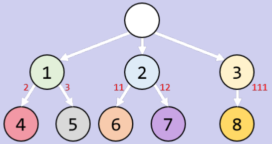


Master Thesis Seminar Talk

Progress Upade

Fabrice Beaumont

Department of Information Systems and Artificial Intelligence - **Dr. Pascal Welke**

11. May 2022

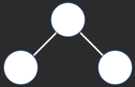
Progress overview

1. Task formulation, registration of the thesis:
   "**Learning graph similarity measures using the Weisfeiler-Lehman label hierarchy**"
   Definition of several sub-goals a programming road-map.

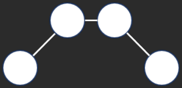
2. Implementation of a dynamic **Dataset Loader** (*GarKel*, *OGB*, from file).
   Easily expandable for other frameworks.

Example of the whole procedure

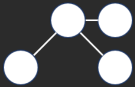
A



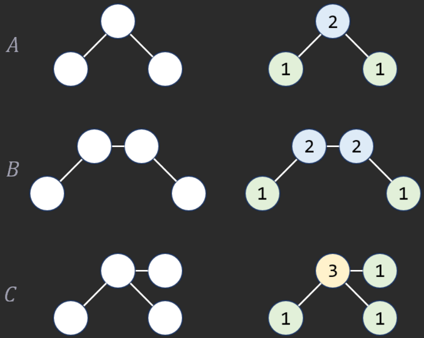
B



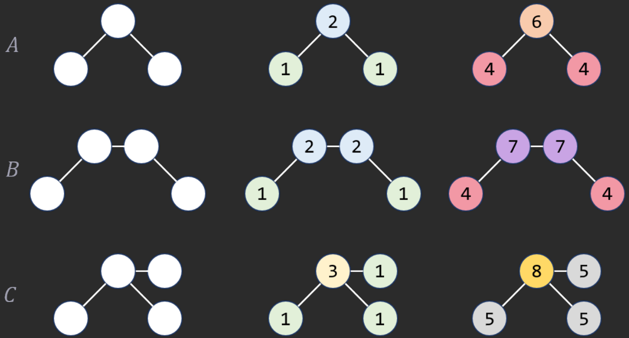
C



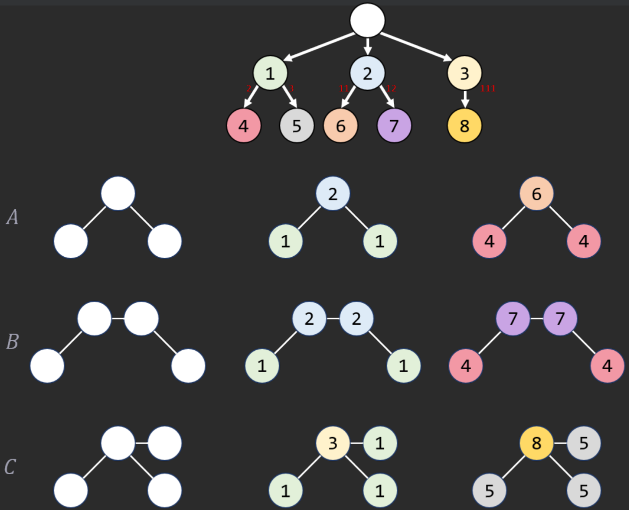
Example of the whole procedure



Example of the whole procedure



Example of the whole procedure



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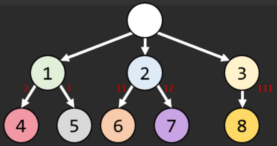

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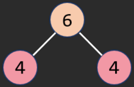

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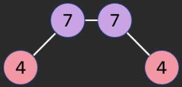

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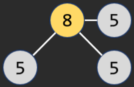
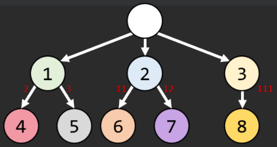
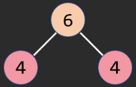


Example of the whole procedure



A



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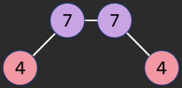
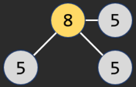


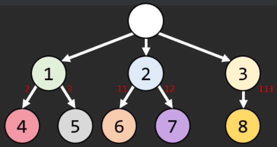
C

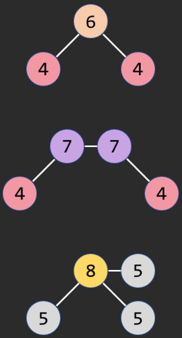


Tree metric between the WL-labels:

$$
\begin{array}{c}
\begin{array}{ccccc} 4 & 5 & 6 & 7 & 8 \end{array} \\
\begin{pmatrix}
\cdot & 2 & 4 & 4 & 4 \\
 & \cdot & 4 & 4 & 4 \\
 & & \cdot & 2 & 4 \\
 & \upuparrows & & \cdot & 4 \\
 & & & & \cdot
\end{pmatrix}
\end{array}
$$

Example of the whole procedure



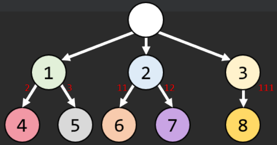


A	2		1		
B	2			2	
C		3			1

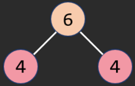
Tree metric:

$$
\begin{array}{c}
\begin{array}{ccccc} 4 & 5 & 6 & 7 & 8 \end{array} \\
\begin{pmatrix}
\cdot & 2 & 4 & 4 & 4 \\
 & \cdot & 4 & 4 & 4 \\
 & & \cdot & 2 & 4 \\
 & \upuparrows & & \cdot & 4 \\
 & & & & \cdot
\end{pmatrix}
\end{array}
$$

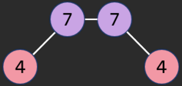
Example of the whole procedure



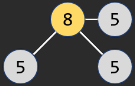
A



B



C

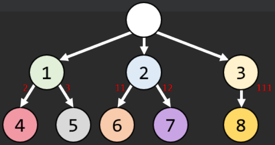


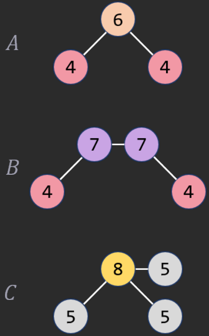
$^2/_3$		$^1/_3$		
$^1/_2$			$^1/_2$	
	$^3/_4$			$^1/_4$

Tree metric:

$$
\begin{array}{ccccc}
4 & 5 & 6 & 7 & 8
\end{array}
$$
$$
\begin{pmatrix}
\cdot & 2 & 4 & 4 & 4 \\
 & \cdot & 4 & 4 & 4 \\
 & & \cdot & 2 & 4 \\
 & \upuparrows & & \cdot & 4 \\
 & & & & \cdot
\end{pmatrix}
$$

Example of the whole procedure





2/3		1/3		
1/2			1/2	
	3/4			1/4

Tree metric:

$$
\begin{array}{c}
\begin{array}{ccccc} 4 & 5 & 6 & 7 & 8 \end{array} \\
\begin{pmatrix}
\cdot & 2 & 4 & 4 & 4 \\
 & \cdot & 4 & 4 & 4 \\
 & & \cdot & 2 & 4 \\
 & \upuparrows & & \cdot & 4 \\
 & & & & \cdot
\end{pmatrix}
\end{array}
$$

Wasserstein Dist.:

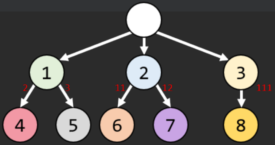
$\mathcal{W}_t(A, B) = \frac{4}{3}$

$\mathcal{W}_t(A, C)$

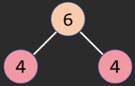
$\mathcal{W}_t(B, C)$

$$d_{\text{WLLT}}(A, B) = 0 * \frac{3}{6} + 4 * \frac{1}{6} + 2 * \frac{2}{6} = \frac{8}{6} = \frac{4}{3}$$

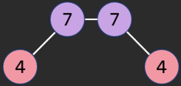
Example of the whole procedure



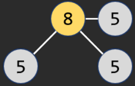
A



B



C



A	$^2/_3$		$^1/_3$		
B	$^1/_2$			$^1/_2$	
C		$^3/_4$			$^1/_4$

Tree metric:

$$\begin{array}{c} \begin{array}{ccccc} 4 & 5 & 6 & 7 & 8 \end{array} \\ \begin{pmatrix} \cdot & 2 & 4 & 4 & 4 \\ & \cdot & 4 & 4 & 4 \\ & & \cdot & 2 & 4 \\ & \upuparrows & & \cdot & 4 \\ & & & & \cdot \end{pmatrix} \end{array}$$

Wasserstein Dist.:

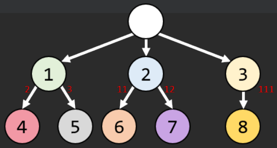
$\mathcal{W}_t(A, B) = \frac{4}{3}$

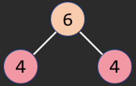
$\mathcal{W}_t(A, C) = 3$

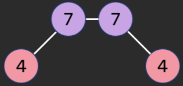
$\mathcal{W}_t(B, C)$

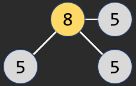
$$d_{\mathrm{WLLT}}(A, C) = 2 * \frac{8}{12} + 4 * \frac{1}{12} + 4 * \frac{4}{12} = \frac{18}{6} = 3$$

Example of the whole procedure









	4	5	6	7	8
A	$^{2}/_{3}$		$^{1}/_{3}$		
B	$^{1}/_{2}$			$^{1}/_{2}$	
C		$^{3}/_{4}$			$^{1}/_{4}$

Tree metric:

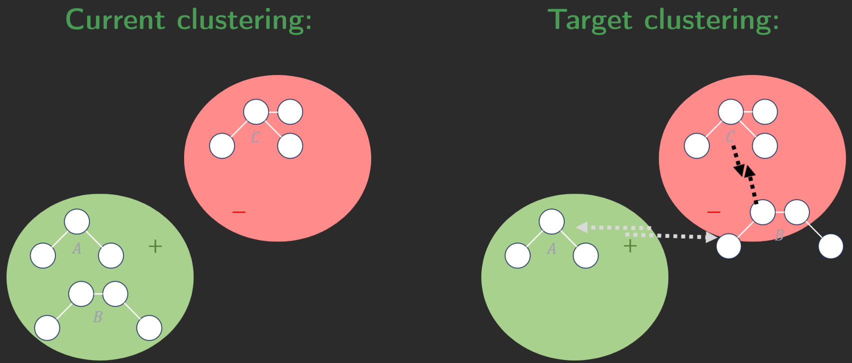
$$\begin{array}{c} \begin{matrix} 4 & 5 & 6 & 7 & 8 \end{matrix} \\ \begin{pmatrix} \cdot & 2 & 4 & 4 & 4 \\ & \cdot & 4 & 4 & 4 \\ & & \cdot & 2 & 4 \\ & \upuparrows & & \cdot & 4 \\ & & & & \cdot \end{pmatrix} \end{array}$$

Wasserstein Dist.:

$$\mathcal{W}_t(A, B) = \frac{4}{3}$$
$$\mathcal{W}_t(A, C) = 3$$
$$\mathcal{W}_t(B, C) = 3$$

$$d_{\mathrm{WLLT}}(B, C) = 2 * \frac{2}{4} + 4 * \frac{1}{4} + 4 * \frac{1}{4} = \frac{12}{4} = 3$$

Example of the whole procedure



Idea: Reduce distance between B and C, by updating the edge weights.

Example of the whole procedure

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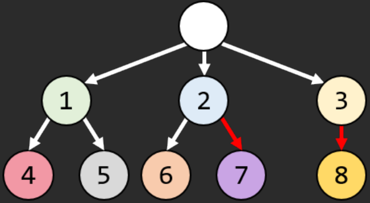
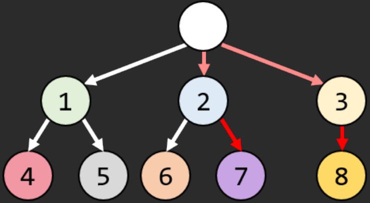
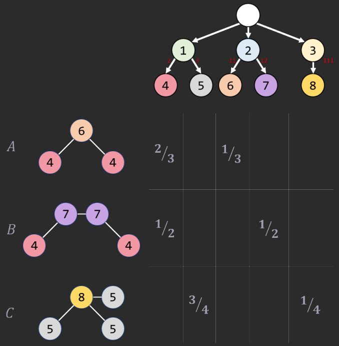
Local update $P_{7,8}$:



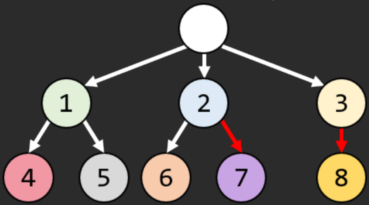
Weighted path update $P_{7,8}$:



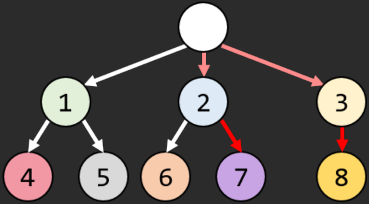


Example of the whole procedure

Local update $P_{7,8}$:



Weighted path update $P_{7,8}$:



Update rule:

Value:

- Constant λ.
- *Gradient descent*.

Location:

- *Local*: Only update the first and last edge weights of the connecting path.
- *Weighted path*: Update all edge weights on the path, with less magnitude for edges closer to the root.
- *Path*: ...
- *Global*: ...

...

Next steps

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- Implement the usage of the **Wasserstein Distance**.
- Implement a “naive” **feedback loop** to update the WLLT edge weights.
  (And the more and more complex variations.)

Thank you all for listening.

I will be happy to answer any **questions** and hear your **comments**.

Implementation road-map 1/2

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- **WLLT Construction**:
  - Write to file and read from file. Construct WL-iteration based.
  - All weights *equal*.
  - (*Random* initial weights.)
  - (Use *a priori* knowledge.)
- **Wasserstein-Distance feedback**:
  - "Biggest pile of dirt". ("Smallest", to increase the distance.)
  - Distribution proportional to the pile size.
  - Distribution proportional to the cost of moving the pile size.

Implementation road-map 2/2

UNIVERSITÄT BONN ML AI lab

- **Update rule**:
  - Value:
    - Constant λ.
    - *Gradient descent*.
  - Location:
    - *Local*: Only update the first and last edge weights of the connecting path.
    - *Weighted path*: Update all edge weights on the path, with less magnitude for edges closer to the root.
    - *Path*: Update all edges on the path.
    - *Global*: Update all edges, related to all occurring labels.