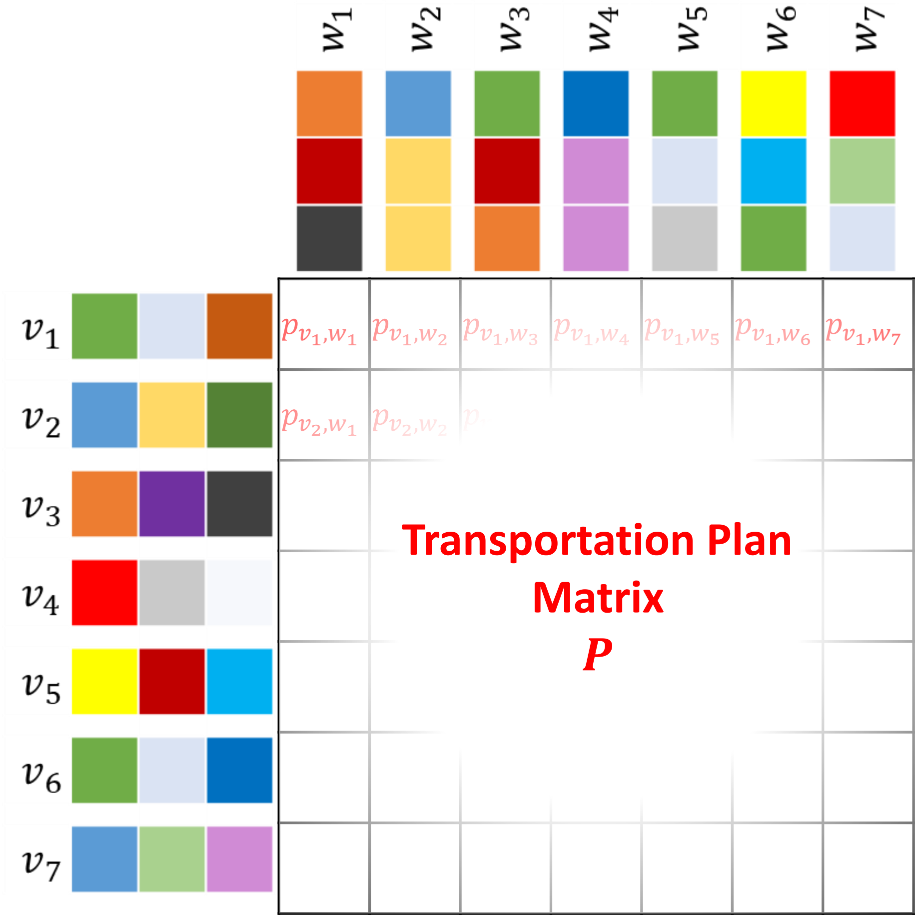
$$\Rightarrow d_{Ham} = \frac{1}{3}2$$

$$d_{Ham}\left(X_G^H(v_6), X_G^H(w_6)\right) = \frac{1}{H+1}\sum_{h=0}^{H}\rho(x^h(v_6), x^h(w_6))$$

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

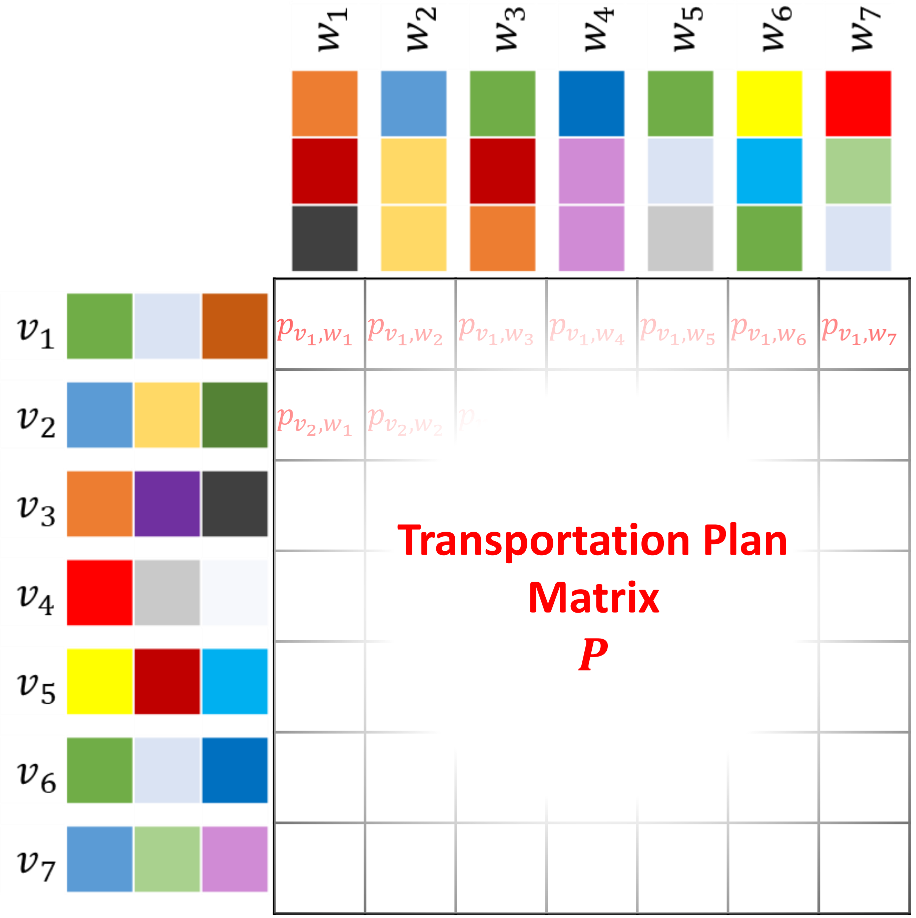
DISCRETE node labels	CONTINUOUS node labels
Normalised Hamming distance: $d_{Ham}(v,v') = \frac{1}{H+1}\sum_{i=0}^{H}\rho(v_i, v'_i)$	Euclidean distance: $d_E(v,v') = \lVert v - v' \rVert_2$

2. Graph Wasserstein distance

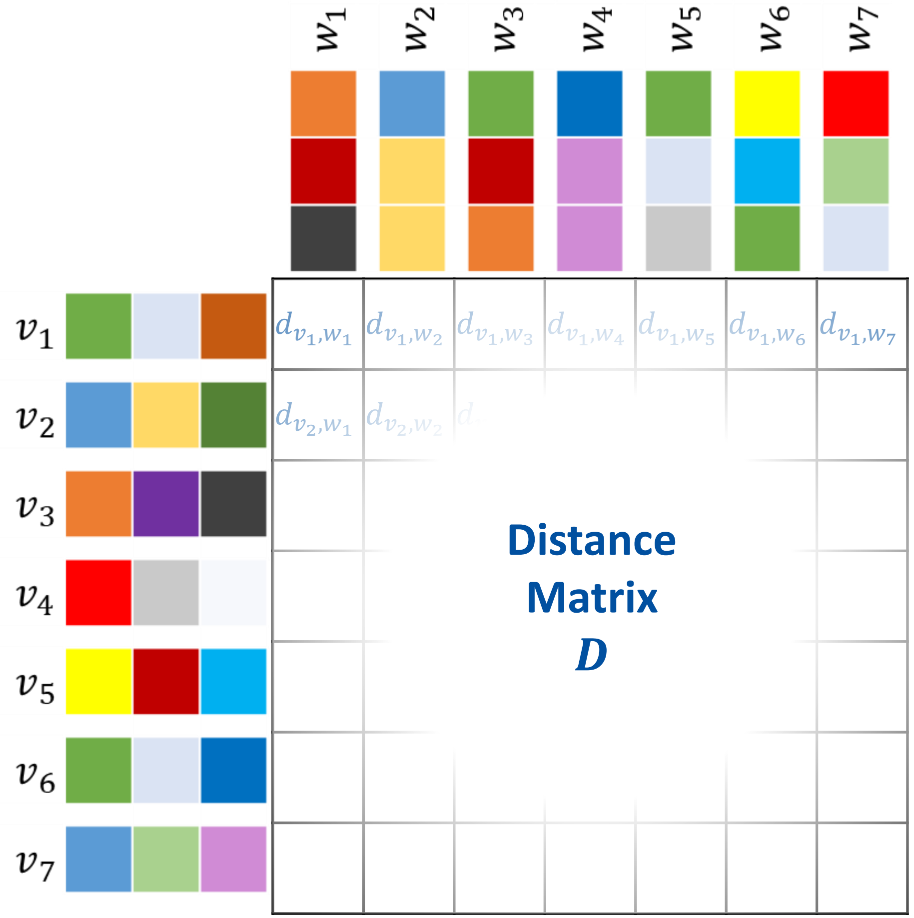


$\in \mathbb{R}^{n_G \times n_{G'}}$

2. Graph Wasserstein distance

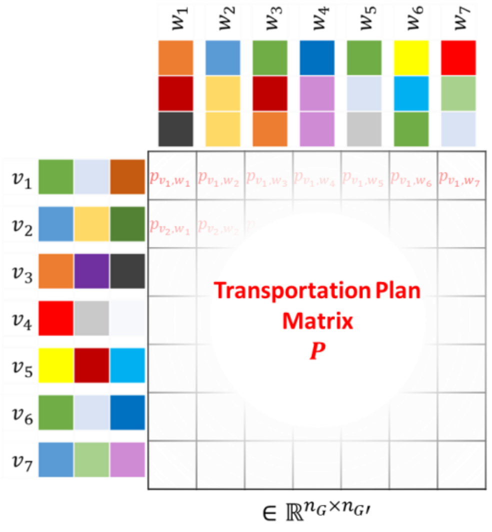


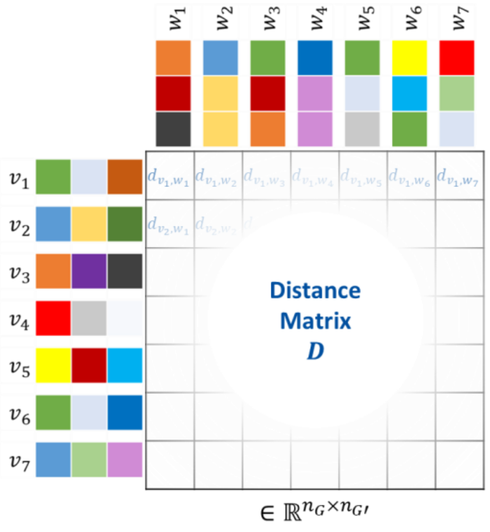
$\in \mathbb{R}^{n_G \times n_{G'}}$



$\in \mathbb{R}^{n_G \times n_{G'}}$

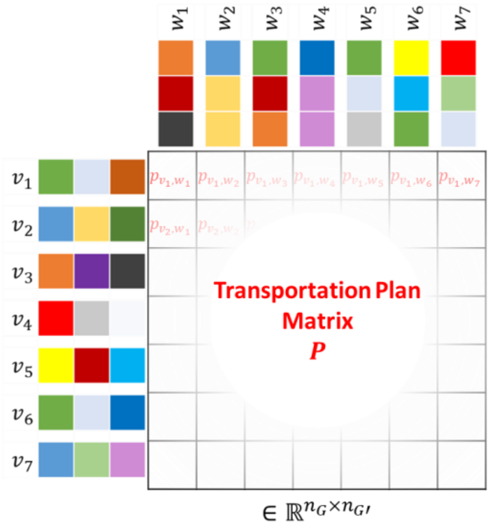
2. Graph Wasserstein distance

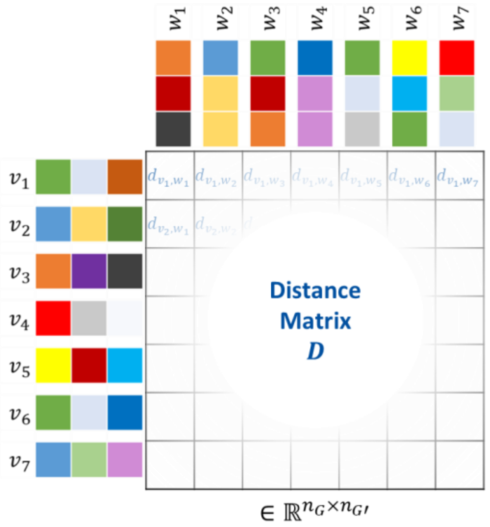




$$W_1(f(G), f(G')) := \min_{P} \sum_{\substack{v \in G, \\ w \in G'}} p_{v,w}\, d(v,w)$$

2. Graph Wasserstein distance





$$W_1(f(G), f(G')) := \min_P \sum_{\substack{v \in G, \\ w \in G'}} p_{v,w}\, d(v,w)$$

$$:= \min_{P \in \Gamma(f(G), f(G'))} \langle P, D \rangle$$

3 Kernel definition

Use a Laplacian kernel:

$$K_{WWL} = e^{-\lambda W_1(f(G), f(G'))}$$

(Leads to favourable conditions for the positive definiteness in case of non-Euclidean Distances)

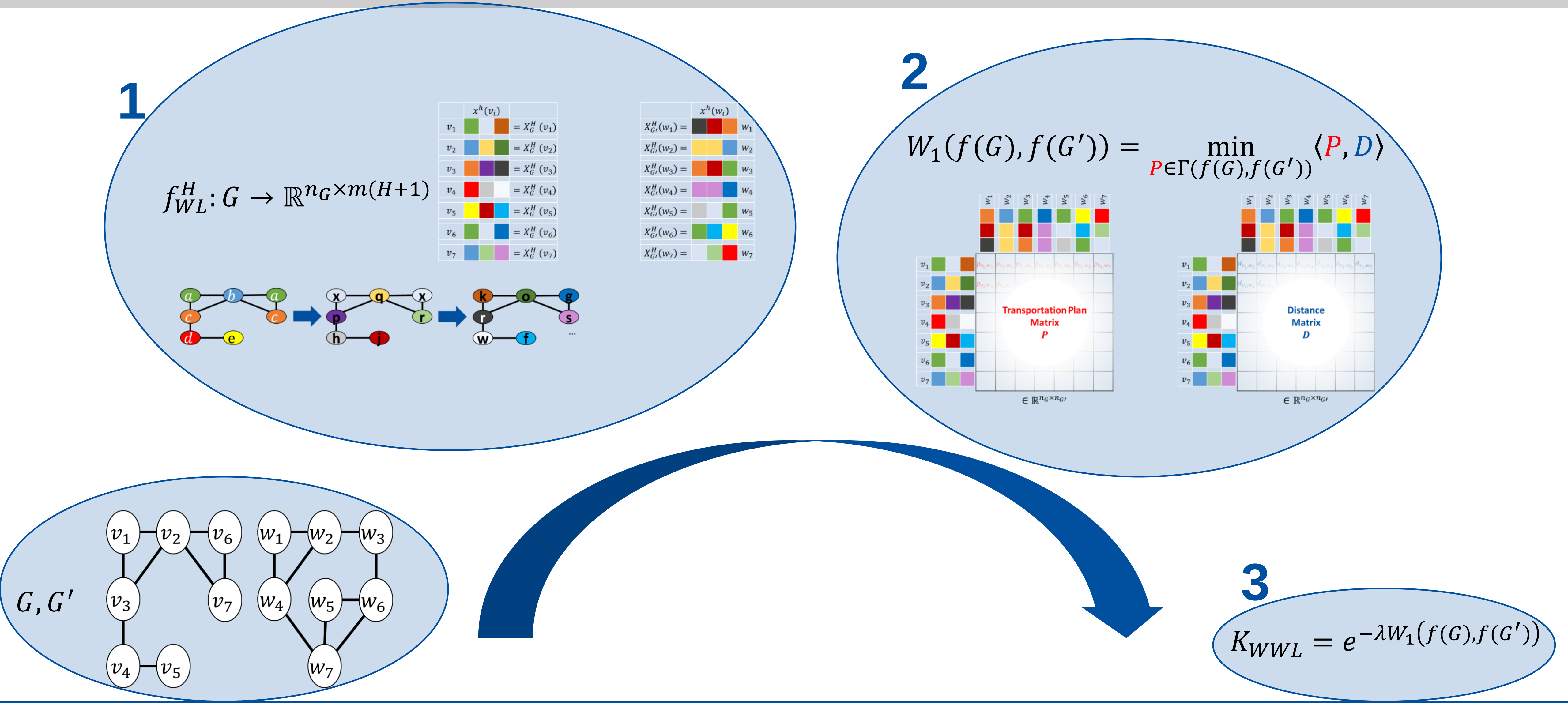
3 Kernel definition

DISCRETE node labels	CONTINUOUS node labels
• The kernel is positive definite for all $\lambda > 0$	? Open problem

3 Kernel definition

DISCRETE node labels	CONTINUOUS node labels
• Positive definite for all $\lambda > 0$ • SVM	• Positive definite? *Open problem* Workaround: • RKKS (reproducing kernel Krein spaces) • KSVM (Krein SVM)

4 OVERVIEW



1
$f_{WL}^H: G \to \mathbb{R}^{n_G \times m(H+1)}$
2
$W_1(f(G), f(G')) = \min_{P \in \Gamma(f(G), f(G'))} \langle P, D \rangle$
Transportation Plan Matrix P
Distance Matrix D
$\in \mathbb{R}^{n_G \times n_{G'}}$
G, G'
3
$K_{WWL} = e^{-\lambda W_1(f(G), f(G'))}$

5 Experimental evaluation

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DISCRETE node labels

SVM accuracies [%], 10-fold cross-validation, trained parameters

	METHOD	MUTAG	PTC-MR	NCI1	PROTEINS	D&D	ENZYMES	
Vertex histogram	V	85.39±0.73	58.35±0.20	64.22±0.11	72.12±0.19	78.24±0.28	22.72±0.56	
Edge histogram	E	84.17±1.44	55.82±0.00	63.57±0.12	72.18±0.42	75.49±0.21	21.87±0.64	
Weisfeiler-Lehman kernel	WL	85.78±0.83	61.21±2.28	85.83±0.09	74.99±0.28	78.29±0.30	53.33±0.93	
Optimal assignment kernel	WL-OA	**87.15±1.82**	60.58±1.35	**86.08±0.27**	**76.37±0.30***	79.15±0.33	**58.97±0.82**	State of art
	WWL	**87.27±1.50**	**66.31±1.21***	85.75±0.25	74.28±0.56	**79.69±0.50**	**59.13±0.80**	

5 Experimental evaluation

DISCRETE node labels

SVM accuracies [%], 10-fold cross-validation, trained parameters

	METHOD	MUTAG	PTC-MR	NCI1	PROTEINS	D&D	ENZYMES
Vertex histogram	V	85.39±0.73	58.35±0.20	64.22±0.11	72.12±0.19	78.24±0.28	22.72±0.56
Edge histogram	E	84.17±1.44	55.82±0.00	63.57±0.12	72.18±0.42	75.49±0.21	21.87±0.64
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Optimal assignment kernel	WL-OA	**87.15±1.82**	60.58±1.35	**86.08±0.27**	**76.37±0.30***	79.15±0.33	**58.97±0.82**
	WWL	**87.27±1.50**	**66.31±1.21***	85.75±0.25	74.28±0.56	**79.69±0.50**	**59.13±0.80**

State of art

CONTINUOUS node labels

KSVM accuracies [%], 10-fold cross-validation, trained parameters

	METHOD	ENZYMES	PROTEINS	IMDB-B	BZR	COX2	BZR-MD	COX2-MD
Vertex histogram	VH-C	47.15±0.79	60.79±0.12	71.64±0.49	74.82±2.13	48.51±0.63	66.58±0.97	64.89±1.06
WWL with RBF-kernel	RBF-WL	68.43±1.47	75.43±0.28	72.06±0.34	80.96±1.67	75.45±1.53	**69.13±1.27**	71.83±1.61
Hash graph kernel	HGK-WL	63.04±0.65	75.93±0.17	73.12±0.40	78.59±0.63	**78.13±0.45**	**68.94±0.65**	74.61±1.74
	HGK-SP	66.36±0.37	75.78±0.17	73.06±0.27	76.42±0.72	72.57±1.18	66.17±1.05	68.52±1.00
GraphHopper kernel	GH	65.65±0.80	74.78±0.29	72.35±0.55	76.49±0.99	76.41±1.39	**69.14±2.08**	66.20±1.05
	WWL	**73.25±0.87***	**77.91±0.80***	**74.37±0.83***	**84.42±2.03***	**78.29±0.47**	**69.76±0.94**	**76.33±1.02**

New state of art

5 Experimental evaluation

DISCRETE node labels	CONTINUOUS node labels
• Competitive with best graph kernel	• Outperforms all state-of-the art graph kernels

Thank you

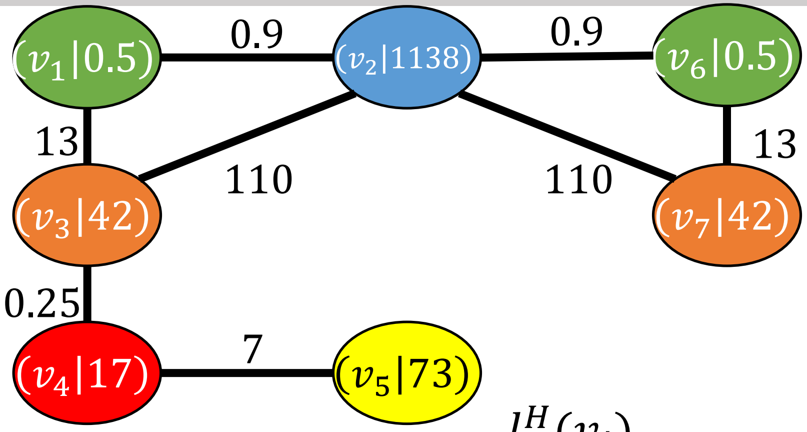
for your attention!

Appendix

Other slides

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

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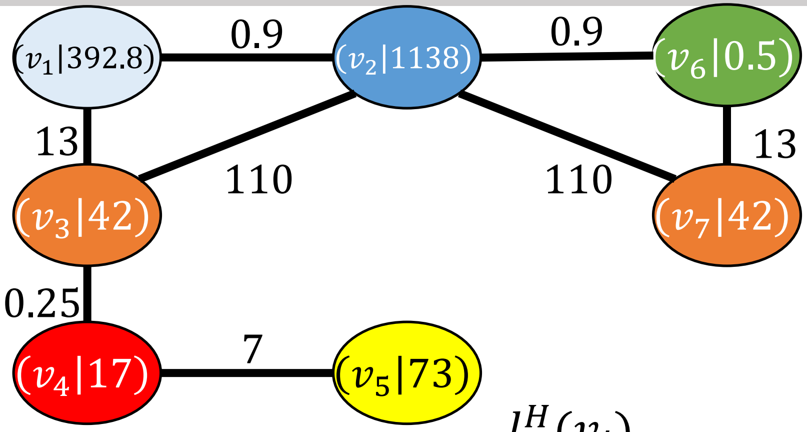
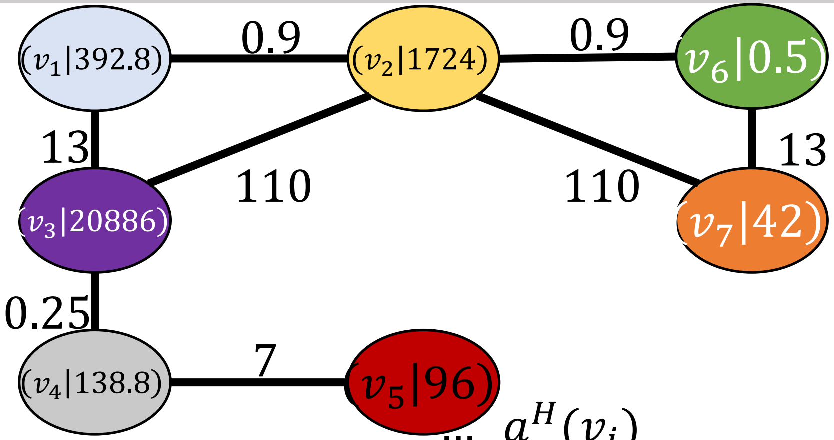
$$a^{h+1}(v) = \frac{1}{2}\left(a^h(v) + \frac{1}{\deg(v)} \sum_{u \in N(v)} w((u,v))\, a^h(u)\right)$$



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

1.1 Weisfeiler-Lehman node embedding scheme
Example – Attribute labels

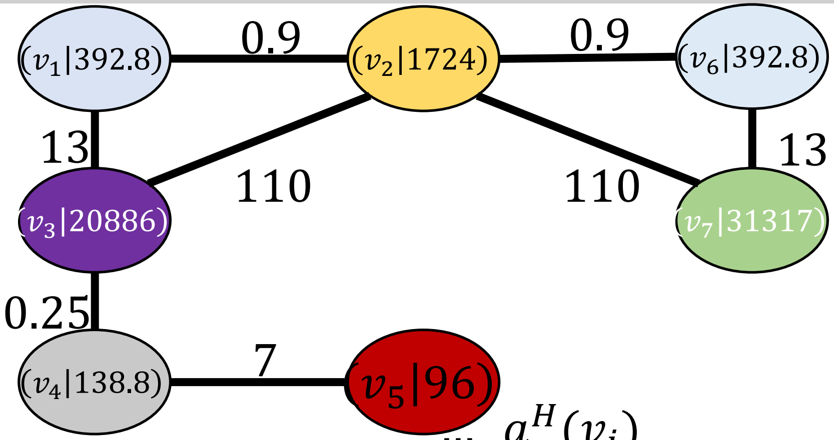
$$a^{h+1}(v) = \frac{1}{2}\left(a^h(v) + \frac{1}{\deg(v)} \sum_{u \in N(v)} w((u,v))\, a^h(u) \right)$$



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

1.1 Weisfeiler-Lehman node embedding scheme Example – Attribute labels

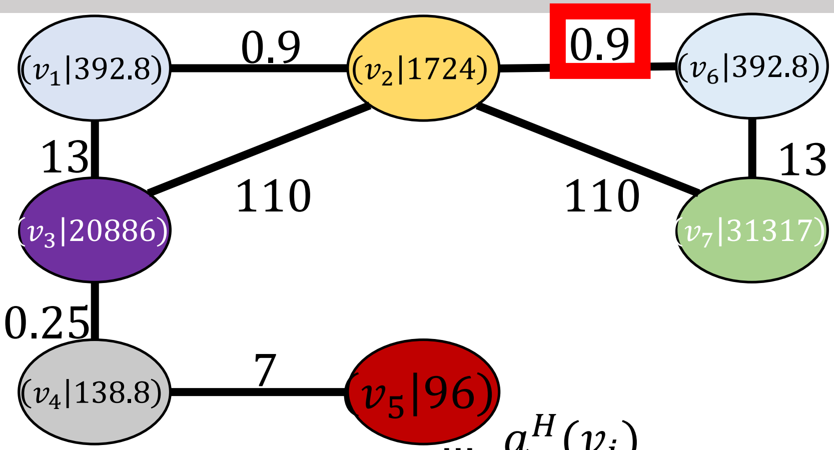
$$a^{h+1}(v) = \frac{1}{2}\left(a^h(v) + \frac{1}{\deg(v)} \sum_{u \in N(v)} w((u,v))\, a^h(u)\right)$$



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

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



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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	$^1/_2\left(1138 + {}^1/_4\,[0.9 * 0.5 + 110 * 42 + \boxed{0.9} * 0.5 + 110 * 42]\right) = 1724.1125$	…	…
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	$^1/_2\left(0.5 + {}^1/_2\,[\boxed{0.9} * 1138 + 13 * 42]\right) = 392.8$	…	…
7	42	$^1/_2\left(42 + {}^1/_2\,[13 * 0.5 + 110 * 1138]\right) = 31317.625$	…	…

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 $\boldsymbol{M}$

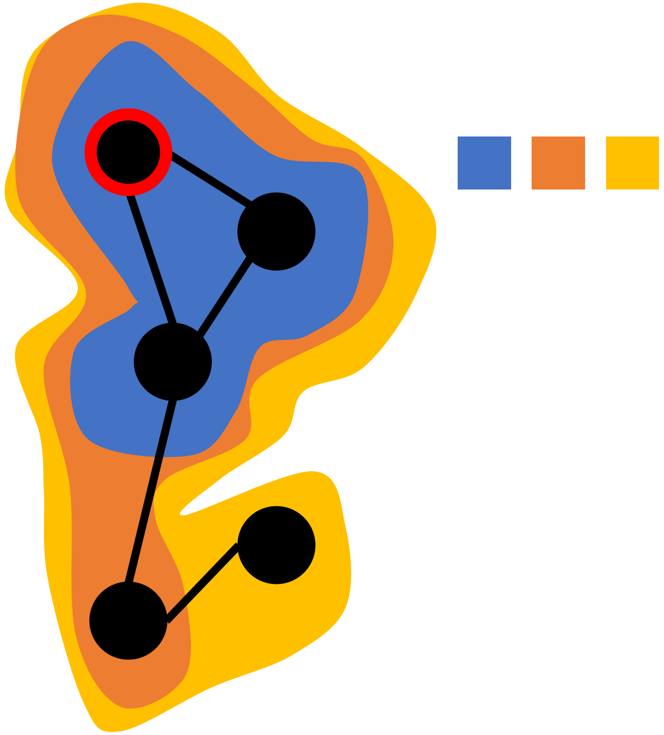
$d: \mathbb{R}^m x \mathbb{R}^m \rightarrow \mathbb{R}^m$: ground distance (on M)

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

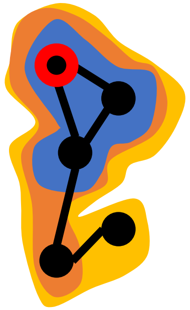
$$W_p(\sigma, \mu) := \left(\lim_{\gamma \in \Gamma(\sigma, \mu)} \int_{MxM} d(x, y)^p d\gamma(x, y) \right)^{\frac{1}{p}}$$

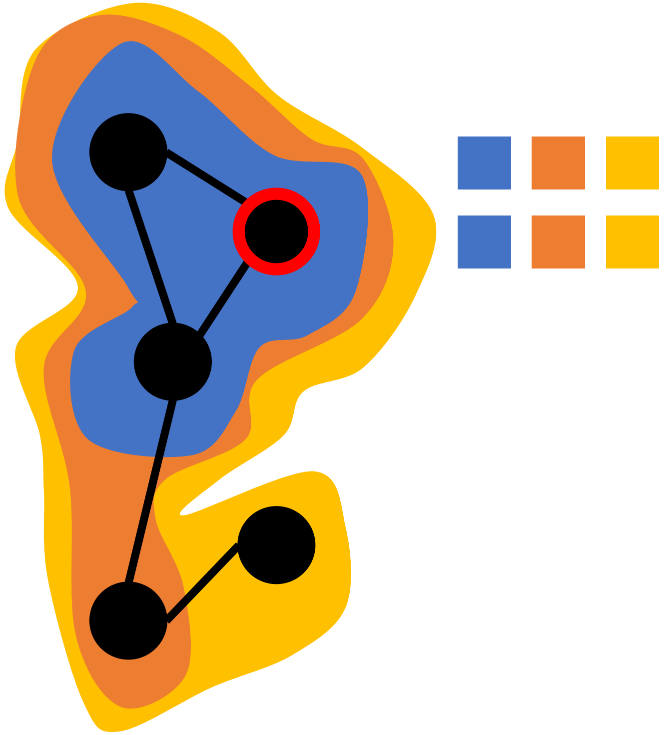
1.1 Weisfeiler-Lehman node embedding scheme
Idea

TODO: Fix this example: use different labels for the Node.
Mention formula next to example

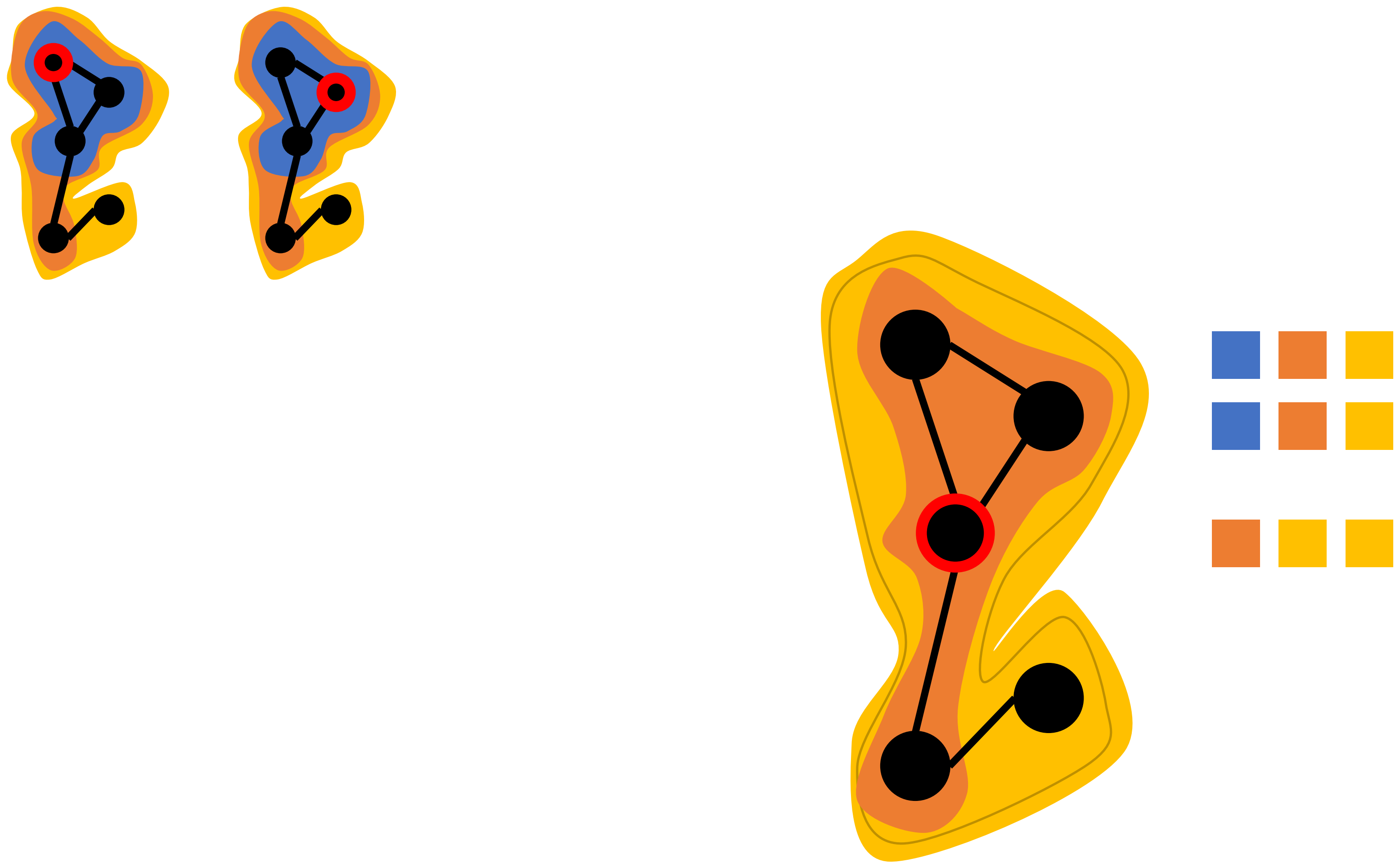


1.1 Weisfeiler-Lehman node embedding scheme
Idea

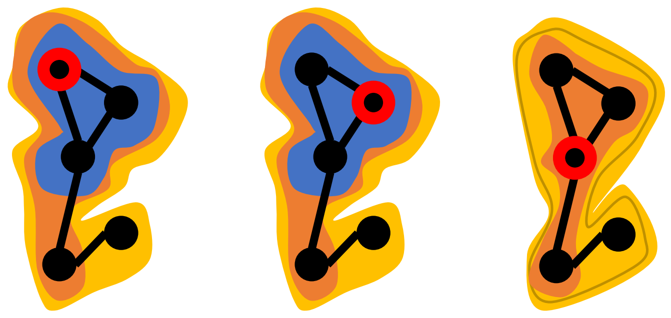


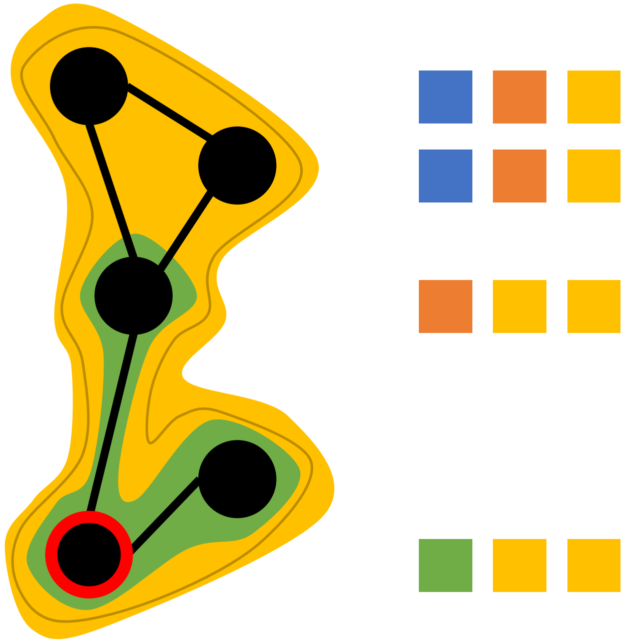


1.1 Weisfeiler-Lehman node embedding scheme
Idea

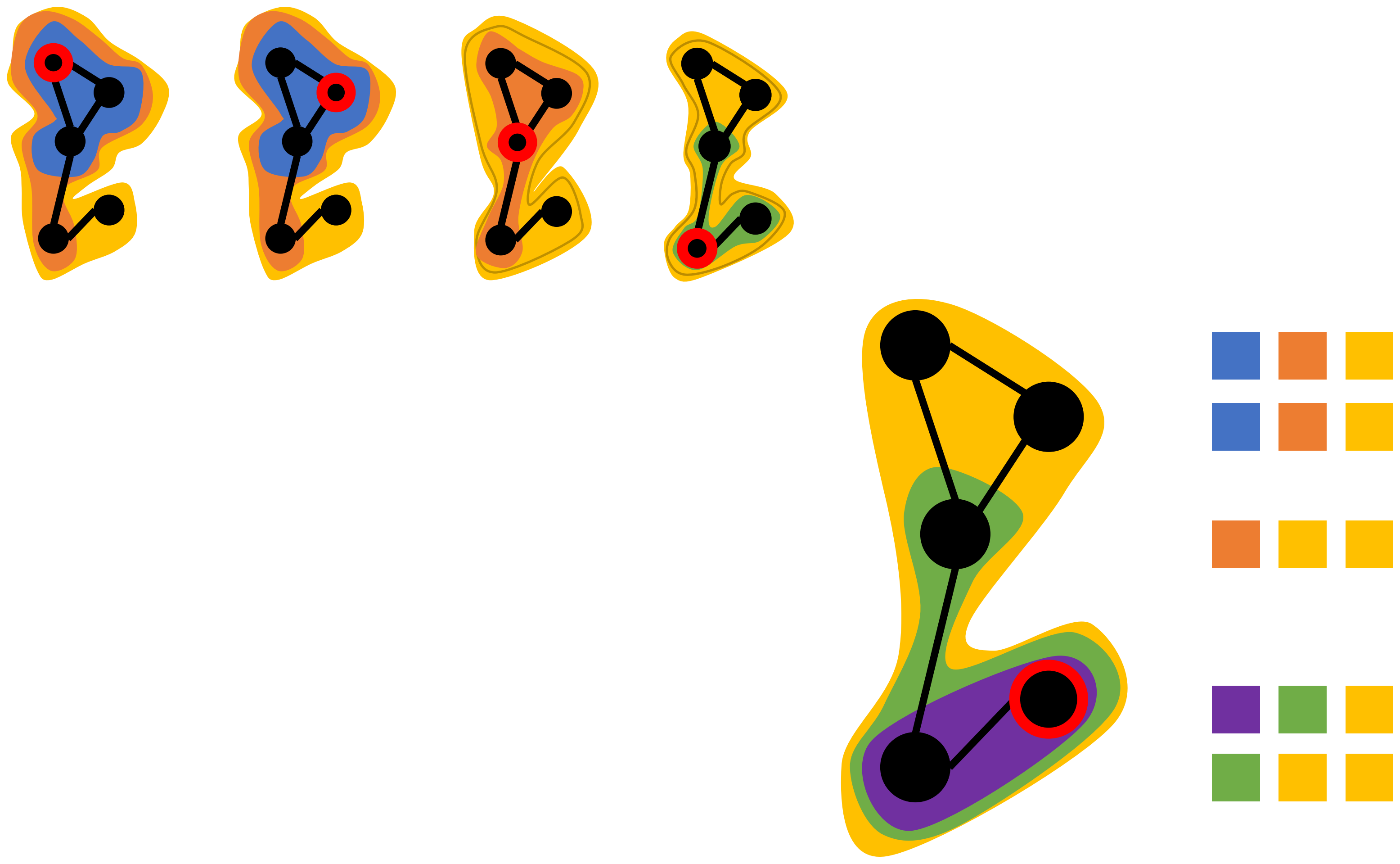


1.1 Weisfeiler-Lehman node embedding scheme
Idea

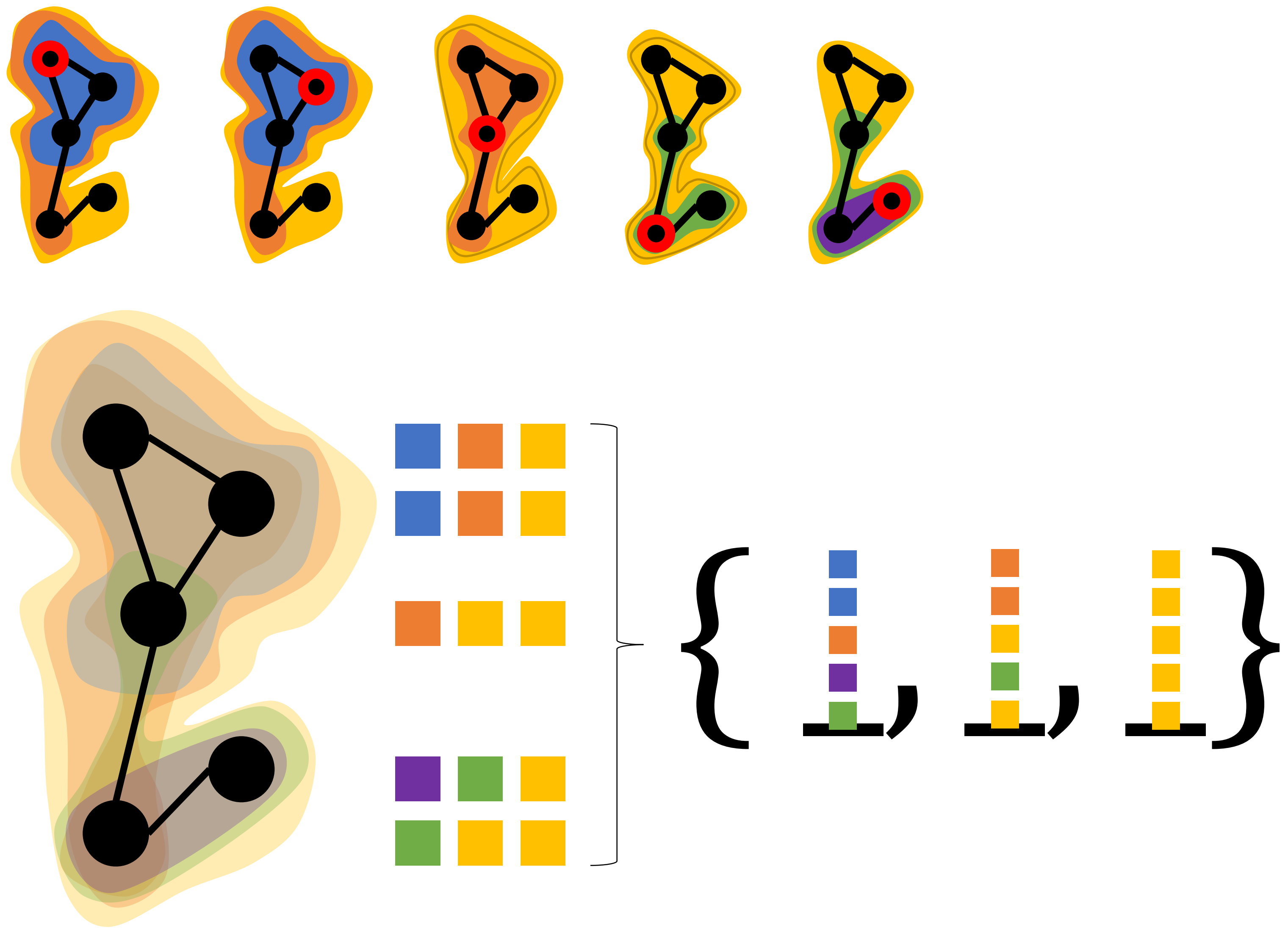




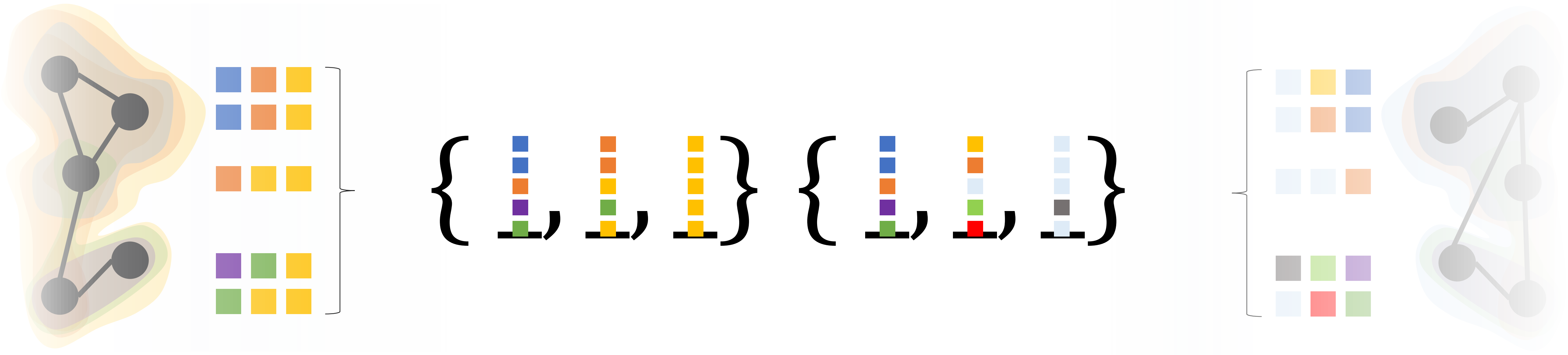
1.1 Weisfeiler-Lehman node embedding scheme
Idea



1.1 Weisfeiler-Lehman node embedding scheme
Idea

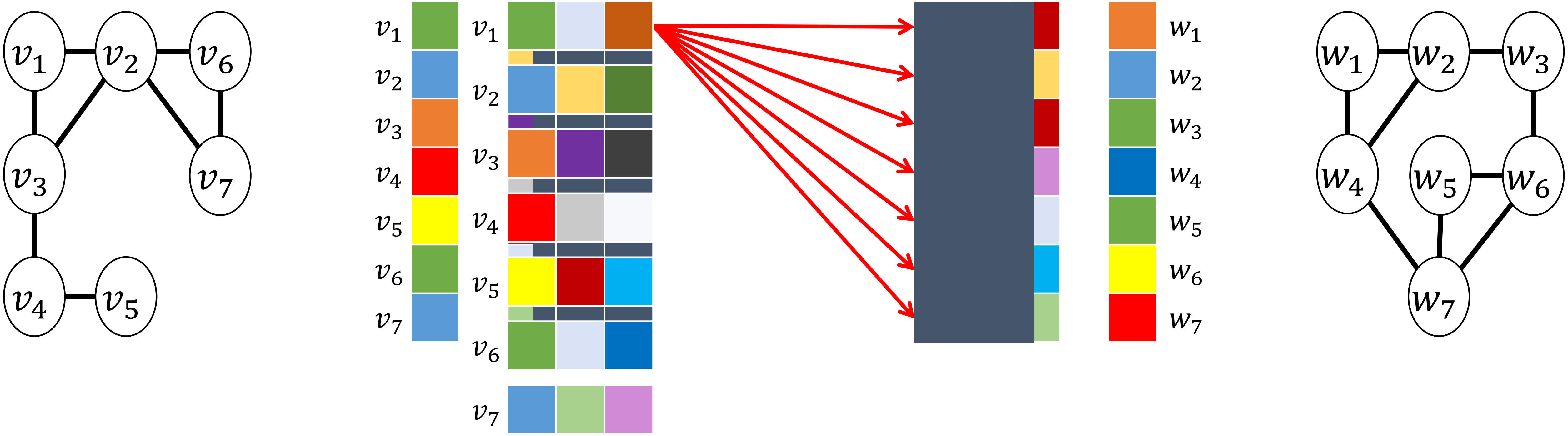


1.1 Weisfeiler-Lehman node embedding scheme
Idea

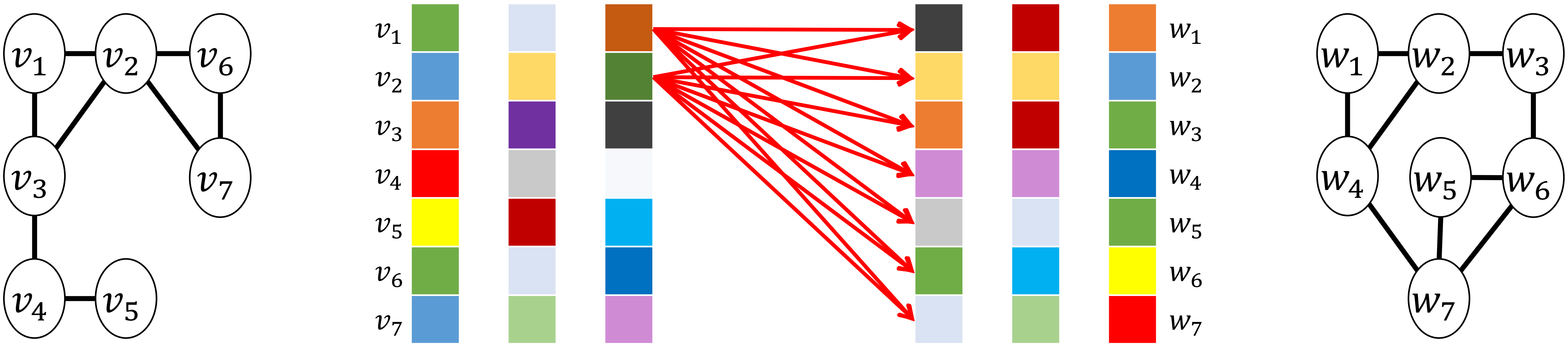


TODO: second version, encapsulating every step from
The method

1.1 Weisfeiler-Lehman node embedding scheme
Idea



1.1 Weisfeiler-Lehman node embedding scheme
Idea



1.1 Weisfeiler-Lehman node embedding scheme Theory

m: dimensionality of the node labels

n_G: cardinality of the node set

$N(v)$: neighbourhood of v

$$N^h(v) = \{x^h(u_1), \dots, x^h(u_{|N(v)|})\}$$

DISCRETE node labels	CONTINUOUS node labels
$x^{h+1}(v) = hash(x^h(v), N^h(v))$	$x^{h+1}(v) = x^h(v) + \sum_{u \in N(v)} x^h(u)$

1.1 Weisfeiler-Lehman node embedding scheme
Theory

m: dimensionality of the node labels

n_G: cardinality of the node set

$N(v)$: neighbourhood of v

$$N^h(v) = \left\{x^h(u_1), \dots, x^h\left(u_{|N(v)|}\right)\right\}$$

DISCRETE node labels	CONTINUOUS node labels
$x^{h+1}(v) = hash(x^h(v), N^h(v))$	$x^{h+1}(v) = x^h(v) + \sum_{u \in N(v)} w((u,v))x^h(u)$

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

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

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

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

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

2.2 Graph Wasserstein distance

$p \in [1, \infty)$: 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

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

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