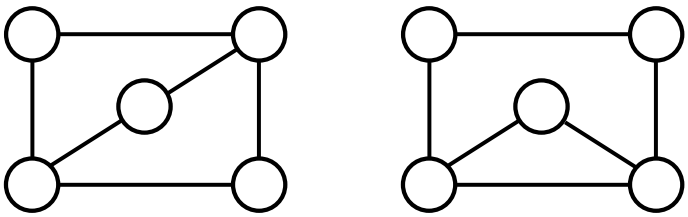
Exercises for the course
Deep Learning 2
Summer Semester 2025

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

Exercise Sheet **Graph Neural Networks**

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.

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

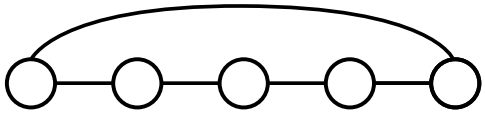
$$L = \tilde{\mathbf{D}}^{-\frac{1}{2}} \tilde{\mathbf{A}} \tilde{\mathbf{D}}^{-\frac{1}{2}}$$
$$\text{with } \tilde{\mathbf{A}} = \mathbf{A} + I_N, \quad \tilde{D}_{ii} = \sum_j \tilde{A}_{ij}$$

(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.

(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.

Exercise 3: Programming (50 P)

Download the programming files on ISIS and follow the instructions.