CS224W Homework 3

Due: November 14, 2024

1 GNNs as MLP of eigenvectors [20 points]

1.1 Batch Node Update [2 points]

Consider the update for Graph Isomorphism Network:

$$\mathbf{x}_v^{(l+1)} = \texttt{MLP}\left((1+\epsilon)\,\mathbf{x}_v^{(l)} + \sum_{u \in \mathcal{N}(v)} \mathbf{x}_u^{(l)}\right), \tag{1}$$

where $\mathbf{x}_v^{(l)} \in \mathbb{R}^{d_l}$ is the embedding of node v at layer l. Let $\mathbf{X}^{(l)} \in \mathbb{R}^{N \times d_l}$ be a matrix containing the embeddings of all the nodes in the graph, i.e., $\mathbf{X}^{(l)}[:, v] = \mathbf{x}_v^{(l)}$. Also, let $\mathbf{A} \in \{0,1\}^{N \times N}$ represent the adjacency matrix of the graph. Write down the update of $\mathbf{X}^{(l+1)}$ as a function of $\mathbf{X}^{(l)}$ and $\mathbf{A}$.

★ **Solution** ★

$$\mathbf{X}^{(l+1)} = \texttt{MLP}\left(((1+\epsilon)\,\mathbf{I} + \mathbf{A})\,\mathbf{X}^{(l)}\right)$$

1.2 Single Layer MLP [2 points]

Assume that $\texttt{MLP}()$ represents a single layer MLP with no bias term. Write down the update of $\mathbf{X}^{(l+1)}$ as a function of $\mathbf{X}^{(l)}$ and $\mathbf{A}$, and the trainable parameters $\mathbf{W}^{(l)}$ of layer l.

★ **Solution** ★

$$\mathbf{X}^{(l+1)} = \sigma\left((\mathbf{A} + (1+\epsilon)\ \mathbf{I})\ \mathbf{X}^{(l)}\mathbf{W}^{(l)}\right)$$

1.3 Eigenvector Extension [4 points]

Let $\{\lambda_n, \mathbf{v}_n\}_{n=1}^{N}$ represent the eigenvalues and eigenvectors of the graph adjacency. Then we can write $\mathbf{A} = \mathbf{V}\boldsymbol{\Lambda}\mathbf{V}^T$, where $\mathbf{V} \in \mathbb{R}^{N\times N}$ is the matrix of eigenvectors with $\mathbf{V}[:, n] = \mathbf{v}_n$ and $\boldsymbol{\Lambda} \in \mathbb{R}^{N\times N}$ is the diagonal matrix of eigenvalues with $\boldsymbol{\Lambda}[n, n] = \lambda_n$. Show that

$$\mathbf{X}^{(l+1)} = \sigma\left(\mathbf{V}\hat{\mathbf{W}}^{(l)}\right), \quad \hat{\mathbf{W}}^{(l)}[n, j] = (\lambda_n + 1 + \epsilon)\sum_{i=1}^{d_l}\mathbf{W}^{(l)}[i, j]\langle \mathbf{v}_n, \mathbf{X}^{(l)}[:, i]\rangle,$$

where $\langle\cdot\rangle$ denotes the dot product. Hint: Use the fact that the eigenvectors are orthonormal. Next, show that each feature across all nodes, $\mathbf{X}^{(l+1)}[:, i]$, can be expressed as a linear combination of eigenvectors, followed by a pointwise nonlinearity.

★ **Solution** ★

$$\hat{\mathbf{W}}^{(l)}[n, j] = (\lambda_n + 1 + \epsilon)\sum_{i=1}^{d_l}\mathbf{W}^{(l)}[i, j]\langle \mathbf{v}_n, \mathbf{X}^{(l)}[:, i]\rangle$$

$$= (\lambda_n + 1 + \epsilon)\sum_{i=1}^{d_l}\langle \mathbf{v}_n, \mathbf{X}^{(l)}[:, i]\rangle\mathbf{W}^{(l)}[i, j]$$

$$= (\lambda_n + 1 + \epsilon)\sum_{i=1}^{d_l}\left(\mathbf{v}_n^{\mathbf{T}}\,\mathbf{X}^{(l)}[:, i]\right)\mathbf{W}^{(l)}[i, j]$$

$$= (\lambda_n + 1 + \epsilon)\;\mathbf{v}_n^{\mathbf{T}}\,\mathbf{X}^{(l)}\,\mathbf{W}^{(l)}[:, j]$$

$$\hat{\mathbf{W}}^{(l)}[n, :] = (\lambda_n + 1 + \epsilon)\;\mathbf{v}_n^{\mathbf{T}}\,\mathbf{X}^{(l)}\,\mathbf{W}^{(l)}$$

$$\hat{\mathbf{W}}^{(l)} = (\Lambda + (1 + \epsilon))\;\mathbf{V}^{\mathbf{T}}\,\mathbf{X}^{(l)}\,\mathbf{W}^{(l)}$$

$$\mathbf{V}\hat{\mathbf{W}}^{(l)} = \mathbf{V}\,(\Lambda + (1 + \epsilon))\;\mathbf{V}^{\mathbf{T}}\,\mathbf{X}^{(l)}\,\mathbf{W}^{(l)}$$

$$= (\mathbf{V}\Lambda + \mathbf{V}\,(1 + \epsilon))\;\mathbf{V}^{\mathbf{T}}\,\mathbf{X}^{(l)}\,\mathbf{W}^{(l)}$$

$$= \left(\mathbf{V}\Lambda\mathbf{V}^{\mathbf{T}} + \mathbf{V}\mathbf{V}^{\mathbf{T}}\,(1 + \epsilon)\right)\,\mathbf{X}^{(l)}\,\mathbf{W}^{(l)}$$

$$= (\mathbf{A} + (1 + \epsilon)\,\mathbf{I})\;\mathbf{X}^{(l)}\,\mathbf{W}^{(l)}$$

$$\sigma(\mathbf{V}\hat{\mathbf{W}}) = \sigma\left((\mathbf{A} + (1 + \epsilon)\,\mathbf{I})\;\mathbf{X}^{(l)}\,\mathbf{W}^{(l)}\right) = \mathbf{X}^{(l+1)}$$

1.4 GraphSAGE [4 points]

Perform the same analysis for the GraphSAGE update when the aggregation function is sum pooling. Recall that the GraphSAGE update function is

$$\begin{aligned}\mathbf{x}_v^{(l+1)} &= \sigma\left(\mathbf{W}^{(l)} \cdot \mathrm{CONCAT}\left(\mathbf{x}_v^{(l)}, \mathbf{x}_{N(v)}^{(l)}\right)\right)\\ &= \sigma\left(\mathbf{W}_1^{(l)}\mathbf{x}_v^{(l)} + \mathbf{W}_2^{(l)}\mathrm{AGG}\left(\mathbf{x}_u^{(l)}, \forall u \in N(v)\right)\right)\end{aligned}$$

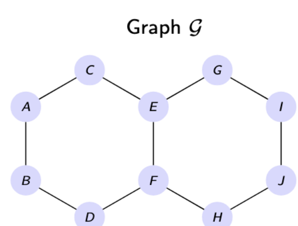
★ **Solution** ★

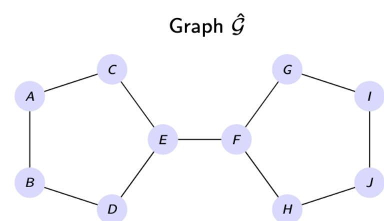
$$\mathbf{X^{(l+1)}} = \sigma\left(\mathbf{X^{(l)}W_1^{(l)}} + \mathbf{AX^{(l)}W_2^{(l)}}\right) = \sigma\left(\mathbf{V\hat{W}}\right)$$

Where

$$\hat{\mathbf{W}}^{(l)}[n, j] = \sum_{i=1}^{d_l}(\mathbf{W_1^{(l)}}[i, j] + \lambda_n \mathbf{W_2^{(l)}}[i, j])\langle \mathbf{v}_n, \mathbf{X}^{(l)}[:, i]\rangle$$

1.5 Eigendecomposition Analysis [8 points]





For graphs $\mathcal{G}$ and $\hat{\mathcal{G}}$ instantiate the graph adjacencies in Numpy, PyTorch, or PyG, and compute their eigenvalue decompositions. What do you observe?

★ **Solution** ★

Both graphs have the same eigenvalue decompositions for the adjacency matrix.

Consider a GIN where all nodes start with the same initial color, i.e., $\mathbf{x}_v^{(0)} = 1$ for all nodes $v \in \mathcal{V}$. This setup is equivalent to having $\mathbf{X}^{(0)} = \mathbf{1}$, where $\mathbf{1}$ denotes the all-one vector. This is the initialization of the WL test. Using the equations in 1.3, derive the expression for $\mathbf{X}^{(1)}$.

★ **Solution** ★

$$\mathbf{X}^{(1)} = \sigma\left(\mathbf{V}\hat{\mathbf{W}}^{(0)}\right), \quad \hat{\mathbf{W}}^{(0)}[n, j] = (\lambda_n + 1 + \epsilon)\sum_{i=1}^{d_l}\mathbf{W}^{(l)}[i, j]\langle \mathbf{v}_n, \mathbf{X}^{(0)}\rangle,$$

Observe that each column $\mathbf{X}^{(1)}[:, j]$ is a linear combination of eigenvectors, followed by a pointwise nonlinearity. What is the weight associated with each eigenvector? What factors determine this weight?

★ Solution ★

The weight associated with the n-th eigenvector in the column j of the new $\mathbf{X}$ matrix is equal to:

$$\hat{\mathbf{W}}^{(0)}[n, j] = (\lambda_n + 1 + \epsilon) \sum_{i=1}^{d_l} \mathbf{W}^{(l)}[i, j] \langle \mathbf{v}_n, \mathbf{X}^{(0)} \rangle,$$

It is determined by the associated eigenvalue, the ϵ parameter, the weight associated with column j in the original layer, and the dot product $\langle \mathbf{v}_n, \mathbf{X}^{(0)} \rangle$.

Compute the dot product $\langle \mathbf{v}_n, \mathbf{X}^{(0)} \rangle$, for each eigenvector across both graphs. What do you observe?

★ Solution ★

The result for each corresponding eigenvector is the same across both graphs.

What does the previous result suggest about $\mathbf{X}^{(1)}$ for the graphs $\mathcal{G}$ and $\hat{\mathcal{G}}$?

★ Solution ★

The result suggests that both graphs will have the same resulting $\mathbf{X}^{(1)}$ matrix.