

# CS224W-Fall 2021 Homework 1 Solutions

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## 1 Link Analysis

### 1.1 Personalized PageRank I

We first calculate the PageRank vector for each page  $i \in \{1, 2, 3, 4, 5\}$ .

$$v_1 = \frac{1}{3}v_a + \frac{1}{3}v_c + v_d$$

$$v_2 = \frac{1}{3}v_a$$

$$v_3 = \frac{1}{3}v_a + \frac{1}{3}v_b$$

$$v_4 = \frac{1}{3}v_b + \frac{1}{3}v_c$$

$$v_5 = \frac{1}{3}v_b + \frac{1}{3}v_c$$

Therefore the Personalized PageRank of Eloise, whose interests are represented by the teleport set  $\{2\}$ , is  $v_e = v_2 = \frac{1}{3}v_a$

### 1.2

$$v_f = v_5 = \frac{1}{3}v_b + \frac{1}{3}v_c$$

### 1.3

$$v_g = 0.1v_1 + 0.2v_2 + 0.3v_3 + 0.2v_4 + 0.2v_5 = \frac{1}{30}v_a + \frac{1}{30}v_c + \frac{1}{10}v_d + \frac{1}{15}v_a + \frac{1}{10}v_a + \frac{1}{10}v_b + \frac{1}{15}v_b + \frac{1}{15}v_c + \frac{1}{15}v_b + \frac{1}{15}v_c = \frac{1}{5}v_a + \frac{7}{30}v_b + \frac{1}{6}v_c + \frac{1}{10}v_d$$

### 1.4

As we have shown above, we can compute the personalized PageRank of the items that belongs to the user's teleport set.

## 1.5

Since  $\sum_{i=1}^N r_i = 1$  we have  $\mathbf{1}^\top r = 1$  Therefore:

$$\begin{aligned} r &= Ar \\ r &= (\beta M + \frac{1-\beta}{N} \mathbf{1} \mathbf{1}^\top) r \\ r &= \beta M r + \frac{1-\beta}{N} \mathbf{1} (\mathbf{1}^\top r) \\ r &= \beta M r + \frac{1-\beta}{N} \mathbf{1} \end{aligned}$$

## 2 Relational Classification I

After first iteration:  $v_1 = [\frac{1}{2}, \frac{1}{2}]$ ,  $v_2 = [\frac{3}{8}, \frac{5}{8}]$ ,  $v_3 = [\frac{5}{8}, \frac{3}{8}]$ ,  $v_4 = [\frac{15}{32}, \frac{17}{32}]$ ,  $v_8 = [\frac{31}{64}, \frac{33}{64}]$ ,  $v_9 = [\frac{31}{128}, \frac{97}{128}]$

After second iteration:  $v_1 = [\frac{1}{2}, \frac{1}{2}]$ ,  $v_2 = [\frac{51}{128}, \frac{77}{128}]$ ,  $v_3 = [\frac{81}{128}, \frac{47}{128}]$ ,  $v_4 = [\frac{241}{512}, \frac{271}{512}]$ ,  $v_8 = [\frac{365}{1024}, \frac{659}{1024}]$ ,  $v_9 = [\frac{365}{2048}, \frac{1683}{2048}]$

### 2.1

$$P(Y_3 = +) = \frac{81}{128}$$

### 2.2

$$P(Y_4 = +) = \frac{241}{512}$$

### 2.3

$$P(Y_8 = +) = \frac{365}{1024}$$

### 2.4

Vertices 1, 2, 4, 8, 9 would be classified to "-" after the second iteration.

## 3 Relational Classification II

### 3.1

The initial Node - Label pairs are Node1 - 0, Node2 - 1, Node3 - 1, Node4 - 1, Node5 - 1, Node6 - 0, Node7 - 0.

### 3.2

The link vectors for each node are  $\text{LinkV1} = (0, 1)$ ,  $\text{LinkV2} = (1, 0)$ ,  $\text{LinkV3} = (1, 1)$ ,  $\text{LinkV4} = (1, 0)$ ,  $\text{LinkV5} = (1, 1)$ ,  $\text{LinkV6} = (1, 1)$ ,  $\text{LinkV7} = (1, 1)$

After the first iteration, the predicted labels are Node1 - 0, Node2 - 0, Node3 - 0, Node4 - 0, Node5 - 0, Node6 - 0, Node7 - 0.

### 3.3

After the second iteration, the link vector for each node are the same  $(1, 0)$   
The predicted labels are all 0.

### 3.4

The labels assigned by the iterative classification algorithm have converged.

## 4 GNN Expressiveness

### 4.1

The two nodes would have different representations after 3 iterations(layers) of message passing. The red node in the first graph would have representation 18, and the red node in the second graph would have representation 17.

### 4.2

The random walk matrix  $M$  is defined as follow

$$M = \begin{bmatrix} 0 & 0.5 & 0 & 0.5 \\ 0.5 & 0 & 0 & 0.5 \\ 0 & 0 & 0 & 1 \\ \frac{1}{3} & \frac{1}{3} & \frac{1}{3} & 0 \end{bmatrix}$$

Where the  $i$ th row corresponds with node  $i$  in the graph.

The eigenvector has an eigenvalue of 1 is  $[\frac{1}{4}, \frac{1}{4}, \frac{1}{4}, \frac{1}{4}]$

### 4.3

The transition matrix  $M = D^{-1}A$

### 4.4

The new transition matrix  $\tilde{M} = I + D^{-1}A$  where  $I$  is the identity matrix with same dimensions as  $A$ .

## 4.5

A non rigorous proof:

Since the graph is connected and has no bipartite components, the transtion matrix  $M = D^{-1}A$  has eigenvalue 1 with eigenvector  $r$ . After a sufficient amount of iterations, the node features would converge to  $r$  and applying the transition matrix  $M$  to it does not change since  $r = Mr$ .

## 4.6

The aggregation function for Breadth-First-Search is defined as follow

$$h_i^{(l+1)} = \begin{cases} 0 & \sum_{j \in \mathcal{N}_i} h_j^{(l)} \\ 1 & \text{else} \end{cases}$$

# 5 Node Embedding and its relation to Matrix Factorization

## 5.1

Here the decoder is the inner product of the encoded vectors  $z_u^T z_v$

## 5.2

The minimization objective becomes  $\min_z \|A - Z^T W Z\|_2$

## 5.3

(I am not sure of my answer right here.) If we want the matrix factorization of  $\min_z \|A - Z^T W Z\|_2$  equivalent to the learning of the eigendecomposition of adjacent matrix  $A$ , we need the weight matrix  $W$  to be an diagonal matrix with  $A$ 's eigenvalues on its diagonal entries.

## 5.4

Let  $A'$  be the matrix where  $A'_{ij} = 1$  if  $i$  and  $j$  are connected or  $i$  is  $j$ 's two hop neighbor. Then the matrix factorization problem would be

$$\min_z \|A - Z^T Z\|_2$$

## 5.5

The nodes in the left clique would have a representation, whereas the nodes in the right clique would have an entirely different representation, even through they are structurally the same.

## 5.6

In `node2vec`, you can arrive at any node within that clique with same probability.

In `struct2vec`, you can also arrive at any node within the second clique. But the probability for the green node is not the same as the probability for the blue node.

## 5.7

Because different  $g_k$  capture different types of structural information.

## 5.8

All of the nodes with same degrees are represented with the same color (shown in the picture in blue), whereas the node with an additional degree have a different representation (shown in green).