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A Note on the Kirchhoff and Additive Degree-Kirchhoff Indices of Graphs

Abstract: Two resistance-distance-based graph invariants, namely, the Kirchhoff index and the additive degree-Kirchhoff index, are studied. A relation between them is established, with inequalities for the additive degree-Kirchhoff index arising via the Kirchhoff index along with minimum, maximum, and average degrees. Bounds for the Kirchhoff and additive degree-Kirchhoff indices are also determined, and extremal graphs are characterised. In addition, an upper bound for the additive degree-Kirchhoff index is established to improve a previously known result.

Keywords: Additive Degree-Kirchhoff Index; Average Degree; Kirchhoff Index; Maximum Degree; Minimum Degree; Resistance Distance.

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1 Introduction

Let $G = (V, E)$ be a connected graph. For any two distinct vertices $i, j \in V$, the *resistance distance* [1] between them, denoted by Ω_{ij}, is defined as the net effective resistance between nodes i and j in the electrical network constructed from G when each edge is identified as a unit resistor.

Since the appearance of the concept of resistance distance, some resistance distance-based graph invariants have been defined. Among these invariants, a famous one is the *Kirchhoff index* $R(G)$ [1] (or *total effective resistance* [2], or *effective graph resistance* [3]), which is defined as the sum of resistance distances between all pairs of vertices of G:

$$R(G) = \sum_{\{i,j\} \subseteq V} \Omega_{ij}. \tag{1}$$

Then, two modifications of the Kirchhoff index have been made to take the degrees of vertices into account. The first one is the *multiplicative degree-Kirchhoff index* $R^*(G)$ introduced by Chen and Zhang [4] as

$$R^*(G) = \sum_{\{i,j\} \subseteq V} d_i d_j \Omega_{ij}, \tag{2}$$

where d_i is the degree (i.e., the number of neighbours) of the vertex i. The second one is the *additive degree-Kirchhoff* introduced by Gutman et al. [5] as

$$R^+(G) = \sum_{\{i,j\} \subseteq V} (d_i + d_j) \Omega_{ij}. \tag{3}$$

The Kirchhoff index has been widely studied, and we refer the reader to recent papers [6–19] and references therein. However, the study of the additive degree-Kirchhoff index is at an initial stage. In Ref. [5], Gutman et al. characterised n-vertex unicyclic graphs having minimum and second minimum additive degree-Kirchhoff indices. Then, Palacios and his collaborators [20, 21] exhibited various bounds for this index using elegant random walks, majorization, and Schur-convexity techniques. In Refs. [16, 18], the current authors obtained formulae for these Kirchhoffian indices of the subdivision and triangulation of a graph G, which neatly relates their Kirchhoffian indices to that of the original graph G.

In this article, first of all, we establish a relation between the Kirchhoff index and the additive degree-Kirchhoff index by expressing the additive degree-Kirchhoff index in terms of the Kirchhoff index and the Moore–Penrose inverse of the Laplacian matrix of G, so as to yield inequalities for the additive degree-Kirchhoff index via the Kirchhoff index, minimum, maximum, and average degrees. Then, we determine bounds for the Kirchhoff and additive degree-Kirchhoff indices via maximum and minimum degrees, with extremal graphs being characterised. Finally, we obtain an upper bound for the additive degree-Kirchhoff index, which improves the result obtained in Ref. [21].

2 A Relation between the Kirchhoff Index and the Additive Degree-Kirchhoff Index

Let G be a connected graph with n vertices. The *adjacency matrix* $A = (a_{ij})$ of G is the matrix with $a_{ij} = 1$ if i and j are

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adjacent and 0 otherwise. Let $D = \mathrm{diag}\{d_1, d_2, \ldots, d_n\}$ be the diagonal matrix of vertex degrees. Then, the *Laplacian matrix* of G is defined as $L = D - A$. Because the sum of each row and of each column is zero, L is singular and does not admit an (ordinary) inverse.

Let M be an $n \times m$ matrix. Then, the *Moore–Penrose inverse* of M, denoted by M^+, is [22] an $m \times n$ matrix satisfying the equations:

$$MM^+M = M, M^+MM^+ = M^+, (MM^+)^H = MM^+, (M^+M)^H = M^+M,$$

where M^H denotes the conjugate transpose of M. It is well known [22] that the Moore–Penrose inverse of a matrix exists and is unique. Let $L^+ = (l^+_{ij})$ be the Moore–Penrose inverse of L. It is shown that L^+ plays an essential role in the computation of resistance distance and the Kirchhoff index.

Theorem 1 [1] *The resistance distance between vertices i and j can be computed as*

$$\Omega_{ij} = l^+_{ii} + l^+_{ii} - 2l^+_{ij}. \tag{4}$$

Theorem 2 [23, 24] *Let G be a connected graph with n vertices. Then,*

$$R(G) = n\sum_{i=1}^{n} l^+_{ii}. \tag{5}$$

Using Theorems 1 and 2, a formula for the additive degree-Kirchhoff index is obtained.

Theorem 3 *Let G be a connected graph with n vertices and m edges. Then,*

$$R^+(G) = \frac{2m}{n}R(G) + n\sum_{i=1}^{n} d_i l^+_{ii} \tag{6}$$

Proof. By the definition of the additive degree-Kirchhoff index, we have

$$\begin{aligned}
R^+(G) &= \frac{1}{2}\sum_{i=1}^{n}\sum_{j=1}^{n}(d_i + d_j)\Omega_{ij}\\
&= \frac{1}{2}\sum_{i=1}^{n}\sum_{j=1}^{n}(d_i + d_j)(l^+_{ii} + l^+_{jj} - 2l^+_{ij})\\
&= \frac{1}{2}\sum_{i=1}^{n}\sum_{j=1}^{n}[d_i l^+_{ii} + d_j l^+_{jj} + d_i l^+_{jj} + d_j l^+_{ii} - 2(d_i l^+_{ij} + d_j l^+_{ij})]\\
&= \frac{1}{2}\sum_{i=1}^{n}\sum_{j=1}^{n}(d_i l^+_{ii} + d_j l^+_{jj}) + \frac{1}{2}\sum_{i=1}^{n}\sum_{j=1}^{n}(d_i l^+_{jj} + d_j l^+_{ii})\\
&\quad - \sum_{i=1}^{n}\sum_{j=1}^{n}(d_i l^+_{ij} + d_j l^+_{ij})\\
&= n\sum_{i=1}^{n} d_i l^+_{ii} + \sum_{i=1}^{n} d_i \sum_{j=1}^{n} l^+_{jj} - \sum_{i=1}^{n}\sum_{j=1}^{n}(d_i l^+_{ij} + d_j l^+_{ij}).
\end{aligned} \tag{7}$$

By the fact that $\sum_{i=1}^{n} d_i = 2m$ and $n\sum_{j=1}^{n} l^+_{jj} = R(G)$, it follows that

$$\sum_{i=1}^{n} d_i \sum_{j=1}^{n} l^+_{jj} = \frac{2m}{n}R(G). \tag{8}$$

On the other hand, by the fact that L^+ is symmetric and that the n–vector $\mathbf{1}$ with all entries equal to 1 is a 0-eigenvalue eigenvector of L^+, that is, $L^+\mathbf{1} = \mathbf{0}$, we have

$$\sum_{i=1}^{n}\sum_{j=1}^{n}(d_i l^+_{ij} + d_j l^+_{ij}) = \sum_{i=1}^{n} d_i \sum_{j=1}^{n} l^+_{ij} + \sum_{j=1}^{n} d_j \sum_{i=1}^{n} l^+_{ji} = 0. \tag{9}$$

Then, (6) is obtained by substitution of (8) and (9) into (7).

Let δ, Δ, and $\bar{d} = (2m/n)$ denote the minimum, maximum, and average degrees of G, respectively. Then, from the definition of the additive degree-Kirchhoff index, it is obvious that

$$2\delta R(G) \le R^+(G) \le 2\Delta R(G).$$

As a consequence of Theorem 3, bounds in the earlier equation can be improved as follows.

Theorem 4 *$R^+(G)$ and $R(G)$ satisfy the following inequalities:*

$$(\delta + \bar{d})R(G) \le R^+(G) \le (\Delta + \bar{d})R(G), \tag{10}$$

with equality if and only if G is d-regular, that is, $d = \bar{d} = \delta = \Delta$.

Proof. Noting that $\bar{d} = (2m/n)$ and $n\sum_{i=1}^{n} l^+_{ii} = R(G)$, one invokes the inequalities arising upon noting that $l^+_{ii} \ge 0$ (since L^+ is non-negative definite) and replacing d_i in Theorem 3 successively by either δ or Δ. ☐

3 Bounds for the Kirchhoff and Additive Degree-Kirchhoff Indices via Maximum and Minimum Degrees

We first consider the Kirchhoff index to give an upper bound via the maximum degree as well as a lower bound via the minimum degree. A natural way to bound the Kirchhoff index is first to find the extremal graphs and use their values as bounds. It turns out that $T_{n,\Delta}$ and K_n^{δ} as given in the following definitions are extremal graphs.

Definition 1 [25] *The broom graph $T_{n,\Delta}$ is a tree on n vertices obtained by taking a path $P_{n-\Delta+1}$ and an edgeless graph*

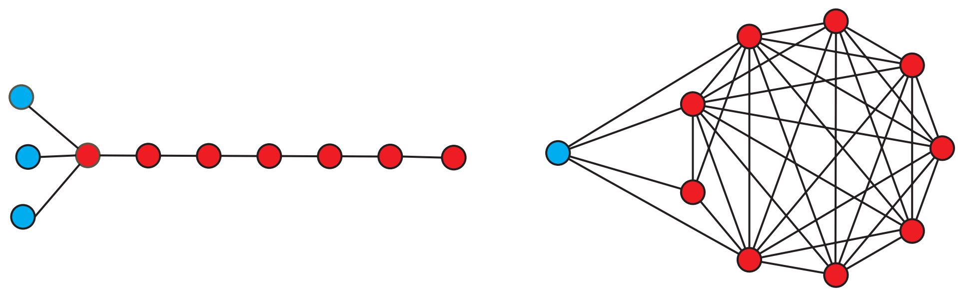

Figure 1: Graphs $T_{10,4}$ (left) and K_{10}^{4} (right).

$\overline{K_{\Delta-1}}$, and joining one end vertex of the path with every vertex of this edgeless graph.

Definition 2 *Let K_n^{δ} be the graph obtained by taking a complete graph K_{n-1} and an isolated vertex, and joining δ vertices of K_{n-1} with the isolated vertex.*

For example, graphs $T_{10,4}$ and K_{10}^{4} are shown in Figure 1.

Let $\mathcal{G}_{n,\Delta}$ be the set of all graphs with n vertices and maximum degree Δ. In Refs. [25, 26], it is shown that among all graphs in $\mathcal{G}_{n,\Delta}$, the graph $T_{n,\Delta}$ has the maximum Wiener index.

Theorem 5 *For every graph $G \in \mathcal{G}_{n,\Delta}$,*

$$W(G) \le W(T_{n,\Delta}),$$

with equality if and only if G is isomorphic to $T_{n,\Delta}$.

Recall [1] that for any graph G, $R(G) \le W(G)$ with equality if and only if G is a tree. Then, from Theorem 5, for every graph $G \in \mathcal{G}_{n,\Delta}$,

$$R(G) \le W(G) \le W(T_{n,\Delta}) \le R(T_{n,\Delta}),$$

with equality if and only if G is isomorphic to $T_{n,\Delta}$.

Let $\mathbb{G}_{n,\delta}$ be the set of graphs with n vertices and minimum degree δ. Next, we characterise the extremal graph in $\mathbb{G}_{n,\delta}$ with the minimum Kirchhoff index. The following property, known as the non-increasing property of the Kirchhoff index, is used.

Proposition 1 [27] *Let G be a connected graph, and let H be a spanning subgraph of G. Then,*

$$R(G) \le R(H)$$

with equality if and only if $G \cong H$.

From Proposition 1, it is easily observed as follows.

Lemma 1 *For every graph $G \in \mathbb{G}_{n,\delta}$,*

$$R(G) \ge R(K_n^{\delta}),$$

with equality if and only if G is isomorphic to K_n^{δ}.

Now, we compute Kirchhoff indices for the two extremal graphs $T_{n,\Delta}$ and K_n^{δ}. It is shown in Refs. [25, 26] that

$$R(T_{n,\Delta}) = \binom{n-\Delta+2}{3} + (\Delta-1)\binom{n-\Delta+2}{2} + (\Delta-1)(\Delta-2). \tag{11}$$

To compute the Kirchhoff index of K_n^{δ}, we first address resistance distances in K_n^{δ}. Given a graph $G=(V, E)$, let $N(u)=\{i \in V : iu \in E\}$ and $N[u]=N(u)\cup\{u\}$.

Lemma 2 [28] *Let i and j be vertices of G such that they have the same neighbourhood N in $V-\{i, j\}$. Then,*

$$\Omega_{ij} = \begin{cases} \dfrac{2}{|N|+2}, & \text{if } i \text{ and } j \text{ are adjacent}, \\[2ex] \dfrac{2}{|N|}, & \text{otherwise}. \end{cases}$$

Lemma 3 [29] *Let $G=(V, E)$ be a connected graph. Then, for any two vertices, $a, b \in V$ $(a \ne b)$,*

$$d_a \Omega_{ab} + \sum_{i \in N(a)} (\Omega_{ia} - \Omega_{ib}) = 2.$$

Theorem 6 *Let u be the exceptional vertex in K_n^{δ}, and let $\overline{N[u]} = V - N[u]$. Then, resistance distances in K_n^{δ} are given as*

$$\Omega_{ij} = \begin{cases} \dfrac{2}{n}, & i,j \in N(u), \\[1ex] \dfrac{2}{n-1}, & i,j \in \overline{N[u]}, \\[1ex] \dfrac{n+\delta-1}{n\delta}, & i=u \text{ and } j \in N(u), \\[1ex] \dfrac{n+\delta}{(n-1)\delta}, & i=u \text{ and } j \in \overline{N[u]}, \\[1ex] \dfrac{2n\delta-\delta+1}{n(n-1)\delta}, & i \in N(u) \text{ and } j \in \overline{N[u]}. \end{cases}$$

Proof. If $i, j \in N(u)$, then i and j are adjacent and have the same neighbourhood $N = V - \{i, j\}$ with $|N| = n-2$. Hence, by Lemma 2, it follows that $\Omega_{ij} = (2/n)$. If $i, j \in N[u]$, then again i and j are adjacent and Lemma 2 yields $\Omega_{ij} = (2/(n-1))$.

Now, suppose that $j \in N(u)$. To compute Ω_{uj}, we apply Lemma 3 to u and j, to obtain that

$$\delta\Omega_{uj} + \sum_{k \in N(u)} (\Omega_{uk} - \Omega_{jk}) = 2.$$

By symmetry, it is easily seen that for any $k \in N(u)$, $\Omega_{uk} = \Omega_{uj}$. Thus, the preceding equation becomes

$$2\delta\Omega_{uj} = 2 - \sum_{k \in N(u)} \Omega_{jk} = 2 - (\delta - 1)\frac{2}{n},$$

which yields that $\Omega_{uj} = ((n + \delta - 1)/n\delta)$. The case for Ω_{uj} with $j \in N[u]$ could be obtained in the same way.

Finally, we consider Ω_{ij} with $i \in N(u)$ and $j \in N[u]$. Again by Lemma 3, we have

$$d_j\Omega_{ji} + \sum_{k \in N(j)} (\Omega_{kj} - \Omega_{ki}) = 2,$$

that is,

$$(n-2)\Omega_{ji} + \sum_{k \in N(u)} (\Omega_{kj} - \Omega_{ki}) + \sum_{k \in N[u]-j} (\Omega_{kj} - \Omega_{ki}) = 2.$$

By symmetry, the preceding equation becomes

$$(n-2)\Omega_{ji} + \delta\Omega_{ij} - \sum_{k \in N(u)} \Omega_{ki} + \sum_{k \in N[u]-j} \Omega_{kj} - (n-2-\delta)\Omega_{ij} = 2.$$

Simple calculation leads to

$$2\delta\Omega_{ji} = 2 + \sum_{k \in N(u)} \Omega_{ki} - \sum_{k \in N[u]-j} \Omega_{kj} = 2 + (\delta - 1)\frac{2}{n} - (n - \delta - 2)\frac{2}{n-1} = \frac{4n\delta - 2\delta + 2}{n(n-1)}.$$

This gives $\Omega_{ji} = (2n\delta - \delta + 1)/(n(n-1)\delta)$.

Thus, the proof is complete. □

As a corollary of Lemma 2, the Kirchhoff index of K_n^δ is obtained.

Corollary 1

$$R(K_n^\delta) = n - 1 + \frac{n}{\delta} - \frac{\delta + 1}{n-1}. \tag{12}$$

Proof.

$$R(K_n^\delta) = \binom{\delta}{2}\frac{2}{n} + \binom{n-1-\delta}{2}\frac{2}{n-1} + \delta\frac{n+\delta-1}{n\delta} + (n-1-\delta)\frac{n+\delta}{(n-1)\delta} + \delta(n-1-\delta)\frac{2n\delta - \delta + 1}{n(n-1)\delta}$$

$$= \frac{\delta(\delta-1)}{n} + \frac{(n-1-\delta)(n-2-\delta)}{n-1} + \frac{n+\delta-1}{n} + \frac{(n+\delta)(n-1-\delta)}{(n-1)\delta} + \frac{(n-1-\delta)(2n\delta - \delta + 1)}{n(n-1)}$$

$$= n - 1 + \frac{n}{\delta} - \frac{\delta+1}{n-1}.$$

Recalling the results in Theorem 5 and Lemma 1, together with (11) and (12), the main result is obtained.

Theorem 7 *Let G be a n-vertex connected graph with minimum degree δ and maximum degree Δ ($\Delta \geq 2$). Then,*

$$n - 1 + \frac{n}{\delta} - \frac{\delta+1}{n-1} \leq R(G) \leq \binom{n-\Delta+2}{3} + (\Delta - 1)\binom{n-\Delta+2}{2} + (\Delta-1)(\Delta-2).$$

The first equality holds if and only if $G \cong K_n^\delta$, and the second holds if and only if $G \cong T_{n,\Delta}$.

According to Theorems 4 and 7, bounds for the additive degree-Kirchhoff index follow directly.

Theorem 8 *Let G be a connected graph with n vertices, m edges, minimum degree δ, and maximum degree Δ ($\Delta \geq 2$). Then,*

$$\left(\delta + \frac{2m}{n}\right)\left(n - 1 + \frac{n}{\delta} - \frac{\delta+1}{n-1}\right) \leq R^+(G) < \left(\Delta + \frac{2m}{n}\right)\left[\binom{n-\Delta+2}{3} + (\Delta-1)\binom{n-\Delta+2}{2} + (\Delta-1)(\Delta-2)\right],$$

the first equality holds if and only if G is complete.

4 An Upper Bound for the Additive Degree-Kirchhoff Index

In Ref. [21], it was shown that for any G,

$$R^+(G) \leq \frac{1}{3}(n^4 - n^3 - n^2 + n).$$

In addition, it was conjectured that the maximum of $R^+(G)$ over all graphs is attained by the (1/3,1/3,1/3) barbell graph, which consists of two complete graphs on $n/3$ vertices united by a path of length $n/3$ and for which $R^+(G) \geqslant (2/27)n^4$. As given in the following result, we improve the bound to $\geqslant (1/8)n^4$.

Theorem 9 *Let G be a connected graph with n vertices. Then,*

$$R^+(G) \leq \frac{1}{8}(n-1)^3(n+14),$$

with equality if and only if $G \cong K_2$.

Proof. Let d_{ij} denote the distance between i and j in G. Then, by the definition of the additive degree-Kirchhoff index, we have

$$\begin{aligned} R^+(G) &= \sum_{\{i,j\}\subset V} (d_i + d_j)\Omega_{ij} \\ &= \sum_{\substack{\{i,j\}\subset V \\ d_{ij}=1}} (d_i + d_j)\Omega_{ij} + \sum_{\substack{\{i,j\}\subset V \\ d_{ij}=2}} (d_i + d_j)\Omega_{ij} + \sum_{\substack{\{i,j\}\subset V \\ d_{ij}\geq 3}} (d_i + d_j)\Omega_{ij}. \end{aligned} \tag{13}$$

By the Foster formula [30], which states that the sum of resistance distances between pairs of adjacent vertices is equal to $n-1$, we have

$$\sum_{\substack{\{i,j\}\subset V \\ d_{ij}=1}} (d_i + d_j)\Omega_{ij} \leq 2(n-1) \sum_{\substack{\{i,j\}\subset V \\ d_{ij}=1}} \Omega_{i,j} = 2(n-1)^2. \tag{14}$$

Then, by the fact that $\Omega_{ij} \leq d_{ij}$, it follows that

$$\begin{aligned} \sum_{\substack{\{i,j\}\subset V \\ d_{ij}=2}} (d_i + d_j)\Omega_{ij} &\leq 2 \sum_{\substack{\{i,j\}\subset V \\ d_{ij}=2}} (d_i + d_j) \leq 2(n-1+n-1) \sum_{\substack{\{i,j\}\subset V \\ d_{ij}=2}} 1 \\ &\leq 4(n-1)\left[\binom{n}{2} - (n-1)\right]. \end{aligned} \tag{15}$$

For $i, j \in V$ such that $d_{ij} \geq 3$, since i and j have no common neighbours, it follows that

$$d_{ij} \leq n + 1 - (d_i + d_j),$$

which gives

$$(d_i + d_j)\Omega_{ij} \leq (d_i + d_j)d_{ij} \leq (d_i + d_j)[n-1-(d_i + d_j)] \leq \frac{(n-1)^2}{4}.$$

Noting that pairs of vertices at distance 3 is less than or equal to

$$\frac{n(n-1)}{2} - (n-1) = \frac{(n-2)(n-1)}{2},$$

it follows that

$$\begin{aligned} \sum_{\substack{\{i,j\}\subset V \\ d_{ij}\geq 3}} (d_i + d_j)\Omega_{ij} &\leq \frac{(n-1)^2}{4} \sum_{\substack{\{i,j\}\subset V \\ d_{ij}\geq 3}} 1 = \frac{(n-1)^2}{4}\frac{(n-2)(n-1)}{2} \\ &= \frac{(n-2)(n-1)^3}{8}. \end{aligned} \tag{16}$$

Substitution of (14)–(16) back into (13) yields the desired result.

Equality in (14) holds only when the end vertices of each edge of G are $n-1$, which means G is $n-1$ regular, in other words, G is a complete graph. On the other hand, equality in (15) holds also requires that G has $n-1$ edges, which indicates G is a tree. Thus, equality in Theorem 9 holds only when $G \cong K_2$, and it is easily verified that $R^+(K_2)$ does attain the upper bound.

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