Article

Resistance Distance and Kirchhoff Index of Graphs with Pockets

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Abstract: Let $G[F, V_k, H_{uv}]$ be the graph with k pockets, where F is a simple graph of order $n \geq 1$, $V_k = \{v_1, v_2, \cdots, v_k\}$ is a subset of the vertex set of F and H_v is a simple graph of order $m \geq 2$, v is a specified vertex of H_v. Also let $G[F, E_k, H_{uv}]$ be the graph with k edge pockets, where F is a simple graph of order $n \geq 2$, $E_k = \{e_1, e_2, \cdots e_k\}$ is a subset of the edge set of F and H_{uv} is a simple graph of order $m \geq 3$, uv is a specified edge of H_{uv} such that $H_{uv} - u$ is isomorphic to $H_{uv} - v$. In this paper, we derive closed-form formulas for resistance distance and Kirchhoff index of $G[F, V_k, H_v]$ and $G[F, E_k, H_{uv}]$ in terms of the resistance distance and Kirchhoff index F, H_v and F, H_{uv}, respectively.

Keywords: Kirchhoff index; resistance distance; generalized inverse.

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0. Introduction

All graphs considered in this paper are simple and undirected. The resistance distance between vertices u and v of G was defined by Klein and Randić [1] to be the effective resistance between nodes u and v as computed with Ohm's law when all the edges of G are considered to be unit resistors. The Kirchhoff index $Kf(G)$ was defined in [1] as $Kf(G) = \sum_{u<v} r_{uv}$, where $r_{uv}(G)$ denote the resistance distance between u and v in G. Resistance distance are, in fact, intrinsic to the graph, with some nice purely mathematical interpretations and other interpretations. The Kirchhoff index was introduced in chemistry as a better alternative to other parameters used for discriminating different molecules with similar shapes and structures [1]. The resistance distance and the Kirchhoff index have attracted extensive attention due to its wide applications in physics, chemistry and others. Up till now, many results on the resistance distance and the Kirchhoff index are obtained. See ([2], [3], [4], [5]) and the references therein to know more. However, the resistance distance and Kirchhoff index of the graph is, in general, a difficult thing from the computational point of view. Therefore, the bigger is the graph, the more difficult is to compute the resistance distance and Kirchhoff index, so a common strategy is to consider complex graph as composite graph, and to find relations between the resistance distance and Kirchhoff indices of the original graphs.

Let $G = (V(G), E(G))$ be a graph with vertex set $V(G)$ and edge set $E(G)$. Let d_i be the degree of vertex i in G and $D_G = diag(d_1, d_2, \cdots d_{|V(G)|})$ the diagonal matrix with all vertex degrees of G as its diagonal entries. For a graph G, let A_G and B_G denote the adjacency matrix and vertex-edge incidence matrix of G, respectively. The matrix $L_G = D_G - A_G$ is called the Laplacian matrix of G, where D_G is the diagonal matrix of vertex degrees of G. We use $\mu_1(G) \geq u_2(G) \geq \cdots \geq \mu_n(G) = 0$ to denote the eigenvalues of L_G. For other undefined notations and terminology from graph theory, the readers may refer to [6] and the references therein ([7]-[10]).

Recently Barik [11] described the Laplacian spectrum of graph with pockets except $n+k$ Laplacian eigenvalues. Nath and Paul [12] gave the Laplacian spectrum of graph with edge pockets except $n+k$ Laplacian eigenvalues. Tian [13] gave the spectrum and signless Laplacian spectrum of graph with pockets and edge pockets except $n+k$ signless Laplacian eigenvalues. This paper

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considers the resistance distance and Kirchhoff index of graphs with pockets and edge pockets of these two new graph operations below, which come from [11] and [12], respectively.

Definition 1 [11] Let F, H_v be graphs of orders n and m, respectively, where $m \geq 2$, v be a specified vertex of H_v and $V_k = \{v_1, v_2, \cdots v_k\}$ is a subset of the vertex set of F. Let $G = G[F, V_k, H_v]$ be the graph obtained by taking one copy of F and k vertex disjoint copies of H_v, and then attaching the i-th copy of H_v to the vertex $v_i, i = 1, ..., k$, at the vertex v of H (identify v_i with the vertex v of the i-th copy). Then the copies of the graph H_v that are attached the vertices v_i, $i = 1, ..., k$, are referred to as pockets , and G is described as a graph with k pockets.

Definition 2 [12] Let F and H_{uv} be two graphs of orders n and m , respectively, where $n \geq 2$, $m \geq 3$, $E_k = \{e_1, e_2, \cdots e_k\}$ is a subset of the edge set of F and H_{uv} has a specified edge uv such that $H_{uv} - u$ is isomorphic to $H_{uv} - v$. Assume that E_k denote the subgraph of F induced by E_k. Let $G = G[F, E_k, H_{uv}]$ be the graph obtained by taking one copy of F and k vertex disjoint copies of H_{uv}, and then pasting the edge uv in the i-th copy of H_{uv} with the edge $e_i \in E_k$, where $i = 1, ..., k$. Then the copies of the graph H_{uv} that are pasted to the edges e_i, $i = 1, ..., k$, are called as edge-pockets , and G is described as a graph with k edge pockets.

Note that if a copy of H_v is attached to every vertex of F, each at the vertex v of H_v, that is, if G has n pockets, then the graph $G = G[F, V_k, H_v]$ is nothing but the corona $F \circ H$. If a copy of H_{uv} is pasted to every edge of F, each at the edge uv of H_{uv}, that is, if G has m edge-pockets, then the graph $G = G[F, E_k, H_{uv}]$ is nothing but the edge corona $F \diamond H$, where $H = H_{uv} - \{u, v\}$.

Bu et al. investigated resistance distance in subdivision-vertex join and subdivision-edge join of graphs [14]. Liu et al. [15] gave the resistance distance and Kirchhoff index of R-vertex join and R-edge join of two graphs. Motivated by the results, in this paper we obtain formulas for resistance distances and Kirchhoff index $G = G[F, V_k, H_v]$ and $G = G[F, E_k, H_{uv}]$ in terms of the resistance distance and Kirchhoff index of F, H_v and F, H_{uv}.

1. Preliminaries

The $\{1\}$-inverse of M is a matrix X such that $MXM = M$. If M is singular, then it has infinite $\{1\}$-inverse [17]. For a square matrix M, the group inverse of M, denoted by $M^{\#}$, is the unique matrix X such that $MXM = M$, $XMX = X$ and $MX = XM$. It is known that $M^{\#}$ exists if and only if $rank(M) = rank(M^2)$ ([17],[18]). If M is real symmetric, then $M^{\#}$ exists and $M^{\#}$ is a symmetric $\{1\}$-inverse of M. Actually, $M^{\#}$ is equal to the Moore-Penrose inverse of M since M is symmetric [18].

It is known that resistance distances in a connected graph G can be obtained from any $\{1\}$-inverse of G ([6], [16]). We use $M^{(1)}$ to denote any $\{1\}$-inverse of a matrix M, and let $(M)_{uv}$ denote the (u, v)- entry of M.

Lemma 1.1 ([6],[18]) Let G be a connected graph. Then

$$r_{uv}(G) = (L_G^{(1)})_{uu} + (L_G^{(1)})_{vv} - (L_G^{(1)})_{uv} - (L_G^{(1)})_{vu} = (L_G^{\#})_{uu} + (L_G^{\#})_{vv} - 2(L_G^{\#})_{uv}.$$

Let 1_n denote the column vector of dimension n with all the entries equal one. We will often use 1 to denote all-ones column vector if the dimension can be read from the context.

Lemma 1.2 ([14]) For any graph, we have $L_G^{\#} 1 = 0$.

Lemma 1.3 ([19]) Let

$$M = \begin{pmatrix} A & B \\ C & D \end{pmatrix}$$

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be a nonsingular matrix. If A and D are nonsingular, then

$$\begin{aligned} M^{-1} &= \begin{pmatrix} A^{-1}+A^{-1}BS^{-1}CA^{-1} & -A^{-1}BS^{-1} \\ -S^{-1}CA^{-1} & S^{-1} \end{pmatrix} \\ &= \begin{pmatrix} (A-BD^{-1}C)^{-1} & -A^{-1}BS^{-1} \\ -S^{-1}CA^{-1} & S^{-1} \end{pmatrix}, \end{aligned}$$

where $S = D - CA^{-1}B$.

Lemma 1.4 ([20]) Let G be a connected graph on n vertices. Then

$$Kf(G) = ntr(L_G^{(1)}) - 1^T L_G^{(1)} 1 = ntr(L_G^{\#}).$$

Lemma 1.5 ([21]) Let

$$L = \begin{pmatrix} A & B \\ B^T & D \end{pmatrix}$$

be the Laplacian matrix of a connected graph. If D is nonsingular, then

$$X = \begin{pmatrix} H^{\#} & -H^{\#}BD^{-1} \\ -D^{-1}B^T H^{\#} & D^{-1}+D^{-1}B^T H^{\#} BD^{-1} \end{pmatrix}$$

is a symmetric $\{1\}$-inverse of L, where $H = A - BD^{-1}B^T$.

2. The resistance distance and Kirchhoff index of $G[F, V_k, H_v]$

In this section, we focus on determing the resistance distance and Kirchhoff index of $G[F, V_k, H_v]$ in terms of the resistance distance and Kirchhoff index of F, H_v.

Theorem 2.1 Let F, H_v be graphs of orders n and m, respectively, where $m \geq 2$, v be a specified vertex of H_v and $V_k = \{v_1, v_2, \cdots v_k\}$ is a subset of the vertex set of F. Let $G = G[F, V_k, H_v]$ be the graph as defined in Definition 1. Then $G = G[F, V_k, H_v]$ have the resistance distance and Kirchhoff index as follows:

(i) For any $i, j \in V(F)$, we have

$$r_{ij}(G[F, V_k, H_v]) = (L^{\#}(F))_{ii} + (L^{\#}(F))_{jj} - 2(L^{\#}(F))_{ij}.$$

(ii) For any $i, j \in V(H)$, we have

$$r_{ij}(G[F, V_k, H_v]) = ((L(H)+I_{m-1})^{-1})_{ii} + (L(H)+I_{m-1})^{-1})_{jj} - 2(L(H)+I_{m-1})^{-1})_{ij}.$$

(iii) For any $i \in V(G), j \in V(H)$, we have

$$r_{ij}(G[F, V_k, H_v]) = (L^{\#}(F))_{ii} + ((L(H)+I_{m-1})^{-1} \otimes I_k)_{jj} - 2L^{\#}(F)_{ij}.$$

(iv)

$$\begin{aligned} Kf(G[F, V_k, H_v]) &= (n + k(m-1)) \left(\frac{1}{n} Kf(F) + k \sum_{i=1}^{m-1} \frac{1}{\mu_i(H)+1} \right. \\ &+ tr \left[\left(1_{m-1} \otimes \begin{pmatrix} 0^T \\ I_k \end{pmatrix} \right)^T L^{\#}(F) \left(1_{m-1}^T \otimes \begin{pmatrix} 0^T \\ I_k \end{pmatrix} \right) \right] \\ &- 1^T \left(1_{m-1}^T \otimes \begin{pmatrix} 0^T \\ I_k \end{pmatrix} \right) L^{\#}(F) \left(1_{m-1}^T \otimes \begin{pmatrix} 0^T \\ I_k \end{pmatrix} \right) 1 - k(m-1). \end{aligned}$$

Proof Since v is of degree $m-1$, H_v can be written as $H_v = \{v\} \vee H$, where H is the graph obtained from H_v, after deleting the vertex v and the edges incident to it, the Laplacian matrix of $G = G[F, V_k, H_v]$ can be written as

$$L(G) = \begin{pmatrix} L(F) + \begin{pmatrix} 0 & 0^T \\ 0 & (m-1)I_k \end{pmatrix} & -1_{m-1}^T \otimes \begin{pmatrix} 0^T \\ I_k \end{pmatrix} \\ -1_{m-1} \otimes \begin{pmatrix} 0^T \\ I_k \end{pmatrix}^T & (L(H) + I_{m-1}) \otimes I_k \end{pmatrix}.$$

By Lemma 1.5, we have

$$\begin{aligned} H &= L(F) + \begin{pmatrix} 0 & 0^T \\ 0 & (m-1)I_k \end{pmatrix} - \left(-1_{m-1}^T \otimes \begin{pmatrix} 0^T \\ I_k \end{pmatrix}\right) ((L(H) + I_{m-1}) \otimes I_k)^{-1} \\ &\quad \left(-1_{m-1} \otimes \begin{pmatrix} 0^T \\ I_k \end{pmatrix}^T\right) \\ &= L(F) + \begin{pmatrix} 0 & 0^T \\ 0 & (m-1)I_k \end{pmatrix} - (1_{m-1}^T (L(H) + I)^{-1} 1_{m-1}) \otimes \begin{pmatrix} 0 & 0^T \\ 0 & I_k \end{pmatrix} \\ &= L(F) + \begin{pmatrix} 0 & 0^T \\ 0 & (m-1)I_k \end{pmatrix} - \begin{pmatrix} 0 & 0^T \\ 0 & (m-1)I_k \end{pmatrix} \\ &= L(F), \end{aligned}$$

so $H^\# = L^\#(F)$.

According to Lemma 1.5, we calculate $-H^\# B D^{-1}$ and $-D^{-1} B^T H^\#$.

$$\begin{aligned} -H^\# B D^{-1} &= -L^\#(F) \left(-1_{m-1}^T \otimes \begin{pmatrix} 0^T \\ I_k \end{pmatrix}\right) ((L(H) + I_{m-1}) \otimes I_k)^{-1}) \\ &= L^\#(F) \left(1_{m-1}^T \otimes \begin{pmatrix} 0^T \\ I_k \end{pmatrix}\right) \end{aligned}$$

and

$$\begin{aligned} -D^{-1} B^T H^\# &= -((L(H) + I_{m-1}) \otimes I_k)^{-1}) \left(-1_{m-1} \otimes \begin{pmatrix} 0^T \\ I_k \end{pmatrix}^T\right) L^\#(F) \\ &= \left(1_{m-1} \otimes \begin{pmatrix} 0 & I_k \end{pmatrix}\right) L^\#(F). \end{aligned}$$

We are ready to compute the $D^{-1} B^T H^\# B D^{-1}$.

$$\begin{aligned} D^{-1} B^T H^\# B D^{-1} &= ((L(H) + I_{m-1})^{-1} \otimes I_k)) \left(-1_{m-1} \otimes \begin{pmatrix} 0^T \\ -I_k \end{pmatrix}^T\right) L^\#(F) \\ &\quad \left(-1_{m-1}^T \otimes \begin{pmatrix} 0^T \\ -I_k \end{pmatrix}\right) ((L(H) + I_{m-1})^{-1} \otimes I_k)) \\ &= \left(1_{m-1} \otimes \begin{pmatrix} 0^T \\ I_k \end{pmatrix}^T\right) L^\#(F) \left(1_{m-1}^T \otimes \begin{pmatrix} 0^T \\ I_k \end{pmatrix}\right). \end{aligned}$$

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Let $P = (L(H) + I_{m-1}) \otimes I_k$, $M = \left(1_{m-1} \otimes \begin{pmatrix} 0^T \\ I_k \end{pmatrix}^T\right) L^{\#}(F) \left(1^T_{m-1} \otimes \begin{pmatrix} 0^T \\ I_k \end{pmatrix}\right)$. Based on Lemma 1.5, the following matrix

$$N = \begin{pmatrix} L^{\#}(F) & L^{\#}(F)\left(1^T_{m-1} \otimes \begin{pmatrix} 0^T \\ I_k \end{pmatrix}\right) \\ \left(1_{m-1} \otimes \begin{pmatrix} 0 & I_k \end{pmatrix}\right) L^{\#}(F) & P^{-1} + M \end{pmatrix} \quad (1)$$

is a symmetric $\{1\}$-inverse of $G = G[F, V_k, H_v]$.

For any $i, j \in V(F)$, by Lemma 1.1 and the Equation (1), we have

$$r_{ij}(G[F, V_k, H_v]) = (L^{\#}(F))_{ii} + (L^{\#}(F))_{jj} - 2(L^{\#}(F))_{ij},$$

as stated in (i).

For any $i, j \in V(H)$, by Lemma 1.1 and the Equation (1), we have

$$\begin{aligned} r_{ij}(G[F, V_k, H_v]) &= ((L(H) + I_{m-1})^{-1} \otimes I_k)_{ii} + ((L(H) + I_{m-1})^{-1} \otimes I_k) \\ &\quad -2((L(H) + I_{m-1})^{-1} \otimes I_k)_{ij}, \end{aligned}$$

as stated in (ii).

For any $i \in V(F), j \in V(H)$, by Lemma 1.1 and the Equation (1), we have

$$r_{ij}(G[F, V_k, H_v]) = (L^{\#}(F))_{ii} + ((L(H) + I_{m-1})^{-1} \otimes I_k)_{jj} - 2L^{\#}(F)_{ij},$$

as stated in (iii).

By Lemma 1.4, we have

$$\begin{aligned} Kf(G[F, V_k, H_v]) &= (n + k(m-1))tr(N) - 1^T N 1 \\ &= (n + k(m-1)) \Big[tr(L^{\#}(F)) + tr((L(H) + I_{m-1})^{-1} \otimes I_k) + \\ &\quad + tr\left(\left(1_{m-1} \otimes \begin{pmatrix} 0^T \\ I_k \end{pmatrix}^T\right) L^{\#}(F) \left(1^T_{m-1} \otimes \begin{pmatrix} 0^T \\ I_k \end{pmatrix}\right)\right)\Big] - 1^T N 1. \end{aligned}$$

Note that the eigenvalues of $(L(H) + I)$ are $\mu_1(H) + 1, \mu_2(H) + 1, ..., \mu_{m-1}(H) + 1$. Then

$$tr((L(H) + I_{m-1})^{-1} \otimes I_k) = k \sum_{i=1}^{m-1} \frac{1}{\mu_i(H) + 1}. \quad (2)$$

Note that the eigenvalues of $(L(H) + I)$ are $\mu_1(H) + 1, \mu_2(H) + 1, ..., \mu_{m-1}(H) + 1$. Then

$$tr((L(H) + I_{m-1})^{-1} \otimes I_k) = k \sum_{i=1}^{m-1} \frac{1}{\mu_i(H) + 1}. \quad (3)$$

Let $P = (L(H) + I_{m-1}) \otimes I_k$, then

$$1^T P^{-1} 1 = \begin{pmatrix} 1^T_{m-1} & 1^T_{m-1} & \cdots & 1^T_{m-1} \end{pmatrix} \begin{pmatrix} P^{-1} & 0 & 0 & ... & 0 \\ 0 & P^{-1} & 0 & ... & 0 \\ 0 & 0 & ... & ... & 0 \\ 0 & 0 & 0 & ... & P^{-1} \end{pmatrix} \begin{pmatrix} 1_{m-1} \\ 1_{m-1} \\ \cdots \\ 1_{m-1} \end{pmatrix}$$

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$$= k1_{m-1}^T(L(H)+I_{m-1})^{-1}1_{m-1} = k(m-1), \tag{4}$$

Plugging (2) and (3) into $Kf(G[F,V_k,H_v])$, we obtain the required result in (iv).

3. Resistance distance and Kirchhoff index of $G[F,E_k,H_{uv}]$

In this section, we focus on determing the resistance distance and Kirchhoff index of $G[F,E_k,H_{uv}]$ in terms of the resistance distance and Kirchhoff index of F, H_{uv}.

Theorem 3.1 Let F and H_{uv} be two graphs of orders n and m , respectively, where $n \geq 2$, $m \geq 3$, $E_k = \{e_1, e_2, \cdots e_k\}$ is a subset of the edge set of F and H_{uv} has a specified edge uv such that $H_{uv} - u$ is isomorphic to $H_{uv} - v$. Let F_s be an r-regular subgraph of F induced by E_k in Definition 2. Also let $G = G[F,E_k,H_{uv}]$ and $|E_k| = k$. Then $G = G[F,E_k,H_{uv}]$ have the resistance distance and Kirchhoff index as follows:

(i) For any $i,j \in V(F)$, we have

$$\begin{aligned} r_{ij}(G[F,E_k,H_{uv}]) &= \left(L(F)+\begin{pmatrix} \frac{m-2}{2}L(F_s) & 0 \\ 0 & 0 \end{pmatrix}\right)^{\#}_{ii} + \left(L(F)+\begin{pmatrix} \frac{m-2}{2}L(F_s) & 0 \\ 0 & 0 \end{pmatrix}\right)^{\#}_{jj} \\ &\quad -2\left(L(F)+\begin{pmatrix} \frac{m-2}{2}L(F_s) & 0 \\ 0 & 0 \end{pmatrix}\right)^{\#}_{ij}. \end{aligned}$$

(ii) For any $i,j \in V(H)$, we have

$$\begin{aligned} r_{ij}(G[F,E_k,H_{uv}]) &= ((L(H)+2I_{m-2})^{-1} \otimes I_k)_{ii} + ((L(H)+2I_{m-2})^{-1} \otimes I_k)_{jj} \\ &\quad -2\left((L(H)+2I_{m-2})^{-1} \otimes I_k\right)_{ij}. \end{aligned}$$

(iii) For any $i \in V(G), j \in V(H)$, we have

$$\begin{aligned} r_{ij}(G[F,E_k,H_{uv}]) &= \left(L(F)+\begin{pmatrix} \frac{m-2}{2}L(F_s) & 0 \\ 0 & 0 \end{pmatrix}\right)^{\#}_{ii} + (L(H)+2I_{m-2})^{-1} \otimes I_k)_{jj} \\ &\quad -2\left(L(F)+\begin{pmatrix} \frac{m-2}{2}L(F_s) & 0 \\ 0 & 0 \end{pmatrix}\right)^{\#}_{ij}. \end{aligned}$$

(iv) $Kf(G[F,E_k,H_{uv}])$

$$\begin{aligned} &= (n+k(m-2))\left(tr(L(F)+\begin{pmatrix} \frac{m-2}{2}L(F_s) & 0 \\ 0 & 0 \end{pmatrix})^{\#} + k\sum_{i=1}^{m-2}\frac{1}{\mu_i(H)+2}\right. \\ &\quad +\frac{1}{4}tr\left[\left(1_{m-2}\otimes\begin{pmatrix} -R^T(F_s) & 0 \end{pmatrix}\right)\left(L(F)+\begin{pmatrix} \frac{m-2}{2}L(F_s) & 0 \\ 0 & 0 \end{pmatrix}\right)^{\#}\left(1_{m-2}^T\otimes\begin{pmatrix} -R(F_s) \\ 0 \end{pmatrix}\right)\right]\Bigg) \\ &\quad -1^T\left(1_{m-2}\otimes\begin{pmatrix} R^T(F_s) & 0 \end{pmatrix}\right)\left(L(F)+\begin{pmatrix} \frac{m-2}{2}L(F_s) & 0 \\ 0 & 0 \end{pmatrix}\right)^{\#}\left(1_{m-2}^T\otimes\begin{pmatrix} R(F_s) \\ 0 \end{pmatrix}\right)1-\frac{k}{2}(m-2). \end{aligned}$$

Proof Let F_S be an r-regular subgraph of F on the first p vertices, then the Laplacian matrix of $G = G[F,E_k,H_{uv}]$ can be written as

$$L(G) = \begin{pmatrix} L(F)+r(m-2)\begin{pmatrix} I_p & 0 \\ 0 & 0 \end{pmatrix} & 1_{m-2}^T\otimes\begin{pmatrix} -R(F_s) \\ 0 \end{pmatrix} \\ 1_{m-2}\otimes\begin{pmatrix} -R^T(F_s) & 0 \end{pmatrix} & (L(H)+2I_{m-2})\otimes I_k \end{pmatrix}.$$

By Lemma 1.5, we have

$$\begin{aligned}
H &= L(F)+r(m-2)\begin{pmatrix} I_p & 0 \\ 0 & 0 \end{pmatrix} - \left(1_{m-2}^T \otimes \begin{pmatrix} -R(F_s) \\ 0 \end{pmatrix}\right)((L(H)+2I_{m-2})\otimes I_k)^{-1} \\
&\quad \left(1_{m-2}\otimes \begin{pmatrix} -R^T(F_s) & 0 \end{pmatrix}\right) \\
&= L(F)+\begin{pmatrix} r(m-2)I_p & 0 \\ 0 & 0 \end{pmatrix} - (1_{m-2}^T(L(H)+2I_{m-2})^{-1}1_{m-2})\otimes \begin{pmatrix} R(F_s)R(F_s)^T & 0 \\ 0 & 0 \end{pmatrix} \\
&= L(F)+r(m-2)\begin{pmatrix} I_p & 0 \\ 0 & 0 \end{pmatrix} - \frac{m-2}{2}\begin{pmatrix} R(F_s)R(F_s)^T & 0 \\ 0 & 0 \end{pmatrix} \\
&= L(F)+r(m-2)\begin{pmatrix} I_p & 0 \\ 0 & 0 \end{pmatrix} - \frac{m-2}{2}\begin{pmatrix} rI_p + A(F_s) & 0 \\ 0 & 0 \end{pmatrix} \\
&= L(F)+\begin{pmatrix} \frac{m-2}{2}L(F_s) & 0 \\ 0 & 0 \end{pmatrix},
\end{aligned}$$

so

$$H^{\#} = \left(L(F)+\begin{pmatrix} \frac{m-2}{2}L(F_s) & 0 \\ 0 & 0 \end{pmatrix}\right)^{\#}.$$

According to Lemma 1.5, we calculate $-H^{\#}BD^{-1}$ and $-D^{-1}B^TH^{\#}$.

$$\begin{aligned}
-H^{\#}BD^{-1} &= -H^{\#}\left(1_{m-2}^T\otimes\begin{pmatrix} -R(F_s) \\ 0 \end{pmatrix}\right)((L(H)+2I_{m-2})\otimes I_k)^{-1}) \\
&= -H^{\#}\,(1_{m-2}^T(L(H)+2I_{m-2})^{-1})\otimes\begin{pmatrix} -R(F_s) \\ 0 \end{pmatrix} \\
&= \frac{1}{2}H^{\#}\left(1_{m-2}^T\otimes\begin{pmatrix} R(F_s) \\ 0 \end{pmatrix}\right)
\end{aligned}$$

and

$$\begin{aligned}
-D^{-1}B^TH^{\#} &= -((L(H)+2I_{m-2})\otimes I_k)^{-1}\left(1_{m-2}\otimes\begin{pmatrix} -R^T(F_s) & 0 \end{pmatrix}\right)H^{\#} \\
&= \frac{1}{2}\left(1_{m-2}\otimes\begin{pmatrix} R^T(F_s) & 0 \end{pmatrix}\right)H^{\#}.
\end{aligned}$$

We are ready to compute the $D^{-1}B^TH^{\#}BD^{-1}$.

$$\begin{aligned}
D^{-1}B^TH^{\#}BD^{-1} &= -\frac{1}{2}1_{m-2}\otimes\begin{pmatrix} R^T(F_s) & 0 \end{pmatrix}H^{\#}\,(1_{m-2}^T(L(H)+2I_{m-2})^{-1})\otimes\begin{pmatrix} -R(F_s) \\ 0 \end{pmatrix} \\
&= \frac{1}{4}\left(1_{m-2}\otimes\begin{pmatrix} -R^T(F_s) & 0 \end{pmatrix}\right)H^{\#}\left(1_{m-2}^T\otimes\begin{pmatrix} -R(F_s) \\ 0 \end{pmatrix}\right).
\end{aligned}$$

Let $P=(L(H)+2I_{m-2})\otimes I_k$, $Q=\left(1_{m-2}^T\otimes\begin{pmatrix} R(F_s) \\ 0 \end{pmatrix}\right)$. Based on Lemma 1.5, the following matrix

$$N=\begin{pmatrix} \left(L(F)+\begin{pmatrix} \frac{m-2}{2}L(F_s) & 0 \\ 0 & 0 \end{pmatrix}\right)^{\#} & \frac{1}{2}\left(L(F)+\begin{pmatrix} \frac{m-2}{2}L(F_s) & 0 \\ 0 & 0 \end{pmatrix}\right)^{\#}Q \\ \frac{1}{2}Q^T\left(L(F)+\begin{pmatrix} \frac{m-2}{2}L(F_s) & 0 \\ 0 & 0 \end{pmatrix}\right)^{\#} & P^{-1}+\frac{1}{4}Q^T\left(L(F)+\begin{pmatrix} \frac{m-2}{2}L(F_s) & 0 \\ 0 & 0 \end{pmatrix}\right)^{\#}Q \end{pmatrix} \quad (5)$$

is a symmetric $\{1\}$-inverse of $G[F,E_k,H_{uv}]$.

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For any $i, j \in V(F)$, by Lemma 1.1 and the Equation (4), we have

$$\begin{aligned} r_{ij}(G[F,E_k,H_{uv}]) &= \left(L(F) + \begin{pmatrix} \frac{m-2}{2}L(F_s) & 0 \\ 0 & 0 \end{pmatrix}\right)^{\#}_{ii} + \left(L(F) + \begin{pmatrix} \frac{m-2}{2}L(F_s) & 0 \\ 0 & 0 \end{pmatrix}\right)^{\#}_{jj} \\ &\quad -2\left(L(F) + \begin{pmatrix} \frac{m-2}{2}L(F_s) & 0 \\ 0 & 0 \end{pmatrix}\right)^{\#}_{ij}, \end{aligned}$$

as stated in (i).

For any $i, j \in V(H)$, by Lemma 1.1 and the Equation (4), we have

$$\begin{aligned} r_{ij}(G[F,E_k,H_{uv}]) &= \left((L(H)+2I_{m-2})^{-1} \otimes I_k\right)_{ii} + \left((L(H)+2I_{m-2})^{-1} \otimes I_k\right)_{jj} \\ &\quad -2\left((L(H)+2I_{m-2})^{-1} \otimes I_k\right)_{ij}, \end{aligned}$$

as stated in (ii).

For any $i \in V(F), j \in (H)$, we have

$$\begin{aligned} r_{ij}(G[F,E_k,H_{uv}]) &= \left(L(F) + \begin{pmatrix} \frac{m-2}{2}L(F_s) & 0 \\ 0 & 0 \end{pmatrix}\right)^{\#}_{ii} + (L(H)+2I_{m-2})^{-1} \otimes I_k)_{jj} \\ &\quad -2\left(L(F) + \begin{pmatrix} \frac{m-2}{2}L(F_s) & 0 \\ 0 & 0 \end{pmatrix}\right)^{\#}_{ij}, \end{aligned}$$

as stated in (iii).

By Lemma 1.4, we have

$Kf(G[F,E_k,H_{uv}])$

$$\begin{aligned} &= (n+k(m-2))tr(N) - 1^T N 1 \\ &= (n+k(m-2))\left[tr\left(L(F) + \begin{pmatrix} \frac{m-2}{2}L(F_s) & 0 \\ 0 & 0 \end{pmatrix}\right)^{\#} + tr\left((L(H)+2I_{m-2})^{-1} \otimes I_k\right) \right. \\ &\quad \left. + \frac{1}{4} tr\left((1_{m-2} \otimes \begin{pmatrix} -R^T(F_s) & 0 \end{pmatrix}\right) H^{\#}\left(1^T_{m-2} \otimes \begin{pmatrix} -R(F_s) \\ 0 \end{pmatrix}\right)\right] - 1^T N 1. \end{aligned}$$

Note that the eigenvalues of $(L(H)+2I_{m-2}) \otimes I_k$ are $\mu_1(H)+2, \mu_2(H)+2, ..., \mu_{m-1}(H)+2$. Then

$$tr\left((L(H)+2I_{m-2}) \otimes I_k\right) = k\sum_{i=1}^{m-2} \frac{1}{\mu_i(H)+2}. \tag{6}$$

Let $P = (L(H)+2I_{m-2}) \otimes I_k$, then

$$\begin{aligned} 1^T P^{-1} 1 &= \begin{pmatrix} 1^T_{m-2} & 1^T_{m-1} & \cdots & 1^T_{m-2} \end{pmatrix} \begin{pmatrix} P^{-1} & 0 & 0 & ... & 0 \\ 0 & P^{-1} & 0 & ... & 0 \\ 0 & 0 & ... & ... & 0 \\ 0 & 0 & 0 & ... & P^{-1} \end{pmatrix} \begin{pmatrix} 1_{m-2} \\ 1_{m-2} \\ \cdots \\ 1_{m-2} \end{pmatrix} \\ &= k 1^T_{m-2}(L(H)+2I_{m-2})^{-1} 1_{m-2} = \frac{k}{2}(m-2). \end{aligned} \tag{7}$$

Plugging (5) and (6) into $Kf(G[F,E_k,H_{uv}])$, we obtain the required result in (iv).

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Conflicts of Interest

The authors declare no conflict of interest.

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Sample Availability: Samples of the compounds ...... are available from the authors.