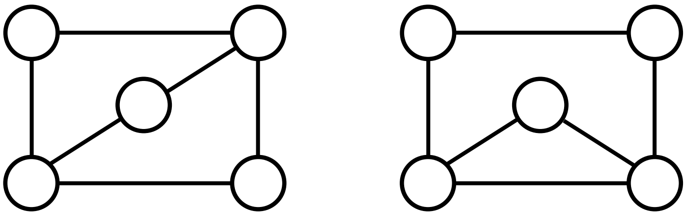
Machine Learning Group
Faculty IV – Electrical Engineering and Computer Science
Technische Universität Berlin

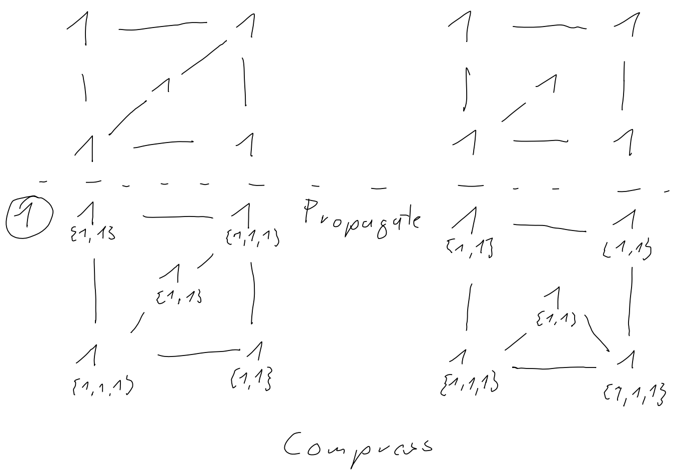
Exercise Sheet 5

Exercise 1: Weisfeiler-Lehman isomorphism test (25 P)

We want to examine whether the following two graphs are isomorphic

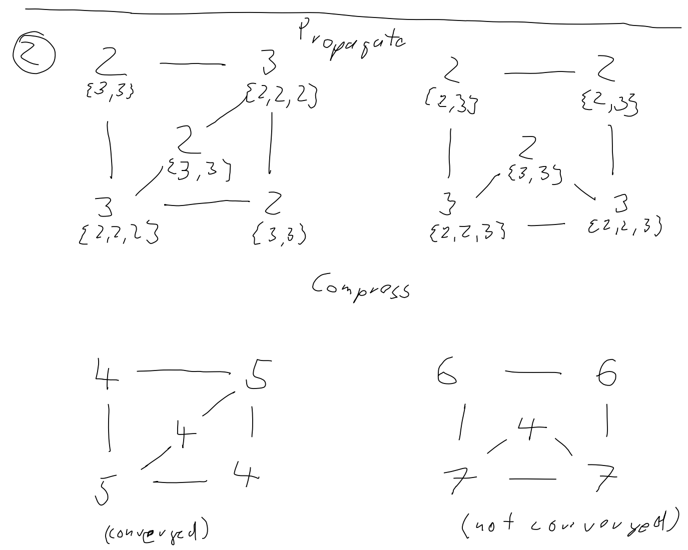


(a) Perform the Weisfeiler-Lehman isomorphism test on the two graphs. You can use sequential indexing to compress the labels (for example: $(1, \{1\}) \to 2$, $(1, \{1, 1\}) \to 3$, $(2, \{2, 2\}) \to 4$, etc.).
Are the graphs isomorphic according to the WL test? Explain whether Weisfeiler-Lehman gives the correct answer in this case.



$\Rightarrow \{2,2,2,3,3\} = \{2,2,2,3,3\}$

converged? no!



$\{4,4,4,5,5\} \neq \{4,6,6,7,7\}$

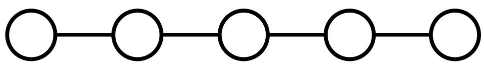
$\Rightarrow$ not isomorpic according to WL

$\Rightarrow$ WL is necessary condition

$\Rightarrow$ not isomorphic

Exercise 2: Relationship between graph convolution and discrete convolution (25 P)

In this exercise, we will treat a 1-D grid (or sequence) as a graph. For this, we will consider a sequence of length 5, corresponding to the following graph:



We will apply a spectral graph convolutional layer

$$g_\theta * x = \tilde{\mathbf{D}}^{-\frac{1}{2}}\tilde{\mathbf{A}}\tilde{\mathbf{D}}^{-\frac{1}{2}}x\Theta,$$

with kernel g_θ to a signal x on this graph. For simplicity, we assume one input and output channel, i.e. $x \in \mathbb{R}^{5\times 1}$ and $\Theta = I_1 = 1$.

(a) Write down an adjacency matrix $\mathbf{A}$ of the 1d grid and calculate the renormalized graph Laplacian

$$L = \tilde{\mathbf{D}}^{-\frac{1}{2}}\tilde{\mathbf{A}}\tilde{\mathbf{D}}^{-\frac{1}{2}}$$
$$\text{with } \tilde{\mathbf{A}} = \mathbf{A} + I_N, \quad \tilde{D}_{ii} = \sum_j \tilde{A}_{ij}$$

a)

$$A = \begin{bmatrix} 0 & 1 & 0 & 0 & 0 \\ 1 & 0 & 1 & 0 & 0 \\ 0 & 1 & 0 & 1 & 0 \\ 0 & 0 & 1 & 0 & 1 \\ 0 & 0 & 0 & 1 & 0 \end{bmatrix}$$

$$\tilde{A} = \begin{bmatrix} 1 & 1 & 0 & 0 & 0 \\ 1 & 1 & 1 & 0 & 0 \\ 0 & 1 & 1 & 1 & 0 \\ 0 & 0 & 1 & 1 & 1 \\ 0 & 0 & 0 & 1 & 1 \end{bmatrix}$$

$$\tilde{D} = \mathrm{diag}([2\ 3\ 3\ 3\ 2])$$

$$\tilde{D}^{-\frac{1}{2}} = \begin{bmatrix} \sqrt{\frac{1}{2}} & 0 & 0 & 0 & 0 \\ 0 & \sqrt{\frac{1}{3}} & 0 & 0 & 0 \\ 0 & 0 & \sqrt{\frac{1}{3}} & 0 & 0 \\ 0 & 0 & 0 & \sqrt{\frac{1}{3}} & 0 \\ 0 & 0 & 0 & 0 & \sqrt{\frac{1}{2}} \end{bmatrix}$$

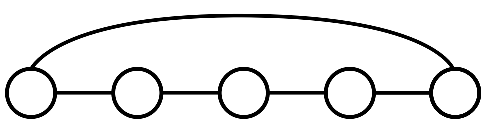
$$L = \begin{bmatrix} \frac{1}{2} & \sqrt{\frac{1}{6}} & 0 & 0 & 0 \\ \sqrt{\frac{1}{6}} & \frac{1}{3} & \frac{1}{3} & 0 & 0 \\ 0 & \frac{1}{3} & \frac{1}{3} & \frac{1}{3} & 0 \\ 0 & 0 & \frac{1}{3} & \frac{1}{3} & \sqrt{\frac{1}{6}} \\ 0 & 0 & 0 & \sqrt{\frac{1}{6}} & \frac{1}{2} \end{bmatrix}$$

(b) Find a convolution filter $W \in \mathbb{R}^3$ for a standard discrete convolution

$$(W * x)_i = \sum_{\tau=-1}^{1} W_\tau x_{i+\tau},$$

which is equivalent to performing the graph convolution above, or explain why it does not exist.
For the graph convolution to have a corresponding discrete convolution, L needs to be a Toeplitz matrix. This is not the case because of the normalization with the node degrees $\tilde{D}$.

(c) Next we will consider the graph convolution on a 1d grid with periodic boundary conditions:



Find a convolution filter $W \in \mathbb{R}^3$ for a standard discrete convolution with periodic boundary conditions

$$(W * x)_i = \sum_{\tau=-1}^{1} W_\tau x_{[(i+\tau) \bmod 5]},$$

which is equivalent to performing the graph convolution above, or explain why it does not exist.
Since all nodes in the graph are of degree 3, the Laplacian is a Toeplitz matrix:

$$L = \begin{bmatrix} \frac{1}{3} & \frac{1}{3} & 0 & 0 & \frac{1}{3} \\ \frac{1}{3} & \frac{1}{3} & \frac{1}{3} & 0 & 0 \\ 0 & \frac{1}{3} & \frac{1}{3} & \frac{1}{3} & 0 \\ 0 & 0 & \frac{1}{3} & \frac{1}{3} & \frac{1}{3} \\ \frac{1}{3} & 0 & 0 & \frac{1}{3} & \frac{1}{3} \end{bmatrix}$$

Therefore, there is a corresponding discrete convolution with $W = \left[\frac{1}{3}\ \frac{1}{3}\ \frac{1}{3}\right]$

Exercise 3: Programming (30 P)

Download the programming files on ISIS and follow the instructions.