Tensorized Graphs

B

26 de Setembro de 2021

1 Definitions

Considering the graph formation rule presented in Equation 1 and input distance matrix $\mathbf{D} = [d_{ij}]$, where $d_{ij} = \|\mathbf{x}_i - \mathbf{x}_j\|_2^2$ so Equation 1 can be rewritten as Equation 2.

$$\begin{aligned}(\mathbf{x}_i, \mathbf{x}_j) \in E \longleftrightarrow \|\mathbf{x}_i - \mathbf{x}_j\|_2^2 \leq \left(\|\mathbf{x}_i - \mathbf{x}_k\|_2^2 + \|\mathbf{x}_j - \mathbf{x}_k\|_2^2\right) \\ \forall\, \mathbf{x}_k \in V, (\mathbf{x}_i, \mathbf{x}_j) \neq \mathbf{x}_k\end{aligned} \tag{1}$$

$$\begin{aligned}(\mathbf{x}_i, \mathbf{x}_j) \in E \longleftrightarrow d_{ij} \leq (d_{ik} + d_{jk}) \\ \forall\, \mathbf{d}_k \in D, (\mathbf{d}_i, \mathbf{d}_j) \neq \mathbf{d}_k\end{aligned} \tag{2}$$

So, considering that $\mathbf{D}$ is given, the operation presented in inequality **??** can be accomplished by summing up all pairs of columns/rows of $\mathbf{D}, \forall i \neq j$.

2 Example

Considering the following data matrix

$$X = \begin{bmatrix} 1 & 2 & 3 \\ 4 & 5 & 6 \\ 7 & 8 & 9 \\ 10 & 11 & 12 \end{bmatrix}_{4\times 3}, \tag{3}$$

its distance matrix is stated as

$$D_X = \begin{bmatrix} \infty & 27 & 108 & 243 \\ 27 & \infty & 27 & 108 \\ 108 & 27 & \infty & 27 \\ 243 & 108 & 27 & \infty \end{bmatrix}_{4\times 4}. \tag{4}$$

The combination of $\binom{4}{2}$ yields in a vector of indexes $C_{indexes}$, such as: $C_{indexes} = [(0,1),(0,2),(0,3),(1,2),(1,3),(2,3)]$. To state the mask matrix, both indexes $i_{0,1}$ of each element $i \in C_{indexes}$ are related to the same row in $\mathbf{M}$. Therefore, in this example, the mask matrix $\mathbf{M}$ is stated as

$$M = \begin{bmatrix} 1 & 1 & 0 & 0 \\ 1 & 0 & 1 & 0 \\ 1 & 0 & 0 & 1 \\ 0 & 1 & 1 & 0 \\ 0 & 1 & 0 & 1 \\ 0 & 0 & 1 & 1 \end{bmatrix}_{6\times 4}. \tag{5}$$

Thus matrix D_{sum} — which represents the sum of every unique element in D — is given as

$$D_{sum} = \begin{bmatrix} 1 & 1 & 0 & 0 \\ 1 & 0 & 1 & 0 \\ 1 & 0 & 0 & 1 \\ 0 & 1 & 1 & 0 \\ 0 & 1 & 0 & 1 \\ 0 & 0 & 1 & 1 \end{bmatrix} \times \begin{bmatrix} \infty & 27 & 108 & 243 \\ 27 & \infty & 27 & 108 \\ 108 & 27 & \infty & 27 \\ 243 & 108 & 27 & \infty \end{bmatrix} \tag{6}$$

$$D_{sum} = \begin{bmatrix} \infty & \infty & 135 & 351 \\ \infty & 54 & \infty & 270 \\ \infty & 135 & 135 & \infty \\ 135 & \infty & \infty & 135 \\ 270 & \infty & 54 & \infty \\ 351 & 135 & \infty & \infty \end{bmatrix}_{6\times 4}. \tag{7}$$

Applying the *minpooling* operation to each row (or layer), the outcome vector is

$$D_{sumpooled} = [135, 54, 135, 135, 54, 135] \tag{8}$$

If the combination indexes $C_{indexes}$ are applied to D_X, it is possible to stack D_X in a vector of thresholds, yielding in:

$$V_{th} = [27, 108, 243, 27, 108, 27]. \tag{9}$$

Considering an element-wise comparison between $D_{sumpooled}$ and V_{th}, evaluating whether $d_{sum} \leq d_{th}, \forall d_{sum} \in D_{sumpooled}$ & $d_{th} \in V_{th}$; it is possible to calculate the adjacency vector as

$$V_A = [0, 1, 1, 0, 1, 0]. \tag{10}$$

3 Additional thoughts

Consider matrix $\mathbf{D}$ represented in Equation 11.

$$\mathbf{D} = \begin{bmatrix} d_{11} & d_{12} & d_{13} & d_{14} & d_{15} \\ d_{21} & d_{22} & d_{23} & d_{24} & d_{25} \\ d_{31} & d_{32} & d_{33} & d_{34} & d_{35} \\ d_{41} & d_{42} & d_{43} & d_{44} & d_{45} \\ d_{51} & d_{52} & d_{53} & d_{54} & d_{55} \end{bmatrix} \tag{11}$$

Consider now that a **sum convolution** is accomplished considering the following:

- Distance matrix 11 is given;
- Convolution mask is the distance matrix itself, shifted up one position, as represented in 12. The mask matrix has dimensions $(N+1) \times N$, since it is augmented with an additional row with ∞ elements for every shift-up of the convolution. In the present example, only one shift up is analysed.

$$\mathbf{D_M} = \begin{bmatrix} d_{11} & d_{12} & d_{13} & d_{14} & d_{15} \\ d_{21} & d_{22} & d_{23} & d_{24} & d_{25} \\ d_{31} & d_{32} & d_{33} & d_{34} & d_{35} \\ d_{41} & d_{42} & d_{43} & d_{44} & d_{45} \\ d_{51} & d_{52} & d_{53} & d_{54} & d_{55} \\ \infty & \infty & \infty & \infty & \infty \end{bmatrix} \tag{12}$$

- In order to accomplish the sum operation, the original distance matrix is also augmented by rows with ∞ every time the mask is shifted-up, as shown in 15 for the present example of a single shift.

$$\mathbf{D_{shifted}} = \begin{bmatrix} \infty & \infty & \infty & \infty & \infty \\ d_{11} & d_{12} & d_{13} & d_{14} & d_{15} \\ d_{21} & d_{22} & d_{23} & d_{24} & d_{25} \\ d_{31} & d_{32} & d_{33} & d_{34} & d_{35} \\ d_{41} & d_{42} & d_{43} & d_{44} & d_{45} \\ d_{51} & d_{52} & d_{53} & d_{54} & d_{55} \end{bmatrix} \tag{13}$$

- The augmentation operation with ∞ is accomplished for every shift up.

For the current example, considering $N = 5$, the mask should be shifted up 4 times in order to assess the full graph. The matrix with sum operations presented in 14, is relative to the first row of 11, after ∞ elements are discarded. In the present example, the resulting matrix has dimensions 4×5 and its extraction from the main sum matrix is subject to the way the method will be further implemented.

$$\begin{bmatrix} d_{11}+d_{21} & d_{12}+d_{22} & d_{13}+d_{23} & d_{14}+d_{24} & d_{15}+d_{25} \\ d_{11}+d_{31} & d_{12}+d_{32} & d_{13}+d_{33} & d_{14}+d_{34} & d_{15}+d_{35} \\ d_{11}+d_{41} & d_{12}+d_{42} & d_{13}+d_{43} & d_{14}+d_{44} & d_{15}+d_{45} \\ d_{11}+d_{51} & d_{12}+d_{52} & d_{13}+d_{53} & d_{14}+d_{54} & d_{15}+d_{55} \end{bmatrix} \tag{14}$$

Considering that the elements $d_{ij} \forall i = j$ of $\mathbf{D}$ can be set to ∞ too, the first column of 14 can also be discarded. Also, the elements of the sum containing $d_{ij} \forall i = j$ are set to ∞, what results finally in matrix D_1 presented in 15, which contain all sum of distances operations that are required in order to evaluate whether edges e_{12}, e_{13}, e_{14} and e_{15} belong to the graph or not.

$$D_1 = \begin{bmatrix} \infty & d_{13}+d_{23} & d_{14}+d_{24} & d_{15}+d_{25} \\ d_{12}+d_{32} & \infty & d_{14}+d_{34} & d_{15}+d_{35} \\ d_{12}+d_{42} & d_{13}+d_{43} & \infty & d_{15}+d_{45} \\ d_{12}+d_{52} & d_{13}+d_{53} & d_{14}+d_{54} & \infty \end{bmatrix} \tag{15}$$

The firs row of 15 should be compared with d_{12}, the second with d_{13} and so the first row of $\mathbf{D}$ can be compared directly with each one of the rows of $\mathbf{D}_1$. Further shifts up should allow the evaluation of the remaining edges of the graph.