

Homework 6: Graph neural networks

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YOUR NAME

Instruction

- This homework is due at 11:59:59 p.m. on ** Aug. 1st, 2022.
- The write-up must be a soft copy .pdf file edited by L^AT_EX.
- The overall submission should be a .pdf file named by xxx(student id)-xxx(name)-Assignment6.pdf

Q1. Permutation-equivalent property of PointNet [50 points]

This problem revisits PointNet, a fundamental tool for 3D point cloud processing. You will show the permutation-equivalent property of PointNet.

Let $X \in \mathbb{R}^{N \times 3}$ be a 3D point cloud with N points. As we mentioned in the lecture, PointNet works as follows

$$y = \text{PointNet}(X) = \text{maxpool}_1(\text{ReLU}(\text{ReLU}(XW_1)W_2)),$$

where $W_1 \in \mathbb{R}^{3 \times d_1}$ and $W_2 \in \mathbb{R}^{d_1 \times d_2}$ are trainable parameters and $\text{maxpool}_1(\cdot)$ is a maximum pooling operation that downsamples the input along its first dimension by taking the maximum value.

- What is the dimension of the output y ?
- Let $P \in \{0, 1\}^{N \times N}$ be a permutation matrix, where each row and each column P sums up to one; see https://en.wikipedia.org/wiki/Permutation_matrix. Let $y' = \text{PointNet}(Px)$. Please show the relationship between y and y' and explain why.
- Does the training of W_1 and W_2 effect the relationship between y and y' ? Please also explain why.

Q2. Oversmoothing issue of GCNs [50 points]

This problem revisits graph convolutional networks (GCNs). You will show the oversmoothing issue of GCNs.

Let $G(\mathcal{V}, \mathcal{E})$ be a graph, where \mathcal{V} is the set with N nodes. The graph adjacency matrix is $A \in \mathbb{R}^{N \times N}$, where each element $A_{i,j}$ reflects the connectivity relationship between the i th node and the j th node. Let $X \in \mathbb{R}^{N \times F}$ be a node feature matrix. One graph convolutional layer works as follows

$$Y = \text{GCL}(X) = \text{ReLU}(AXW),$$

where $W \in \mathbb{R}^{F \times D}$ is a matrix of trainable parameters.

a) What is the dimension of the output Y ?

b) Suppose that we remove $\text{ReLU}(\cdot)$ and the trainable matrix W_i in the i th layer is independent, yet has the same dimension. Please write down the most compact form of K layers of graph convolution and explain why. Note that each W_i is trainable and the multiplication of two trainable matrices is also trainable.

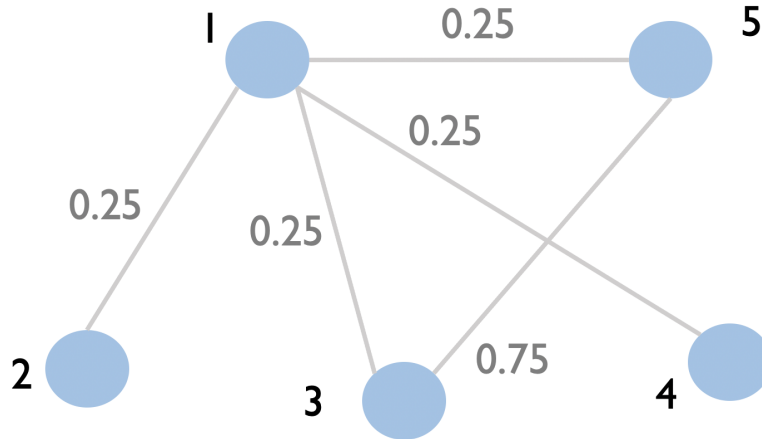


Figure 1: A 5-node graph with undirected, yet weighted edges.

c) Please write down the graph adjacency matrix A in Figure 1.

d) What are A^{10} , A^{100} and A^{1000} ? What is the trend you observe? Also please explain why.

e) Let $x_1 = [1000, 0, 0, 0, 0]^T$ and $x_2 = [0, 0, 0, 1000, 0]^T$. What are $A^{1000}x_1$ and $A^{1000}x_2$? What is the trend you observe? Also please explain why.

Gaussian Mixture Model using 2D Multivariate Gaussians each of as N components: Cholesky decomposition and affine transformation for sampling: