MATCH
Communications in Mathematical and in Computer Chemistry

MATCH Commun. Math. Comput. Chem. **75** (2016) 227-231

ISSN 0340 - 6253

Revisiting Bounds for the Multiplicative Degree–Kirchhoff Index

Monica Bianchi [a], **Alessandra Cornaro** [a], **José Luis Palacios** [b], **José Miguel Renom** [c] **Anna Torriero**[a]

[a] *Department of Mathematics and Econometrics, Catholic University, Milan, Italy*
monica.bianchi@unicatt.it, alessandra.cornaro@unicatt.it, anna.torriero@unicatt.it

[b] *Department of Electrical and Computer Engineering, The University of New Mexico, Albuquerque, NM 87131*
jpalacios@unm.edu

[c] *Department of Scientific Computing and Statistics, Simon Bolivar University, Caracas, Venezuela*
jrenom@usb.ve

(Received March 13, 2015)

Abstract

We revise some bounds found in [2] and give a new general upper bound for the multiplicative degree-Kirchhoff index.

1 Introduction

A finite simple undirected graph $G = (V, E)$ with $|V| = n$ and $|E| = m$ is the basic model for a chemical molecule, where the vertices represent the atoms and the edges in E represent the chemical bonds. Among the descriptors used in Mathematical Chemistry to study these models, one that has received a great deal of attention since its introduction by Klein and Randić in [1] is the Kirchhoff index, defined as

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

where R_{ij} is the effective resistance between vertices i and j computed with Ohm's law when the edges of the graph are supposed to have unit resistances. Two related descriptors that incorporate the degrees (number of neighbors) $d_i, 1 \leq i \leq n$, of the vertices, are the additive degree-Kirchhoff index, introduced by Gutman et al. in [3] and defined as

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

and the multiplicative degree-Kirchhoff index, introduced by Chen and Zhang in [4] and defined as

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

Theorem 2 in [2] claims:

Let G be a connected graph on $n > 2$ vertices and m edges. Then

$$R^{*}(G) \geq 2m\left(n - 2 + \frac{1}{n}\right); \tag{4}$$

$$R^{*}(G) \geq 2m\left(\frac{\Delta}{\Delta+1} + \frac{(n-2)^2}{n-1-\frac{1}{\Delta}}\right); \tag{5}$$

$$R^{*}(G) \geq 2m\left(\frac{\chi}{\chi+1} + \frac{(n-2)^2}{n-1-\frac{1}{\chi}}\right); \tag{6}$$

where Δ and χ are the largest degree and the chromatic number of G, respectively.

It must be noted that claim (4) is a weaker result than our proposition 2 in [6], where using electrical principles we prove that for any G,

$$R^{*}(G) \geq 2m\left(n - 2 + \frac{1}{\Delta+1}\right).$$

It must be noted also that claims (5) and (6) are variants of our lower bounds in [7] of the form

$$R(G) \geq \frac{n}{d_1}\left[\frac{1}{1+\beta} + \frac{(n-2)^2}{n-1-\beta}\right],$$

for the Kirchhoff index $R(G)$, which is our formula (11), and also (17), (18), (19), etc. in [7], and

$$R^{*}(G) \geq 2m\left[\frac{1}{1+\beta} + \frac{(n-2)^2}{n-1-\beta}\right],$$

for the degree-Kirchhoff index, for instance, our formula (30) in [7]. All these inequalities are found with specific bounds for eigenvalues associated to the graph, using majorization techniques. Feng et al. do not contribute in their theorem 2 any new ideas which are not given implicitly or explicitly in our results.

In fact, stronger and more general lower bounds than those in [2] and in [7], for some families of descriptors, were given in [8].

2 A general upper bound

In [5] it was shown that for any n-vertex G, $R^*(G) \leq \frac{1}{6}n^5$ and it was conjectured that the $(1/3, 1/3, 1/3)$-barbell graph which consists of two copies of the complete graph $K_{n/3}$ attached at the endpoints of a linear graph on $n/3$ vertices attains the largest value of $R^*(G)$ among all n-vertex graphs, which is of the order $\frac{2}{243}n^5$. We get closer to the conjecture with the following upper bound whose proof is inspired in that of an upper bound for the additive degree-Kirchhoff index found in [9].

Proposition 1 *For an n-vertex G we have*

$$R^*(G) \leq (n-1)^4 \quad \text{for } n \leq 48,$$

and

$$R^*(G) \leq \frac{n^5 + 50n^3 - 164n^2 + 165n - 52}{54}, \quad \text{for } n \geq 49.$$

Proof. We first remark that $R_{ij} \leq d(i,j)$, where $d(i,j)$ is the distance in the graph between the vertices i and j, and the equality holds when there is only one path from i to j. Now we decompose the descriptor into three sums:

$$R^*(G) = \sum_{i<j:d(i,j)=1} d_i d_j R_{ij} + \sum_{i<j:d(i,j)=2} d_i d_j R_{ij} + \sum_{i<j:d(i,j)\geq 3} d_i d_j R_{ij}. \tag{7}$$

We apply Foster's formula in the first summand in order to obtain

$$\sum_{i<j:d(i,j)=1} d_i d_j R_{ij} \leq (n-1)^2 \sum_{i<j:d(i,j)=1} R_{ij} = (n-1)^3. \tag{8}$$

For the second summand we argue that

$$\sum_{i<j:d(i,j)=2} d_i d_j R_{ij} \leq 2(n-1)^2 \sum_{i<j:d(i,j)=2} 1. \tag{9}$$

Finally, for vertices at distance 3 or larger we argue that the largest path between i and j can be at most of length $d(i,j) \leq n+1-d_i-d_j$. Indeed, the largest possible path between i and j is built with all the vertices in the graph except $d_i - 1$ neighbors of i and $d_j - 1$ neighbors of j, for a total of $n - (d_i - 1) - (d_j - 1) = n - d_i - d_j + 2$ vertices, and the path built with those many vertices has length $(n - d_i - d_j + 2) - 1 = n + 1 - d_i - d_j$. We cannot use $d_i - 1$ neighbors of i and $d_j - 1$ neighbors of j in the path because if we did the path could be shortened and would not have largest length.

Next we observe that the only critical point of the two variable function

$$F(x, y) = xy(n + 1 - x - y),$$

in the region $1 \le x \le n - 1$, $1 \le y \le n - 1$, corresponds to $x = y = \frac{n+1}{3}$, where there is a maximum. Therefore we have

$$\sum_{i<j:d(i,j)\ge 3} d_i d_j R_{ij} \le \sum_{i<j:d(i,j)\ge 3} d_i d_j (n + 1 - d_i - d_j) \le \sum_{i<j:d(i,j)\ge 3} \frac{(n+1)^3}{27},$$

so that

$$\sum_{i<j:d(i,j)\ge 3} d_i d_j R_{ij} \le \frac{(n+1)^3}{27} \sum_{i<j:d(i,j)\ge 3} 1. \qquad (10)$$

Since the number of pairs of vertices at distances 2 or larger is bounded by $\binom{n}{2} - (n-1)$, the sum of (9) and (10) can be bounded thus

$$2(n-1)^2 \sum_{i<j:d(i,j)=2} 1 + \frac{(n+1)^3}{27} \sum_{i<j:d(i,j)\ge 3} 1 \le \frac{(n+1)^3}{27} \sum_{i<j:d(i,j)\ge 2} 1$$

$$\le \frac{(n+1)^3}{27} \frac{(n-1)(n-2)}{2} \quad \text{for } n \ge 49, \qquad (11)$$

and

$$\le (n-1)^3 (n-2) \quad \text{for } n \le 48. \qquad (12)$$

Inserting (8) and either (11) or (12) into (7) we obtain

$$R^*(G) \le \frac{n^5 + 50n^3 - 164n^2 + 165n - 52}{54}, \quad \text{for } n \ge 49$$

and

$$R^*(G) \le (n-1)^4 \quad \text{for } n \le 48,$$

which gives the exact value of $R^*(G)$ for $n = 2$.

References

[1] D. J. Klein, M. Randić, Resistance distance, *J. Math. Chem.* **12** (1993) 81–95.

[2] L. Feng, G. Yu, W. Liu, Further results regarding the degree Kirchhoff index of graphs, *Miskolc Math. Notes* **15** (2014) 97-108.

[3] I. Gutman, L. Feng, G. Yu, Degree resistance distance of unicyclic graphs, *Trans. Comb.* **1** (2012) 27–40.

[4] H. Chen, F. Zhang, Resistance distance and the normalized Laplacian spectrum, *Discr. Appl. Math.* **155** (2007) 654–661.

[5] J. L. Palacios, J. M. Renom, Broder and Karlin's formula for hitting times and the Kirchhoff index, *Int. J. Quantum Chem.* **111** (2011) 35–39.

[6] J. L. Palacios, J. M. Renom, Another look at the degree–Kirchhoff index, *Int. J. Quantum Chem.* **111** (2011) 3453–3455.

[7] M. Bianchi, A. Cornaro, J. L. Palacios, A. Torriero, Bounds for the Kirchhoff index via majorization techniques, *J. Math. Chem.* **51** (2013) 569–587.

[8] M. Bianchi, A. Cornaro, J. L. Palacios, A. Torriero, Bounding the sum of powers of normalized Laplacian eigenvalues of graphs through majorization methods, *MATCH Commun. Math. Comput. Chem.* **70** (2013) 707–716.

[9] Y. Yang, D. Klein, A note on the Kirchhoff and additive–Kirchhoff indices of graphs, *in preparation.*