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** ★

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

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** ★

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

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 $\mathbf{A} = \mathbf{V}\mathbf{\Lambda}\mathbf{V}^T$, where $\mathbf{V} \in \mathbb{R}^{N\times N}$ is the matrix of eigenvectors with $\mathbf{V}[:, n] = \mathbf{v}_n$ and $\mathbf{\Lambda} \in \mathbb{R}^{N\times N}$ is the diagonal matrix of eigenvalues with $\mathbf{\Lambda}[n, n] = \lambda_n$. 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** ★

$$\begin{aligned}
\hat{\mathbf{W}}^{(l)}[n, j] &= (\lambda_n + 1 + \epsilon)\sum_{i=1}^{d_l} \mathbf{W}^{(l)}[i, j]\langle \mathbf{v}_n, \mathbf{X}^{(l)}[:, i]\rangle \\
&= (\lambda_n + 1 + \epsilon)\sum_{i=1}^{d_l} \langle \mathbf{v}_n, \mathbf{X}^{(l)}[:, i]\rangle \mathbf{W}^{(l)}[i, j] \\
&= (\lambda_n + 1 + \epsilon)\sum_{i=1}^{d_l} \left(\mathbf{v}_n^{\mathbf{T}}\, \mathbf{X}^{(l)}[:, i]\right) \mathbf{W}^{(l)}[i, j] \\
&= (\lambda_n + 1 + \epsilon)\; \mathbf{v}_n^{\mathbf{T}}\, \mathbf{X}^{(l)}\, \mathbf{W}^{(l)}[:, j] \\
\hat{\mathbf{W}}^{(l)}[n, :] &= (\lambda_n + 1 + \epsilon)\; \mathbf{v}_n^{\mathbf{T}}\, \mathbf{X}^{(l)}\, \mathbf{W}^{(l)} \\
\hat{\mathbf{W}}^{(l)} &= (\Lambda + (1 + \epsilon))\; \mathbf{V}^{\mathbf{T}}\, \mathbf{X}^{(l)}\, \mathbf{W}^{(l)} \\
\mathbf{V}\hat{\mathbf{W}}^{(l)} &= \mathbf{V}\,(\Lambda + (1 + \epsilon))\; \mathbf{V}^{\mathbf{T}}\, \mathbf{X}^{(l)}\, \mathbf{W}^{(l)} \\
&= (\mathbf{V}\Lambda + \mathbf{V}\,(1 + \epsilon))\; \mathbf{V}^{\mathbf{T}}\, \mathbf{X}^{(l)}\, \mathbf{W}^{(l)} \\
&= \left(\mathbf{V}\Lambda\mathbf{V}^{\mathbf{T}} + \mathbf{V}\mathbf{V}^{\mathbf{T}}\,(1 + \epsilon)\right)\, \mathbf{X}^{(l)}\, \mathbf{W}^{(l)} \\
&= (\mathbf{A} + (1 + \epsilon)\,\mathbf{I})\; \mathbf{X}^{(l)}\, \mathbf{W}^{(l)} \\
\sigma(\mathbf{V}\hat{\mathbf{W}}) &= \sigma\left((\mathbf{A} + (1 + \epsilon)\,\mathbf{I})\; \mathbf{X}^{(l)}\, \mathbf{W}^{(l)}\right) = \mathbf{X}^{(l+1)}
\end{aligned}$$

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

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

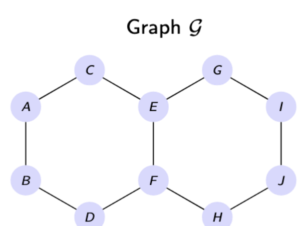
★ **Solution** ★

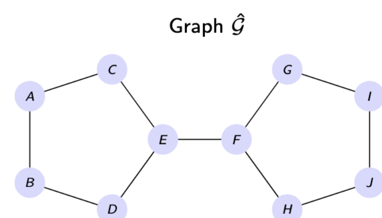
$$\mathbf{X}^{(\mathbf{l+1})} = \sigma\left(\mathbf{X}^{(\mathbf{l})}\mathbf{W}_{\mathbf{1}}^{(\mathbf{l})} + \mathbf{A}\mathbf{X}^{(\mathbf{l})}\mathbf{W}_{\mathbf{2}}^{(\mathbf{l})}\right) = \sigma\left(\mathbf{V}\hat{\mathbf{W}}\right)$$

Where

$$\hat{\mathbf{W}}^{(l)}[n,j] = \sum_{i=1}^{d_l}(\mathbf{W}_{\mathbf{1}}^{(\mathbf{l})}[i,j] + \lambda_n \mathbf{W}_{\mathbf{2}}^{(\mathbf{l})}[i,j])\langle \mathbf{v}_n, \mathbf{X}^{(l)}[:,i]\rangle$$

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 dot product is always equal to 1, because all nodes have their feature value equal to 1 and the vector $\mathbf{v_n}$ has it's norm equal to 1.

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.