Machine Learning for Graphs and Sequential Data Exercise Sheet 13

Graphs: Semi-Supervised Learning

Label Propagation

Problem 1: The goal in Label Propagation is to find a labeling $\boldsymbol{y} \in \{0,1\}^N$ that minimizes the energy $\min_{\boldsymbol{y}} \frac{1}{2} \sum_{ij} \boldsymbol{w}_{ij}(y_i - y_j)^2$ subject to $y_i = \hat{y}_i \ \forall i \in S$ where the set of nodes V has been partitioned into the labeled nodes S and the unlabeled nodes U, $w_{ij} \geq 0$ is the non-negative edge weight and $\hat{y}_i$ are the observed labels.

Following from the first observation regarding the Laplacian, the minimization problem can be rewritten and then relaxed to $\min_{\boldsymbol{y} \in \mathbb{R}^N} \boldsymbol{y}^T \boldsymbol{L} \boldsymbol{y}$ subject to the same constraints. Show that the closed form solution is

$$\boldsymbol{y}_U = -\boldsymbol{L}_{UU}^{-1} \cdot \boldsymbol{L}_{US} \cdot \hat{\boldsymbol{y}}_S$$

where w.l.o.g. we assume that the Laplacian matrix is partitioned into blocks for labeled and unlabeled nodes as

$$\boldsymbol{L} = \begin{pmatrix} \boldsymbol{L}_{SS} & \boldsymbol{L}_{SU} \\ \boldsymbol{L}_{US} & \boldsymbol{L}_{UU} \end{pmatrix}.$$

PPNP

Problem 2: The iterative equation of PPNP is given by

$$\boldsymbol{H}^{(l+1)} = (1-\alpha)\hat{\boldsymbol{A}}\boldsymbol{H}^{(l)} + \alpha \boldsymbol{H}^{(0)}$$

where $\hat{\boldsymbol{A}} = \tilde{\boldsymbol{D}}^{-\frac{1}{2}} \tilde{\boldsymbol{A}} \tilde{\boldsymbol{D}}^{-\frac{1}{2}}$ is the propagation matrix. Derive the closed form solution for infinitely many propagation steps.

Hint: If we have for a matrix $\boldsymbol{T}$ that all its eigenvalues λ are strictly between -1 and 1, an equivalent matrix formulation of the geometric series formula holds and

$$\sum_{k=0}^{\infty} \boldsymbol{T}^k = (\boldsymbol{I} - \boldsymbol{T})^{-1}.$$

Hint: The eigenvalues λ_i of the normalized Laplacian $\boldsymbol{L} = \boldsymbol{I} + \boldsymbol{D}^{-\frac{1}{2}} \boldsymbol{A} \boldsymbol{D}^{-\frac{1}{2}}$ are $0 \leq \lambda_i \leq 2$.