Independent Study – Derivative of Laplacian formula

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

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

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:

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

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

$$D^{\frac{1}{2}} W D^{\frac{1}{2}} = \begin{pmatrix} \frac{1}{\sqrt{d_1}} & 0 & \cdots & 0 \\ 0 & \frac{1}{\sqrt{d_2}} & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & \frac{1}{\sqrt{d_n}} \end{pmatrix} \begin{pmatrix} w_{11} & w_{12} & \cdots & w_{1n} \\ w_{21} & w_{22} & \cdots & w_{2n} \\ \vdots & \vdots & \ddots & \vdots \\ w_{n1} & w_{n2} & \cdots & w_{nn} \end{pmatrix} \begin{pmatrix} \frac{1}{\sqrt{d_1}} & 0 & \cdots & 0 \\ 0 & \frac{1}{\sqrt{d_2}} & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & \frac{1}{\sqrt{d_n}} \end{pmatrix} \tag{1.3}$$

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

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

and can be generalized as followed:

$$L_{i,j} = \begin{cases} \frac{-w_{i,j}}{\sqrt{d_i d_j}} & \text{if } i \neq j \\ 1 - \frac{w_{i,j}}{d_i} & \text{if } i = j \text{, not-scipy} \\ 1 & \text{if } i = j \text{, scipy} \end{cases} \tag{1.5}$$

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 $i \neq j$:

$$\begin{aligned}
L_{i,j} &= L_{j,i} = \frac{-w_{i,j}}{\sqrt{d_i d_j}} \\
\frac{\partial L_{i,j}}{\partial w_{i,j}} &= \frac{\partial L_{j,i}}{\partial w_{i,j}} = \frac{-1}{\sqrt{d_i d_j}} + \frac{w_{i,j}}{2(d_i d_i)^{\frac{3}{2}}}(\frac{\partial d_i}{\partial w_{i,j}} d_j + d_i \frac{\partial d_j}{\partial w_{i,j}}) \\
&= \frac{-1}{\sqrt{d_i d_j}} + \frac{w_{i,j}(d_i + d_j)}{2(d_i d_i)^{\frac{3}{2}}}
\end{aligned} \tag{2.1}$$

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

$$\begin{aligned}
L_{k,k} &= 1 - \frac{w_{k,k}}{d_k} \qquad \text{, where } k \neq i,\ k \neq j \\
\frac{\partial L_{k,k}}{\partial w_{i,j}} &= \frac{w_{k,k}}{d_k^2} \frac{\partial d_k}{\partial w_{i,j}} = \frac{w_{k,k}}{d_k^2}
\end{aligned} \tag{2.2}$$

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

$$\begin{aligned}
L_{i,j} &= 1 - \frac{w_{i,j}}{d_i} \\
\frac{\partial L_{i,j}}{\partial w_{i,j}} &= -(d_i)^{-1} + w_{i,j}(d_i)^{-2} \frac{\partial d_i}{\partial w_{i,j}} \\
&= \frac{w_{i,j} - d_i}{d_i^2}
\end{aligned} \tag{2.3}$$

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

$$\begin{aligned}
L_{i,k} &= L_{k,i} = \frac{-w_{i,k}}{\sqrt{d_i d_k}} \\
\frac{\partial L_{i,k}}{\partial w_{i,j}} &= \frac{\partial L_{k,i}}{\partial w_{i,j}} = \frac{w_{i,k}}{2\sqrt{d_k} d_i^{\frac{3}{2}}}
\end{aligned} \tag{2.4}$$

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

$$\begin{aligned}
L_{k,j} &= L_{j,k} = \frac{-w_{j,k}}{\sqrt{d_j d_k}} \\
\frac{\partial L_{k,j}}{\partial w_{i,j}} &= \frac{\partial L_{j,k}}{\partial w_{i,j}} = \frac{w_{j,k}}{2\sqrt{d_k} d_j^{\frac{3}{2}}}
\end{aligned} \tag{2.5}$$

Therefore the generalized results is as followed:
for w_{ij}, where $i \neq j$:

$$\frac{\partial L}{\partial w_{i,j}} = \begin{cases} \frac{w_{k,k}}{d_k^2} & \text{, for position } (k,k) \text{, where } k = i \text{ or } k = j \text{, not-scipy} \\ 0 & \text{, for position } (k,k) \text{, where } k = i \text{ or } k = j \text{, scipy} \\ \frac{w_{i,k}}{2\sqrt{d_k} d_i^{\frac{3}{2}}} & \text{, for all position } (i,k),(k,i) \text{, where } k \neq i \\ \frac{w_{j,k}}{2\sqrt{d_k} d_j^{\frac{3}{2}}} & \text{, for all position } (j,k),(k,j) \text{, where } k \neq j \\ \frac{-1}{\sqrt{d_i d_j}} + \frac{w_{i,j}(d_i + d_j)}{2(d_i d_i)^{\frac{3}{2}}} & \text{, for position } (i,j),(j,i) \\ 0 & \text{for any other position} \end{cases} \tag{2.6}$$

for w_{ij}, where $i = j$:

$$\frac{\partial L}{\partial w_{i,j}} = \begin{cases} \frac{w_{i,j} - d_i}{d_i^2} & \text{, for position } (k,k) \text{, where } k = i = j \text{, not-scipy} \\ 0 & \text{, for position } (k,k) \text{, where } k = i \text{ or } k = j \text{, scipy} \\ \frac{w_{i,k}}{2\sqrt{d_k} d_i^{\frac{3}{2}}} & \text{, for all position } (i,k),(k,i) \text{, where } k \neq i \\ \frac{w_{j,k}}{2\sqrt{d_k} d_j^{\frac{3}{2}}} & \text{, for all position } (j,k),(k,j) \text{, where } k \neq j \\ 0 & \text{for any other position} \end{cases} \tag{2.7}$$

REFERENCES

[1] A Tutorial on Spectral Clustering