Hands-on: GNN

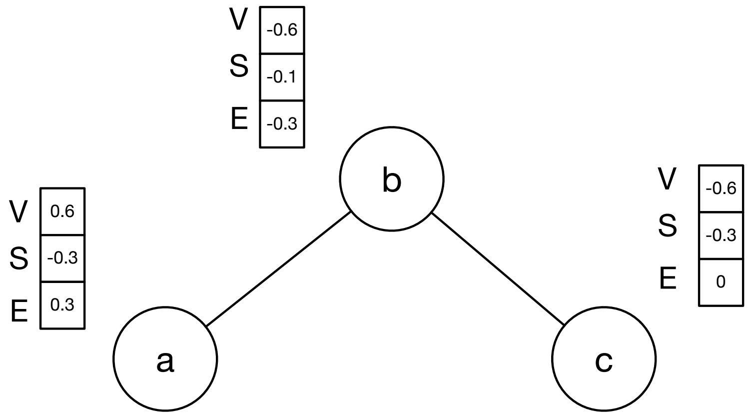

Figure 1: first network

1 Part 1: GNN

1. Forward pass of the GNN: adjacency matrix

   Fig. 1 represent parts of a social network, in which node corresponds to individuals. Let's consider it a network of politicians, with edges corresponding to belonging to a same group (political party or other groups of influence). Each individual has 3 attributes, corresponding to their political opinion, regarding 3 axis: V, Environment, S: social, E: economic . Values range from -1 (leftmost opinion) to +1 (rightmost opinion)

   (a) We will decompose the computation of a forward pass of a GNN. Let us consider the following equation of a simple GCN, using the same terminology as in the class: $\hat{A}H$. Write both matrices, and the result of the appropriate matrix multiplication.

   (b) Write the new attributes/embeddings obtained after a forward pass of the GCN layer, for each node

   (c) Confirm the intepretation of those values directly from the graph

   (d) considering now a GCN defined as $\hat{D}^{-1}\hat{A}H$, write $\hat{D}^{-1}$ and $\hat{D}^{-1}\hat{A}$ in matrix form, compute the resulting embeddings for the nodes, and then check the interpretation in graph terms.

2. Adding the weights

   Consider now that we obtained, by training on the rest of the graph, a weight Matrix W such as

$$W = \begin{vmatrix} -1 \\ 0 \\ 6 \end{vmatrix}$$

   (a) Compute the operation $\hat{D}^{-1}\hat{A}HW$ (you can reuse previous results)

   (b) Report the new attributes/embeddings for nodes A,B,C.

   (c) This weight matrix corresponds, for instance, to the task of predicting the vote of each individual for a particular election, on a particular law. What do you think is the theme of this law, i.e., for/against environment, economy, etc.

   (d) What is the most likely vote for each individual?

(e) Without the network, with the same law W, what would have been the vote of each individual? (HW)

(f) Give a simple (1-2 sentence) description of the role played by the network on each person's decision.

(g) Let us assume that the complete GCN Layer is $ReLU(\hat{D}\hat{A}HW)$. Give the final attributes/embeddings for A,B,C after this layer.

3.

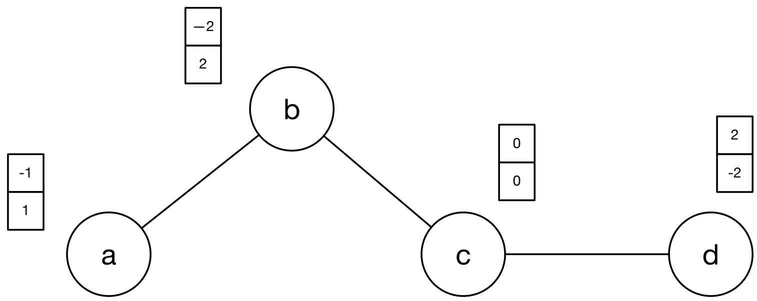

Figure 2: first network

2 Part 2: GAE

Let's consider the network represented in fig. 2.

(a) Write down the corresponding adjacency matrix

(b) Assuming an encoder composed of a single layer of GCN defined as $\hat{D}^{-1}\hat{A}H$ (we do not use learnable weights W for simplicity in this exercise), compute the resulting node embeddings (you do not have to write the full matrix operation)

(c) Using a dot product as Decoder, compute a prediction score for each node pair, seen and unseen. Represent it as a matrix organized as an adjacency matrix.

(d) For a loss function to work on this model, we should be able to compare predicted values with observed values, i.e., the adjacency matrix. Problem: computed values are not between 0 and 1. What function should we use to solve this problem? Compute the adjusted output matrix.

(e) Assuming this transformation, compute the reconstruction error (i.e., comparing with the original adjacency matrix) using the Binary Cross Entropy. Reminder:

$$\text{Loss} = -\frac{1}{N}\sum_{i=1}^{N}\left[y_i \log(\hat{y}_i) + (1-y_i)\log(1-\hat{y}_i)\right]$$

Where:

- N is the total number of elements
- y_i is the actual value from the adjacency matrix.
- $\hat{y}_i$ is the predicted probability from the adjusted output matrix.