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Upper and Lower Bounds for the Mixed Degree-Kirchhoff Index

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Abstract. We introduce the mixed degree-Kirchhoff index, a new molecular descriptor defined by

$$\widehat{R}(G) = \sum_{i<j} \left(\frac{d_i}{d_j} + \frac{d_j}{d_i} \right) R_{ij},$$

where d_i is the degree of the vertex i and R_{ij} is the effective resistance between vertices i and j. We give general upper and lower bounds for $\widehat{R}(G)$ and show that, unlike other related descriptors, it attains its largest asymptotic value (order n^4), among barbell graphs, for the highly asymmetric lollipop graph. We also give more refined lower (order n^2) and upper (order n^3) bounds for c-cyclic graphs in the cases $0 \le c \le 6$. For this latter purpose we use a close relationship between our new mixed degree-Kirchhoff index and the inverse degree, prior bounds we found for the inverse degree of c-cyclic graphs, and suitable expressions for the largest and smallest effective resistances of c-cyclic graphs.

1. Introduction

The Kirchhoff index of an undirected connected simple graph $G = (V, E)$, with $|V| = n$ and $|E| = m$, was defined by Klein and Randić in [16] as

$$R(G) = \sum_{i<j} R_{ij}, \tag{1}$$

where R_{ij} is the effective resistance between the vertices i and j. This molecular descriptor has attracted considerable interest (see [11] and [17]) and the references cited therein. Eventually, it spawned a class of other indices that, in addition to the effective resistance, include other graph information. Among these we can mention the multiplicative degree-Kirchhoff index defined by Cheng and Zhang in [8] (see also [20] and the references cited therein)

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

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where d_i is the degree of the vertex i, and the additive degree-Kirchhoff index defined by Gutman et al. in [13] (see also [14] and [21] and the references cited therein)

$$R^+(G) = \sum_{i<j}(d_i + d_j)R_{ij}. \tag{3}$$

Along these lines we propose in this note a new descriptor, which is inspired in our previous work [3] and we call it the **mixed degree-Kirchhoff index**:

$$\widehat{R}(G) = \sum_{i<j}\left(\frac{d_i}{d_j} + \frac{d_j}{d_i}\right)R_{ij}. \tag{4}$$

In the spirit of references [22] and [23], we justify the introduction of yet another descriptor on the basis of these arguments:

(i) it coincides with $2R(G)$ when G is regular, so it discriminates as well as the indices (1), (2) and (3) within the family of regular graphs;

(ii) The summands $S_{ij} = (\frac{d_i}{d_j} + \frac{d_j}{d_i})R_{ij}$ are symmetric in i and j. This characteristic is shared by the summands of the descriptors (2) and (3), but unlike these, which attain their maxima on graphs with certain symmetry (the barbell graphs), our new index tends to be larger the more asymmetric the graph is, attaining its asymptotic maximum, among the barbell graphs, on the lollipop graph, as will be shown below. These particularly shaped molecules are not unheard of in Chemistry. Lollipop-shaped molecules are mentioned in [7], p. 69, and they are described as being composed of one or two hydrophobic hydrocarbons tails and of a hydrophilic head group. Barbell-shaped molecules are the subject of recent interest as shown in [15];

(iii) It can be written in an attractive way as a probabilistic object, namely

$$\widehat{R}(G) = \frac{1}{2|E|}\sum_{i<j}\left(\frac{\pi_i}{\pi_j} + \frac{\pi_j}{\pi_i}\right)(E_iT_j + E_jT_i),$$

where $\{\pi_i\}$ is the stationary distribution and E_iT_j is the expected hitting time (starting from i) of the vertex j (We refer the reader to [3] for the probabilistic details);

(iv) we proved in [3] that

$$\sum_{i<j}\left(\frac{d_i}{d_j} + \frac{d_j}{d_i}\right) = \sum_j \frac{1-\pi_j}{\pi_j} = 2|E|\sum_{j=1}^{n}\frac{1}{d_j} - n,$$

and therefore we immediately have these upper and lower bounds

$$\widehat{R}(K_n) = 2(n-1) \le rn(n-1) \le r\left(2|E|\sum_{j=1}^{n}\frac{1}{d_j} - n\right) \le \widehat{R}(G) \le R\left(2|E|\sum_{j=1}^{n}\frac{1}{d_j} - n\right), \tag{5}$$

where $r = \min_{i,j} R_{ij} \ge \frac{2}{n}$, $R = \max_{i,j} R_{ij} \le n-1$, and the only nontrivial tool used in (5) is the harmonic mean-arithmetic mean inequality. The bounds on the resistances are consequences of the monotonicity principle (see [12]) because R_{ij} is always greater than the resistance between i and j when we add edges to the graph until it is turned into a complete graph, for which this effective resistance between any pair of vertices is $\frac{2}{n}$; likewise, if $d(i, j) = k$, then R_{ij} is always less than the resistance between i and j when we delete edges of the graph until there is only one path of length k between i and j, in which case $R_{ij} = k$. And clearly, $k \le n-1$.

The inequalities in (5) tell us that the minimal value of $\widehat{R}(G)$ is attained at the complete graph K_n, and also that our new descriptor is linked to another one, called the *inverse degree* and defined as (see [9], [10] and [18])

$$\rho(G) = \sum_{j=1}^{n} \frac{1}{d_j},$$

through the inequalities

$$r(2|E|\rho(G) - n) \leq \widehat{R}(G) \leq R(2|E|\rho(G) - n). \tag{6}$$

The main objectives of this article are to give some general bounds for $\widehat{R}(G)$ and to show that its largest asymptotic value among the barbell graphs is attained by the $L(n/2)$ lollipop graph. Also, from the sizable body of work on the inverse degree, we use recently obtained upper and lower bounds (see [4]) for this index on the particular family of c-cyclic graphs, that is, graphs which contain only c independent cycles (i.e., cycles that do not contain other cycles within themselves). We provide results for $0 \leq c \leq 6$ and apply them to (6) in order to obtain upper and lower bounds for $\widehat{R}(G)$ on these c-cyclic graphs.

2. Further general bounds and the lollipop graph

Since $2 \leq \frac{d_i}{d_j} + \frac{d_j}{d_i} \leq d_i + d_j$, we immediately have that for any G

$$2R(G) \leq \widehat{R}(G) \leq R^+(G). \tag{7}$$

The upper bound in (7) also tells us that $\widehat{R}(G)$ is at most of order $\frac{1}{3}n^4$. Moreover, since $\dfrac{d_i}{d_j}+\dfrac{d_j}{d_i} \leq n-1+\dfrac{1}{n-1}$, directly from the definition we have that

$$\widehat{R}(G) \leq \left(n - 1 + \frac{1}{n-1}\right) R(G) \leq \frac{1}{6}(n^4 - n^3 + 2n),$$

using the well known fact that $R(G)$ is largest for the linear graph, for which $R(G) = \dfrac{n^3 - n}{6}$. We now show that there is a graph G such that $\widehat{R}(G)$ attains the order n^4. In fact we show that the largest asymptotic value among barbell graphs is attained by the $L(n/2)$ lollipop graph, and conjecture that this is the largest value among all graphs.

Indeed, consider the $L(s)$ lollipop graph consisting of a complete graph K_s attached to a linear graph on $n-s$ vertices, $0 \leq s \leq n$. The largest term of $\widehat{R}(L(s))$ arises from considering the terms $\left(\frac{d_i}{d_j} + \frac{d_j}{d_i}\right) R_{ij}$ computed when j runs over all s vertices in the complete part and i is a fixed vertex in the linear part, and then adding over all the vertices in the linear part. This value is at least of order

$$\sum_{i=1}^{n-s} \frac{s^2}{2} i \sim \frac{1}{4} s^2 (n-s)^2.$$

Optimizing this expression over s, the maximum value occurs at $s = \frac{n}{2}$ and the value of the largest term is $\frac{n^4}{64}$.

We consider now a barbell graph $B(s,t)$ consisting of two complete graphs K_s and K_t attached to the endpoints of a $n-s-t$ linear graph, where $0 \leq s, t \leq n, 0 \leq s+t \leq n$. As in the previous calculation, the largest term of $\hat{R}(B(s,t))$ arises from considering the terms $\left(\frac{d_i}{d_j} + \frac{d_j}{d_i}\right) R_{ij}$ computed when j runs over all vertices in the complete parts and i is a fixed vertex in the linear part, and then adding over all i. The contribution of all pairs (i, j) when both i and j are in the linear part of the barbell, or when $i \in K_s$ and $j \in K_t$, is at most cubic in n, and the contribution when both i and j belong to the same complete graph is at most linear in n. So the largest term is roughly

$$\frac{1}{4}(s^2 + t^2)(n - s - t)^2.$$

We maximize this expression on the triangle $0 \le s, t \le n, 0 \le s + t \le n$. The sides of said triangle correspond to lollipop graphs, already studied, and barbells without the linear part that we can discard right away. By partial differentiation we find that the critical points inside the triangle lie on the line $s = t$, and the maximal value on that line occurs at $s = t = n/4$, for which $\hat{R}(B(n/4, n/4)) \sim \frac{1}{128}n^4$, a value that does not improve the one obtained above. Thus the largest asymptotic value of the mixed-degree Kirchhoff index among barbells occurs at the lollipop graph $L(n/2)$ for which $\widehat{R}(L(n/2)) \sim \frac{1}{64}n^4$.

3. Bounds for c-cyclic graphs

In [4] we provided a new characterization of c-cyclic graphs, $0 \le c \le 6$, depending on the degree sequence and we identified their extremal degree sequences with respect to the majorization order. In what follows we briefly recall some basic notations on majorization (for more details see [6] and [19]).

Definition 1. *Given two vectors* $\mathbf{y}, \mathbf{z} \in D = \{\mathbf{x} \in \mathbb{R}^n : x_1 \ge x_2 \ge ... \ge x_n\}$*, the majorization order* $\mathbf{y} \trianglelefteq \mathbf{z}$ *means:*

$$\begin{cases} \left\langle \mathbf{y}, \mathbf{s^k} \right\rangle \le \left\langle \mathbf{z}, \mathbf{s^k} \right\rangle, \; k = 1, ..., (n-1) \\ \langle \mathbf{y}, \mathbf{s^n} \rangle = \langle \mathbf{z}, \mathbf{s^n} \rangle \end{cases}$$

where $\langle \cdot, \cdot \rangle$ *is the inner product in* $\mathbb{R}^n$ *and* $\mathbf{s^j} = [1^j, 0^{n-j}], \quad j = 1, 2, \cdots, n.$

A vector $\mathbf{x}^*(S) \in S$ is said to be maximal for S with respect to the majorization order if $\mathbf{x} \trianglelefteq \mathbf{x}^*(S)$ for each $\mathbf{x} \in S$. Analogously, a vector $\mathbf{x}_*(S) \in S$ is said to be minimal for S with respect to the majorization order if $\mathbf{x}_*(S) \trianglelefteq \mathbf{x}$ for each $\mathbf{x} \in S$. Notice that if $S \subseteq T$, then $\mathbf{x}^*(S) \trianglelefteq \mathbf{x}^*(T)$ and $\mathbf{x}_*(T) \trianglelefteq \mathbf{x}_*(S)$.

A symmetric function $\phi : A \to \mathbb{R}$, $A \subseteq \mathbb{R}^n$, is said to be Schur-convex on A if $\mathbf{x} \trianglelefteq \mathbf{y}$ implies $\phi(\mathbf{x}) \le \phi(\mathbf{y})$. Given an interval $I \subset \mathbb{R}$, and a convex function $g : I \to \mathbb{R}$, the function $\phi(\mathbf{x}) = \sum_{i=1}^n g(x_i)$ is Schur-convex on $I^n = \underbrace{I \times I \times \cdots \times I}_{n-times}$.

If ϕ is a Schur-convex function and S is a subset which admits maximal and minimal elements with respect to the majorization order, the solutions of the constrained optimization problems

$$\begin{cases} \max \; (\min) \; \phi(\mathbf{x}) \\ \text{subject to } \mathbf{x} \in S \end{cases} \tag{P}$$

are the maximal element $\mathbf{x}^*(S)$ and the minimal element $\mathbf{x}_*(S)$, respectively. Let now $F(d_1, d_2, \cdots, d_n)$ be any topological index which is a Schur-convex function of its arguments, defined on a subset S. Then, since the Schur-convex functions preserve the majorization ordering, we get

$$F(\mathbf{x}_*(S)) \le F(d_1, d_2, \cdots, d_n) \le F(\mathbf{x}^*(S)).$$

Using this methodology we determined upper and lower upper bounds of some degree-based topological indices that can be expressed as Schur convex (concave) functions of the degree sequence of the graph (see [1], [2], [4], [3], [5] and [6]). In Table 1 we summarize the bounds obtained in [4] for $\rho(G) = \sum \frac{1}{d_j}$ and point out that when several maximal/minimal degree sequences were identified, we present the best estimate.

c	Lower bound	Upper bound
0	$\frac{n+2}{2}$	$(n-1)+\frac{1}{n-1}$
1	$\frac{n}{2}$	$(n-2)+\frac{1}{n-1}$
2	$\frac{n-2}{2}+\frac{2}{3}$	$(n-3)+\frac{1}{n-1}+\frac{1}{3}$
3 ($n \geq 5$)	$\frac{n-4}{2}+\frac{4}{3}$	$(n-3)+\frac{1}{n-1}$
4 ($n \geq 6$)	$\frac{n-2}{2}$	$\frac{1}{n-1}+\frac{17}{12}$
5 ($n \geq 8$)	$\frac{n-8}{2}+\frac{8}{3}$	$(n-5)+\frac{1}{n-1}+\frac{7}{6}$
6 ($n \geq 10$)	$\frac{n-10}{2}+\frac{10}{3}$	$(n-4)+\frac{1}{n-1}$

Table 1: Lower and upper bounds for $\rho(G)$.

Using the bounds on the inverse degree and the inequalities in (6) we can provide lower and upper bounds for the mixed degree-Kirchhoff index. First we need expressions for r and R in terms of the graph parameters, which are given in the next

Proposition 2. *For a c-cyclic graph,*

(i) If $0 \leq c \leq n-2$ *then*

$$r = \frac{2}{2+c}$$

(ii) If $0 \leq c \leq 6$ *the values of R are given in the following table:*

c	0	1	2	3	4	5	6
R	$n-1$	$n-\frac{7}{3}$	$n-3$	$n-\frac{7}{2}$	$n-\frac{33}{8}$	$n-\frac{13}{3}$	$n-\frac{23}{5}$

Table 2: Maximum resistance R for c-cyclic graphs with $0 \leq c \leq 6$.

Proof. For part (i), take a and b neighbors and set a battery of 1 volt between a and b. To minimize R_{ab}, which is the inverse of the current flowing from a to b, we need to maximize such current, and that is done using c paths of length 2 from a to b which determine exactly c cycles (see Figure 1 for an illustration in the 3-cyclic case). Then by the rule governing resistors placed in parallel we have

$$R_{ab} = \frac{1}{1+\frac{c}{2}} = \frac{2}{2+c},$$

for all $0 \leq c \leq n-2$. When $c = n-2$ we reach the lowest R_{ab} can be, which is $\frac{2}{n}$, as mentioned in Section 1.

Regarding (ii), by the rule stating that the effective resistance of resistors connected in series is the sum of the individual resistances, it is clear that the largest R_{ab} can be is when there is a chain of unit resistors as long as possible between a and b. For a tree (c=0) this happens when there are exactly $n-1$ unit resistors (edges) between a and b.

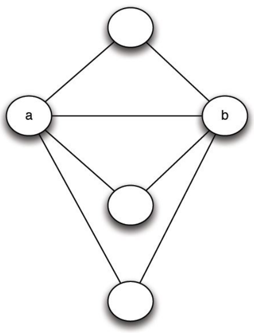

Figure 1: Illustration in the tricyclic case

For a unicyclic graph this is accomplished, as in Figure 2 (I), when we attach a triangle to $n-3$ vertices arranged linearly. For the bicyclic graph we attach a square as in (II), and check that $R_{14} = 1$. For the tricyclic a similar arrangement, as in (III), but now $R_{14} = \frac{1}{2}$. For the tetra- penta- and hexa-cyclic graphs we attach a pentagon as illustrated in Figure 3, (IV), (V) and (VI) respectively, and check that R_{14} is now $\frac{7}{8}$, $\frac{2}{3}$ and $\frac{2}{5}$, respectively.

For all these graphs the maximal effective resistance, computed between vertices 1 and n, results from grouping as few vertices as possible in one end while respecting the c-cyclicity, and using the rest of the vertices in a linear arrangement •

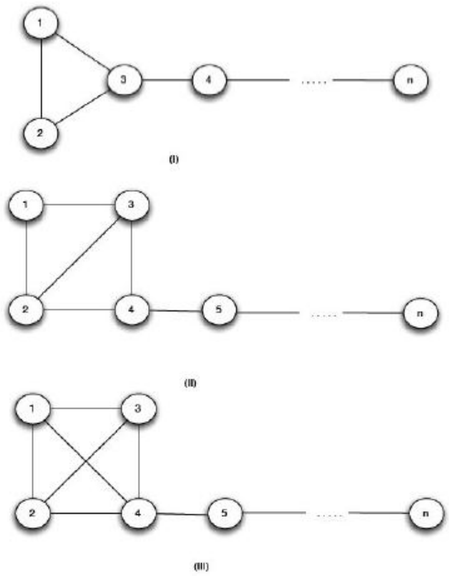

Figure 2: Unicyclic, bicyclic and tricyclic graphs

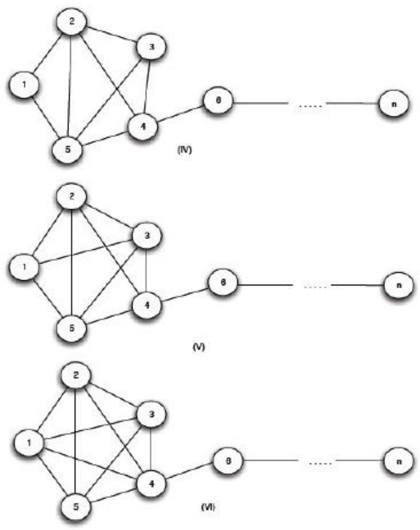

Figure 3: Tetracyclic, pentacyclic and hexacyclic graphs

Now proposition 2 and the inequalities in (6) allow us to present upper and lower bounds for $\widehat{R}(G)$, summarized in Table 3. We remark that the lower bounds are all of order n^2, whereas the upper bounds are of order n^3. Notice also that the results for the tricyclic graphs are valid in case $n \geq 5$; those for tetracyclic graphs in case $n \geq 6$; those for pentacyclic graphs in case $n \geq 8$, and those for hexacyclic graphs in case $n \geq 10$.

c	**Lower bounds**	**Upper bounds**
0	(n^2-2)	$(n-1)(2n^2-5n+4)$
1	$\frac{2}{3}n(n-1)$	$\frac{n(3n-7)\left(2n^2-7n+7\right)}{3(n-1)}$
2	$\frac{1}{6}\left(3n^2-2n-2\right)$	$\frac{(n-2)(n-3)\left(6n^2-7n-11\right)}{3(n-1)}$
3	$\frac{2}{15}\left(3n^2-n-8\right)$	$\frac{\left(2n^3-5n^2-7n+16\right)(2n-7)}{2(n-1)}$
4	$\frac{1}{3}\left(n^2-6\right)$	$\frac{\left(12n^3-25n^2-104n+165\right)(8n-33)}{48(n-1)}$
5	$\frac{2}{21}\left(n+3n^2-32\right)$	$\frac{2\left(3n^3-4n^2-42n+58\right)(3n-13)}{9(n-1)}$
6	$\frac{1}{12}\left(2n+3n^2-50\right)$	$\frac{\left(2n^3-n^2-39n+50\right)(5n-23)}{5(n-1)}$

Table 3: Lower and upper bounds for $\widehat{R}(G)$.

4. Concluding Remarks

We introduced a new molecular descriptor that, while sharing some properties of the Kirchhoff index and its related descriptors, it is asymptotically largest (order n^4) for asymmetric graphs such as the lollipop graph. We gave general upper and lower bounds for this descriptor, as well as more refined lower bounds (order n^2) and upper bounds (order n^3) for c-cyclic graphs, in the cases $0 \leq c \leq 6$. The results were obtained using the bounds we found for the inverse degree of c-cyclic graphs through majorization techniques and closed form expressions for the largest and smallest values of the effective resistance of these c-cyclic graphs that, to the best of our knowledge, are new.

We finally remark that we could define a whole family of descriptors thus:

$$\widehat{R}(G)_\alpha = \sum_{i<j} \left(\left(\frac{d_i}{d_j} \right)^\alpha + \left(\frac{d_j}{d_i} \right)^\alpha \right) R_{ij}, \tag{8}$$

for any non-negative real α.

If $\alpha \geq \beta \geq 0$ then $(\alpha, -\alpha) \succ (\beta, -\beta) \succ (0,0)$, where $\succ$ means "majorizes", and then by majorization (Muirhead's theorem) we have

$$\hat{R}(G)_\alpha \geq \hat{R}(G)_\beta \geq 2R(G),$$

but we will not pursue this matter any further.

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