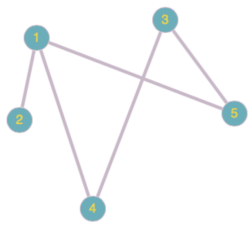
Homework 2

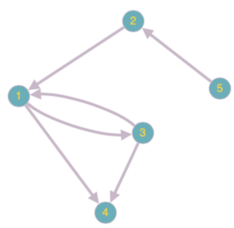
Graph Neural Networks Course

1 Task 1. Constructing a Computation Graph (6 points)

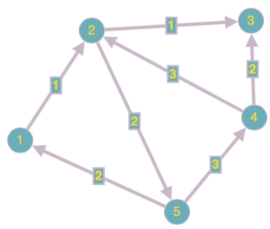
1. Construct a computation graph for vertices 1, 2 (undirected graph).



2. Construct a computation graph for vertices 1, 2 (directed graph).



3. Construct a computation graph for vertices 1, 2 (heterogeneous graph).



2 Task 2. When WL Fails (5 points)

Come up with an example where the WL kernel cannot distinguish between two graphs, even though they are not isomorphic. Can you think of an improvement to the WL algorithm that would allow it to cover the class of your example (a non-trivial improvement)?

3 Task 3. General Form for Message Passing (2 points)

In general, the layer for a vertex is recorded as follows:

$$h_u^{(k)} = \sigma\left(\mathbf{W}_{self} h_u^{(k-1)} + \mathbf{W}_{neigh} \sum_{v \in N(u)} h_v^{(k-1)} + \mathbf{b}^{(k)}\right) \tag{1}$$

where $\mathbf{W}_{self}, \mathbf{W}_{neigh}$ are weight matrices, and $h_u^{(k)}$ is the output at the k-th layer for vertex u.

Rewrite this for the entire graph (the bias term can be omitted). Hint: You may denote the adjacency matrix as A.

4 Task 4. Aggregation Function Properties (2 points)

The three most common aggregation functions are:

$$\text{aggregate}_{\text{sum}}\left(\{h_u^{(k-1)}, \forall u \in \mathcal{N}(v)\}\right) = \sum_{u \in \mathcal{N}(v)} h_u^{(k-1)} \tag{2}$$

$$\text{aggregate}_{\text{mean}}\left(\{h_u^{(k-1)}, \forall u \in \mathcal{N}(v)\}\right) = \frac{1}{|\mathcal{N}(v)|} \sum_{u \in \mathcal{N}(v)} h_u^{(k-1)} \tag{3}$$

$$\text{aggregate}_{\text{max}}\left(\{h_u^{(k-1)}, \forall u \in \mathcal{N}(v)\}\right) = \max_{u \in \mathcal{N}(v)} h_u^{(k-1)} \tag{4}$$

Maximum, mean, and sum. Come up with an example of two graphs where two vertices in each have identical initial features $h^{(0)}$, but their updated features remain the same for maximum and mean aggregations but differ when sum is used as the aggregation function.

Hint: You can take the smallest possible example in terms of size and number of dimensions.