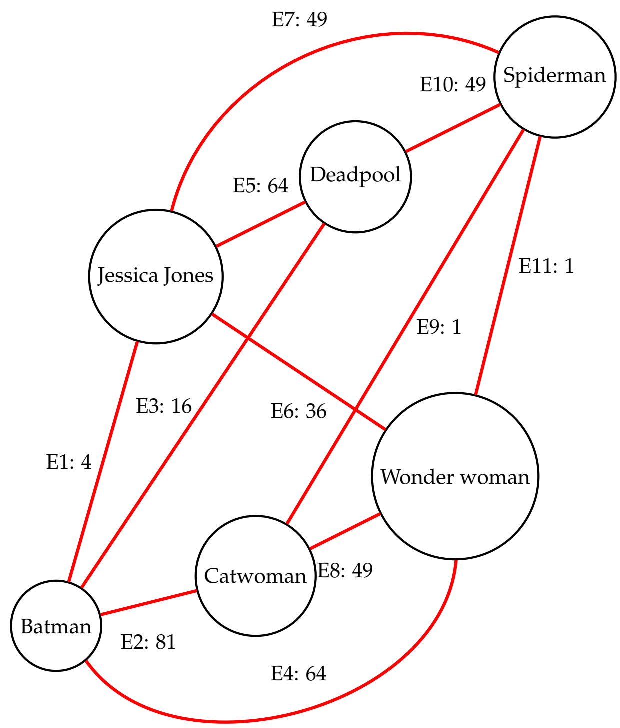
MTH793P Advanced Machine Learning, Semester B, 2023/24

Coursework 1 Example Solution

Graph-based binary classification

1. Write down the incidence matrix for the following weighted, undirected graph:



   Any missing edges correspond to weights of zero between the two nodes. Order the columns of the incidence matrix alphabetically according to the vertex name and the rows according to the edge numbering (E1, E2, E3, ...).

2. Compute the corresponding graph Laplacian for the incidence matrix in Exercise (1).

3. We want to use the graph from Question (1) to determine whether a node in the graph belongs to the class "Marvel" or the class "DC". Suppose we are in a semi-

supervised setting, where the node "Deadpool" is already labelled $v_{\text{Deadpool}} = 0$ (class "Marvel") and the node "Catwoman" is labelled as $v_{\text{Catwoman}} = 1$ (class "DC"). Determine the labels for all remaining nodes, and classify each node.

4. Repeat the previous exercises in Python by following the steps outlined in the template Jupyter notebook.

5. Compute the second eigenvector, i.e. the eigenvector that corresponds to the second smallest eigenvalue, of the graph-Laplacian in Python. What do you observe?

Solution:

1. The incidence matrix for the displayed graph is

$$M = \left(\begin{array}{c|cccccc}
\text{E1} & -2 & 0 & 0 & 2 & 0 & 0 \\
\text{E2} & -9 & 9 & 0 & 0 & 0 & 0 \\
\text{E3} & -4 & 0 & 4 & 0 & 0 & 0 \\
\text{E4} & -8 & 0 & 0 & 0 & 0 & 8 \\
\text{E5} & 0 & 0 & -8 & 8 & 0 & 0 \\
\text{E6} & 0 & 0 & 0 & -6 & 0 & 6 \\
\text{E7} & 0 & 0 & 0 & -7 & 7 & 0 \\
\text{E8} & 0 & -7 & 0 & 0 & 0 & 7 \\
\text{E9} & 0 & -1 & 0 & 0 & 1 & 0 \\
\text{E10} & 0 & 0 & -7 & 0 & 7 & 0 \\
\text{E11} & 0 & 0 & 0 & 0 & -1 & 1 \\
\hline
 & \text{Batman} & \text{Catwoman} & \text{Deadpool} & \text{J. Jones} & \text{Spiderman} & \text{W.woman}
\end{array}\right)$$

2. The corresponding graph Laplacian then reads

$$L = M^\top M = \left(\begin{array}{c|cccccc}
\text{Batman} & 165 & -81 & -16 & -4 & 0 & -64 \\
\text{Catwoman} & -81 & 131 & 0 & 0 & -1 & -49 \\
\text{Deadpool} & -16 & 0 & 129 & -64 & -49 & 0 \\
\text{J. Jones} & -4 & 0 & -64 & 153 & -49 & -36 \\
\text{Spiderman} & 0 & -1 & -49 & -49 & 100 & -1 \\
\text{W.woman} & -64 & -49 & 0 & -36 & -1 & 150 \\
\hline
 & \text{Batman} & \text{Catwoman} & \text{Deadpool} & \text{J. Jones} & \text{Spiderman} & \text{W.woman}
\end{array}\right)$$

3. From the lecture notes we know that the label vector $v \in \mathbb{R}^5$ can be decomposed as

$$v = P_U^\top \tilde{v} + P_L^\top y \,,$$

where P_L denotes the projection of v onto the known (labeled) indices, and P_U onto the unknown indices. The known indices are denoted by y, the unknown by $\tilde{v}$. For

$$v = \begin{pmatrix} v_{\text{Batman}} \\ v_{\text{Catwoman}} \\ v_{\text{Deadpool}} \\ v_{\text{Jessica Jones}} \\ v_{\text{Spiderman}} \\ v_{\text{Wonderwoman}} \end{pmatrix}$$

we know the second and third entry; the second belongs to the class "DC" and therefore takes on the value $v_{\text{Catwoman}} = 1$, whereas the third belongs to the class "Marvel", hence $v_{\text{Deadpool}} = 0$. Thus, for $y = \begin{pmatrix} 1 & 0 \end{pmatrix}^\top$ we have

$$v = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} \tilde{v} + \begin{pmatrix} 0 & 0 \\ 1 & 0 \\ 0 & 1 \\ 0 & 0 \\ 0 & 0 \\ 0 & 0 \end{pmatrix} \begin{pmatrix} 1 \\ 0 \end{pmatrix} .$$

From the lecture notes we also know that we can estimate $\tilde{v}$ via

$$\begin{aligned} \tilde{v} &= \arg\min_{\overline{v}} \left\| M \left(P_U^\top \overline{v} + P_L^\top y \right) \right\|^2 , \\ &= - \left(P_U L P_U^\top \right)^{-1} \left(P_U L P_L^\top y \right) , \end{aligned}$$

which for our matrices reads

$$\begin{pmatrix} 165 & -4 & 0 & -64 \\ -4 & 153 & -49 & -36 \\ 0 & -49 & 100 & -1 \\ -64 & -36 & -1 & 150 \end{pmatrix} \tilde{v} = \begin{pmatrix} 81 \\ 0 \\ 1 \\ 49 \end{pmatrix} ,$$

Solving this linear system leads to the (approximate) solution

$$\tilde{v} \approx \begin{pmatrix} 0.7727 \\ 0.2293 \\ 0.1295 \\ 0.7123 \end{pmatrix} .$$

Rounding all values above $1/2$ to one and below $1/2$ to zero then yields the classification

$$v = \begin{pmatrix} v_{\text{Batman}} \\ v_{\text{Catwoman}} \\ v_{\text{Deadpool}} \\ v_{\text{Jessica Jones}} \\ v_{\text{Spiderman}} \\ v_{\text{Wonderwoman}} \end{pmatrix} = \begin{pmatrix} 1 \\ 1 \\ 0 \\ 0 \\ 0 \\ 1 \end{pmatrix} .$$

4. The solution for the computational parts are given in a separate Jupyter notebook.