Independent Study - Derivative of Laplacian formula

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1. Laplacian formula. Give the definition of normalized Laplacian formula as followed:

$$L := I - D^{\frac{1}{2}}WD^{\frac{1}{2}} \tag{1.1}$$

D is degree matrix defined as the diagnal matrix with degrees d_1, d_2, \ldots, d_n , which d_i is defined as followed:

$$d_i = \sum_{i \neq j}^n w_{ij} \tag{1.2}$$

Althought the condition of $i \neq j$ is not emphasized in [1], but this is the condition when I checked scipy.sparse.csgraph.laplacian.

Here is the steps to calculate equation 1.1

$$D^{\frac{1}{2}}WD^{\frac{1}{2}} = \begin{pmatrix} \frac{1}{\sqrt{d_1}} & 0 & \cdots & 0\\ 0 & \frac{1}{\sqrt{d_2}} & \cdots & 0\\ \vdots & \vdots & \ddots & \vdots\\ 0 & 0 & \cdots & \frac{1}{\sqrt{d_n}} \end{pmatrix} \begin{pmatrix} w_{11} & w_{12} & \cdots & w_{1n}\\ w_{21} & w_{22} & \cdots & w_{2n}\\ \vdots & \vdots & \ddots & \vdots\\ w_{n1} & w_{n2} & \cdots & w_{nn} \end{pmatrix} \begin{pmatrix} \frac{1}{\sqrt{d_1}} & 0 & \cdots & 0\\ 0 & \frac{1}{\sqrt{d_2}} & \cdots & 0\\ \vdots & \vdots & \ddots & \vdots\\ 0 & 0 & \cdots & \frac{1}{\sqrt{d_n}} \end{pmatrix}$$

$$(1.3)$$

After multiplication and the result of equation 1.1 can be rewrite as:

$$L := I - D^{\frac{1}{2}}WD^{\frac{1}{2}} = \begin{pmatrix} 1 - \frac{w_{11}}{d_1} & \frac{-w_{12}}{\sqrt{d_1 d_2}} & \cdots & \frac{-w_{1n}}{\sqrt{d_1 d_n}} \\ \frac{-w_{21}}{\sqrt{d_2 d_1}} & 1 - \frac{w_{22}}{d_2} & \cdots & \frac{-w_{2n}}{\sqrt{d_2 d_n}} \\ \vdots & \vdots & \ddots & \vdots \\ \frac{-w_{n1}}{\sqrt{d_n d_1}} & \frac{-w_{n2}}{\sqrt{d_n d_2}} & \cdots & 1 - \frac{w_{nn}}{d_n} \end{pmatrix}$$
(1.4)

and can be generalized as followed:

$$L_{i,j} = \begin{cases} \frac{-w_{i,j}}{\sqrt{d_i d_j}} & \text{if } i \neq j \\ 1 - \frac{w_{i,j}}{d_i} & \text{if } i = j, \text{ not-scipy} \\ 1 & \text{if } i = j, \text{ scipy} \end{cases}$$

$$(1.5)$$

2. Derivative of Laplacian formula. Now if we would like to take derivative of Laplacian w.r.t variable $w_{i,j}$ in the symmetric matrix W. Basically the components $L_{i,k}$, $L_{k,i}$, $L_{k,j}$, $L_{j,k}$, $L_{i,j}$, and $L_{j,i}$, where $k \neq i, k \neq j$ will need to consider.

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For position $L_{i,j}$, where $i \neq j$:

$$L_{i,j} = L_{j,i} = \frac{-w_{i,j}}{\sqrt{d_i d_j}}$$

$$\frac{\partial L_{i,j}}{\partial w_{i,j}} = \frac{\partial L_{j,i}}{\partial w_{i,j}} = \frac{-1}{\sqrt{d_i d_j}} + \frac{w_{i,j}}{2(d_i d_i)^{\frac{3}{2}}} (\frac{\partial d_i}{\partial w_{i,j}} d_j + d_i \frac{\partial d_j}{\partial w_{i,j}})$$

$$= \frac{-1}{\sqrt{d_i d_j}} + \frac{w_{i,j} (d_i + d_j)}{2(d_i d_i)^{\frac{3}{2}}}$$
(2.1)

For position $L_{i,j}$, where i = j:

$$L_{i,j} = 1 - \frac{w_{i,j}}{d_i}$$

$$\frac{\partial L_{i,j}}{\partial w_{i,j}} = -(d_i)^{-1} + w_{i,j}(d_i)^{-2} \frac{\partial d_i}{\partial w_{i,j}}$$

$$= \frac{w_{i,j} - d_i}{d_i^2}$$
(2.2)

For position $L_{i,k}$, where $k \neq i$ and $k \neq j$:

$$L_{i,k} = L_{k,i} = \frac{-w_{i,k}}{\sqrt{d_i d_k}}$$

$$\frac{\partial L_{i,k}}{\partial w_{i,j}} = \frac{\partial L_{k,i}}{\partial w_{i,j}} = \frac{w_{i,k}}{2\sqrt{d_k}d_i^{\frac{3}{2}}}$$
(2.3)

For position $L_{k,j}$, where $k \neq i$ and $k \neq j$:

$$L_{k,j} = L_{j,k} = \frac{-w_{j,k}}{\sqrt{d_j d_k}}$$

$$\frac{\partial L_{k,j}}{\partial w_{i,j}} = \frac{\partial L_{j,k}}{\partial w_{i,j}} = \frac{w_{j,k}}{2\sqrt{d_k} d_j^{\frac{3}{2}}}$$
(2.4)

Therefore the generalized results is as followed:

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$$\frac{\partial L}{\partial w_{i,j}} = \begin{cases} \frac{w_{i,j} - d_i}{d_i^2} & \text{if } i = j, \text{ for position (i,j), not-scipy} \\ 0 & \text{if } i = j, \text{ for position (i,j), scipy} \\ \frac{-1}{\sqrt{d_i d_j}} + \frac{w_{i,j}(d_i + d_j)}{2(d_i d_i)^{\frac{3}{2}}} & \text{if } i \neq j, \text{ for position (i,j) and (j,i)} \\ \frac{w_{i,k}}{2\sqrt{d_k}d_i^{\frac{3}{2}}} & \text{if } k \neq i \& k \neq j, \text{ for position (i,k) and (k,i)} \\ \frac{w_{j,k}}{2\sqrt{d_k}d_j^{\frac{3}{2}}} & \text{if } k \neq i \& k \neq j, \text{ for position (k,j) and (j,k)} \\ \frac{w_{j,k} - d_i}{d_i^2} & \text{if } k = i, \text{ for position (i,i), not-scipy} \\ \frac{w_{j,k} - d_i}{d_j^2} & \text{if } k = j, \text{ for position (j,j), not-scipy} \\ 0 & \text{for any other position} \end{cases}$$

REFERENCES

[1] A TUTORIAL ON SPECTRAL CLUSTERING