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New Upper Bounds for the ABC Index

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Abstract

For a connected undirected graph $G = (V, E)$ with vertex set $\{1, 2, \ldots, n\}$ and degrees d_i, for $1 \leq i \leq n$, we show that

$$ABC(G) \leq \sqrt{(n-1)(|E| - R_{-1}(G))},$$

where $R_{-1}(G) = \sum_{(i,j)\in E} \frac{1}{d_i d_j}$ is the Randić index. This bound allows us to obtain some maximal results for the ABC index with elementary proofs and to improve all the upper bounds in [20], as well as some in [17], using lower bounds for $R_{-1}(G)$ found in the literature and some new ones found through the application of majorization.

1 Introduction

Among the various descriptors in Mathematical Chemistry, the ABC index has received considerable attention in recent times. For a connected undirected graph $G = (V, E)$ with vertex set $\{1, 2, \ldots, n\}$ and edge set E, the ABC index, proposed by Estrada et al. in [11], and reintroduced in [12] was defined as

$$ABC(G) = \sum_{i\sim j} \sqrt{\frac{d_i + d_j - 2}{d_i d_j}}, \tag{1}$$

where $i \sim j$ means that the vertices i and j are neighbors and d_i is the degree of the vertex i. (For all graph theoretical terms the reader is referred to reference [22])

The index $ABC(G)$ has been studied in a large number of references of which we mention [9], [14] and [18] for their own interest and for many other related references found in them.

In this article we want to give a new upper bound for $ABC(G)$ given in terms of the Randić index $R_{-1}(G)$. This upper bound yields a number of particular bounds (which improve all those in [20] and some in [17]) and maximal results as corollaries of numerous lower bounds for the Randić index found in the literature. We also find new lower bounds for $R_{-1}(G)$ through majorization, yielding additional upper bounds for $ABC(G)$.

In what follows we will assume that the graphs satisfy $n \geq 3$ in order to avoid cases where $i \sim j$ and $d_i = d_j = 1$.

2 New Upper Bounds for the *ABC* Index

In this section we find an upper bound for the ABC index in terms of the Randić index $R_{-1}(G)$, for which there exist a large number of lower bounds in the literature that allow us to obtain some new upper bounds for the ABC index in certain particular cases of graphs. The first main result is a refinement of an argument found in [20].

2.1 The general bound

Proposition 1. *For any graph G we have*

$$ABC(G) \leq \sqrt{(n-1)(|E| - R_{-1}(G))}, \tag{2}$$

where $R_{-1}(G) = \sum_{(i,j)\in E} \frac{1}{d_i d_j}$ *is the Randić index.*

The inequality becomes an equality if G is either the complete graph or the star graph.

Proof.

$$ABC(G) = \sum_{i\sim j} \sqrt{\frac{d_i + d_j - 2}{d_i d_j}} = \sum_{i\sim j} \sqrt{\frac{d_i + d_j - 2}{d_i d_j - 1}} \sqrt{\frac{d_i d_j - 1}{d_i d_j}}$$

$$\leq \sum_{i\sim j} \sqrt{R_{ij}} \sqrt{\frac{d_i d_j - 1}{d_i d_j}},$$

where R_{ij} is the effective resistance between vertices i and j (see Proposition 1 in [20]). Now the Cauchy Schwarz inequality allows us to bound the above with

$$\sqrt{\sum_{i\sim j} R_{ij} \sum_{i\sim j} \frac{d_i d_j - 1}{d_i d_j}} = \sqrt{(n-1) \sum_{i\sim j} \frac{d_i d_j - 1}{d_i d_j}} = \sqrt{(n-1)(|E| - R_{-1}(G))},$$

where the left equality uses Foster's first formula (see [13]).

The maximality of the complete graph and the star graph will be seen below •

The bound (2) is similar to a bound found by Horoldagva and Gutman with different means in [17] stating

$$ABC(G) \leq \sqrt{|E|(n - 2R_{-1}(G))}. \tag{3}$$

Bounds (2) and (3) are not comparable. A bit of algebra shows that our bound is better when

$$R_{-1}(G) \leq \frac{|E|}{2|E| - n + 1} = L_1. \tag{4}$$

Horoldagva and Gutman use their inequality (3) as an intermediate step in order to obtain yet another inequality for $ABC(G)$ in terms of the second Zagreb index, and use upper bounds on this index in order to get upper bounds on $ABC(G)$. They also provide the following general bound:

$$ABC(G) \leq \sqrt{m \left(n - \frac{8m}{\left(\sqrt{8m+1} - 1\right)^2} \right)}. \tag{5}$$

Here we take the alternative path of producing upper bounds for $ABC(G)$ using (2) and (3) with the help of *lower* bounds for $R_{-1}(G)$. Perhaps the best such bound is given in [21], stating

$$R_{-1}(G) \geq \frac{n}{2d_1}, \tag{6}$$

where d_1 is the largest degree of the graph and where the equality is attained in case G is regular. This allows us to prove the following universal bounds

Proposition 2. *For any graph G we have*

$$ABC(G) \leq \sqrt{(n-1)\left(|E| - \frac{n}{2d_1}\right)} \leq n\sqrt{\frac{n-2}{2}}, \tag{7}$$

and

$$ABC(G) \leq \sqrt{|E| n \left(1 - \frac{1}{d_1}\right)} \leq n\sqrt{\frac{n-2}{2}}. \tag{8}$$

Proof. Immediate from (2), (3) and (6) and the fact that $|E| \leq \frac{n(n-1)}{2}$ •

Again, the leftmost inequalities in (7) and (8) are not comparable, with (7) giving better bounds whenever $d_1 \geq n(1 - \frac{n-1}{2|E|})$ as in the case $d_1 = n-1$. Moreover, for the complete graph K_n, it is easily seen that $ABC(K_n) = n\sqrt{\frac{n-2}{2}}$, so either (7) or (8) state that the complete graph is maximal for the ABC index among all graphs. In addition to the maximality of the complete graphs, we can prove another maximal result taking advantage of the literature on the Randić index. Reference [19] mentions that the minimum among trees of $R_{-1}(G)$ is attained by the star graph S_n, and its value is 1. Therefore, (2) implies that for any tree we have that

$$ABC(T) \leq \sqrt{(n-1)(n-2)}. \tag{9}$$

On the other hand, it is not difficult to compute that $ABC(S_n) = \sqrt{(n-1)(n-2)}$, and thus S_n is maximal for the ABC index among trees. This fact can also be shown using (3) and it was cited in [17], Corollary 3.1.

Furthermore, reference [19] founds that the minimum among unicyclic graphs of $R_{-1}(G)$ is attained by the graph S_n^* which consists of the graph S_n with two leaves connected by an edge. Using that $R_{-1}(S_n^*) = \frac{n-2}{n-1} + \frac{1}{4}$ and (3) we get that for unicyclic graphs

$$ABC(G) \leq \sqrt{\frac{n(2n^2 - 7n + 9)}{2(n-1)}}. \tag{10}$$

Notice, however, that in this case we cannot prove that S_n^* is maximal for the ABC index among unicyclic graphs, because $ABC(S_n^*) = (n-3)\sqrt{\frac{n-2}{n-1}} + \frac{3}{\sqrt{2}}$, which is strictly smaller than the upper bound (10) for $n \geq 4$.

2.2 C-cyclic and planar graphs

We now consider a particular class of graph, so-called c-cyclic graphs, where c is the cyclomatic number of a graph G and it is given by $c = |E| - n + 1$. It corresponds to the number of independent cycles in G (see [7]). In particular, graphs with cyclomatic number $c = 0$ are trees and graphs with cyclomatic number $c = 1$ are unicyclic graphs.

Immediate applications of (7) and (8) allow us to provide the following bounds that improve those Propositions 2 and 3 in [20]:

Proposition 3. *If G is c-cyclic, $c \geq 0$, then*

$$ABC(G) \leq \sqrt{(n-1)\left(n-1+c-\frac{n}{2d_1}\right)}, \tag{11}$$

and

$$ABC(G) \leq \sqrt{n(n-1+c)\left(1-\frac{1}{d_1}\right)}. \tag{12}$$

If G is planar then

$$ABC(G) \leq \sqrt{(n-1)\left(3(n-2)-\frac{n}{2d_1}\right)} \leq \sqrt{\frac{6n^2-19n+2}{2}}. \tag{13}$$

The bound (11) is better than the bound (12) in case

$$d_1 \geq \frac{n(n-1+2c)}{2(n-1+c)}. \tag{14}$$

Thus (11) provides the better general bound when taking $d_1 = n-1$ and $n \geq \frac{3+\sqrt{1+8c}}{2}$:

$$ABC(G) \leq \sqrt{(n-1)\left(n-1+c-\frac{n}{2(n-1)}\right)}, \tag{15}$$

There are tight bounds for the ABC index of c-cyclic graphs, for at least $c \leq 4$. For instance, reference [10], through a complex analysis, finds that for any tetracyclic graph with $n \geq 9$ the following tight bound holds:

$$ABC(G) \leq (n-6)\sqrt{\frac{n-2}{n-1}} + \sqrt{\frac{n+2}{5(n-1)}} + 4\sqrt{2}. \tag{16}$$

Our rightmost bound in (15) is slightly worse but asymptotically equivalent to (16): for $n = 10$ the respective values of these bounds are 10.58 and 9.94; for $n = 100$ they are 100.73 and 99.63, etc. Our bound (15) though not optimal, shows a reference value to be improved by any attempt to crack the best bound for c-cyclic graphs for $c \geq 5$.

As expected, for $c = 0$ and $c = 1$, (15) is worse than (9) and (10), respectively.

2.3 Chemical graphs

We briefly recall that a chemical graph is a graph with $d_1 \leq 4$. Of the two bounds (7) and (8), for $d_1 = 4$, (8) produces the best bound whenever $n \geq 9$, allowing us to state the following

Proposition 4. *For any chemical graph G with $n \geq 9$ we have*

$$ABC(G) \leq \sqrt{\frac{3n|E|}{4}}.$$

This yields as particular cases the bounds

$$ABC(T) \leq \sqrt{\frac{3n(n-1)}{4}} \tag{17}$$

for chemical trees T with $n \geq 9$,

$$ABC(U) \leq n\sqrt{\frac{3}{4}} \tag{18}$$

for chemical unicyclic graphs U with $n \geq 9$, etc.

Bounds (17) and (18) are roughly of order $.87n$. There are known bounds for the ABC index of c-cyclic chemical graphs, for $c = 0, 1, 2$, slightly better than ours, as in [8] and [15] (their orders are roughly $.79n$), found with laborious procedures that contrast with the simplicity of the proof of Proposition 4. Even though Proposition 4 may not get the best constants, it shows a path for better bounds of the ABC index to be found in the future for chemical c-cyclic graphs when $c \geq 3$.

3 Bounds via Majorization

In this section we report the methodology based on majorization (for more details see [1], [2], [3], [4], [5] and [6]) that allows us to find further lower bounds for the Randić index and thus new upper bounds for the ABC index.

The Randić index can be equivalently expressed as:

$$R_{-1}(G) = \sum_{(i,j)\in E} \left(\frac{1}{d_i d_j}\right) = \frac{1}{2}\left(\sum_{(i,j)\in E} \left(\frac{1}{d_i} + \frac{1}{d_j}\right)^2 - \sum_{i=1}^{n} \frac{1}{d_i}\right)$$

Let $\pi = (d_1, d_2, .., d_n)$ be a fixed degree sequence and $\mathbf{x} \in \mathbb{R}^m$ be the vector whose components are $\frac{1}{d_i} + \frac{1}{d_j}$, with $(i, j) \in E$. Since $\sum_{i=1}^{n} \frac{1}{d_i}$ is a constant, $R_{-1}(G)$ is a Schur convex function of $\mathbf{x}$ and it is minimal (maximal) if and only $f(\mathbf{x}) = \sum_{i=1}^{m} x_i^2 = \|\mathbf{x}\|_2^2$ is minimal (maximal). It is possible to show that $\sum_{i=1}^{m} x_i = \sum_{(v_i,v_j)\in E} \left(\frac{1}{d_i} + \frac{1}{d_j}\right) = n$ and thus $\sum_{i=1}^{m} x_i$ is a constant. Let

$$\Sigma_n = \{\mathbf{x} \in \mathbb{R}_+^m : \langle \mathbf{x}, \mathbf{s^m} \rangle = n, x_1 \geq x_2 \geq \cdots \geq x_m\}$$

where $\mathbf{s^m}$ is the unit vector of dimension m. By considering a closed subset S of Σ_n whose minimal element with respect to the majorization order is $\mathbf{x}_*(S)$, the Randić index can be bounded below as follows (see (5) in [3]):

$$R_{-1}(G) \geq \frac{\|\mathbf{x}_*(S)\|_2^2 - \sum_{i=1}^{n} \frac{1}{d_i}}{2} = L_2 \tag{19}$$

This lower bound is new, to the best of our knowledge, and of interest in itself when applied to the Randić index. If we can gather more specific information on the degree sequence of G and characterize suitably the set S, then new different numerical bounds can be derived. In the sequel we use the bounds (2) or (3), modified with the introduction of L_1 obtained above through majorization technique, and we get:

$$ABC(G) \leq \sqrt{(n-1)\left(|E| - \frac{\|\mathbf{x}_*(S)\|_2^2 - \sum_{i=1}^{n} \frac{1}{d_i}}{2}\right)} \tag{20}$$

and

$$ABC(G) \leq \sqrt{|E|\left(n - \|\mathbf{x}_*(S)\|_2^2 + \sum_{i=1}^{n} \frac{1}{d_i}\right)}. \tag{21}$$

It is noteworthy that (21) is better than (20) when $L_2 \geq L_1$.

3.1 First type of degree sequence

In what follows we deal with graphs possessing h pendent vertices that is, graphs with degree sequence of the type:

$$\pi = (d_1, \cdots, d_{n-h}, \underbrace{1, \cdots, 1}_{h}), \tag{22}$$

where $h > 0$ and $n - h \geq 2$ (we do not consider the star graph S_n since it is well-known that $R_{-1}(S_n) = 1$). Pointing out that $\frac{1}{d_{n-h}} + \frac{1}{d_{n-h-1}} < 1 + \frac{1}{d_1}$ holds, we face the set

$$\begin{aligned} S_1 = \Big\{ \mathbf{x} \in \mathbb{R}_+^m : \langle \mathbf{x}, \mathbf{s^m} \rangle = n,\ 1 + \frac{1}{d_1} \leq x_h \leq \cdots \leq x_1 \leq \frac{1}{d_{n-h}} + 1\,, \\ \frac{1}{d_1} + \frac{1}{d_2} \leq x_m \leq \cdots \leq x_{h+1} \leq \frac{1}{d_{n-h}} + \frac{1}{d_{n-h-1}} \Big\}, \end{aligned} \tag{23}$$

whose minimal element with respect to the majorization order can be computed by Corollary 10 in [3] as follows:

$$\mathbf{x}_*(S_1) = \begin{cases} \left[\underbrace{m_1, ..., m_1}_{h}, \underbrace{\frac{n-hm_1}{m-h}, ..., \frac{n-hm_1}{m-h}}_{m-h}\right] & \text{if} \quad n < \widetilde{a} \\ \left[\underbrace{\frac{n-m_2(m-h)}{h}, ..., \frac{n-m_2(m-h)}{h}}_{h}, \underbrace{m_2, ..., m_2}_{m-h}\right] & \text{if} \quad n \geq \widetilde{a}, \end{cases}$$

where $\widetilde{a} = hm_1 + (m-h)m_2$, $m_1 = 1 + \frac{1}{d_1}$ and $m_2 = \frac{1}{d_{n-h}} + \frac{1}{d_{n-h-1}}$.

3.2 Second type of degree sequence

In this section we deal with graphs with degree sequences of the type:

$$\pi = (\underbrace{n-1, \cdots, n-1}_{h}, d_{h+1}, \cdots, d_n), \tag{24}$$

where $h > 1$. In this case there are no pendent nodes since necessarily $d_n \geq h$.

First of all, notice that the first h nodes are connected each other, hence we have $\frac{h(h-1)}{2}$ summands of the type $\frac{1}{d_i} + \frac{1}{d_j} = \frac{2}{n-1}$. In this case we face the set:

$$\begin{aligned} S_2 = \big\{\mathbf{x} \in \mathbb{R}^m_+ : \langle \mathbf{x}, \mathbf{s^m} \rangle = n, \;\; x_1 \geq x_2 \geq \cdots \geq x_m \;, \\ x_m = x_{m-1} = \cdots = x_{m-\frac{h(h-1)}{2}+1} = \frac{2}{n-1}\bigg\}. \end{aligned} \tag{25}$$

Now, let $m' = m - \frac{h(h-1)}{2}$. Since $\sum_{i=1}^m x_i = n = \sum_{i=1}^{m'} x_i + \frac{h(h-1)}{n-1}$, in the sequel we can deal with m' variables x_i which add up to $a' = n - \frac{h(h-1)}{n-1}$.

Assuming that the condition

$$\frac{1}{n-1} + \frac{1}{d_n} < \frac{1}{d_{h+1}} + \frac{1}{d_{h+2}} \tag{26}$$

holds, these variables can be split in two separate sequences and opportunely bounded. Hence we can consider the following subset S_2' of S_2:

$$\begin{aligned} S_2' = \bigg\{\mathbf{x} \in \mathbb{R}^{m'}_+ : \left\langle \mathbf{x}, \mathbf{s^{m'}} \right\rangle = a', \;\; \frac{1}{d_{h+1}} + \frac{1}{d_{h+2}} \leq x_{m'-h(n-h)} \leq \cdots \leq x_1 \leq \frac{1}{d_n} + \frac{1}{d_{n-1}} \;, \\ \frac{1}{n-1} + \frac{1}{d_{h+1}} \leq x_{m'} \leq \cdots \leq x_{m'-h(n-h)+1} \leq \frac{1}{n-1} + \frac{1}{d_n}\bigg\}, \end{aligned} \tag{27}$$

whose minimal element with respect to the majorization order is:

$$\mathbf{x}_*(S_2') = \begin{cases} \left[\underbrace{m_1,...,m_1}_{m'-h(n-h)}, \underbrace{\frac{a'-(m'-h(n-h))m_1}{h(n-h)},...,\frac{a'-(m'-h(n-h))m_1}{h(n-h)}}_{h(n-h)}\right] & \text{if} \quad a' < \widetilde{a} \\ \left[\underbrace{\frac{a'-m_2(h(n-h))}{m'-h(n-h)},...,\frac{a'-m_2(h(n-h))}{m'-h(n-h)}}_{m'-h(n-h)}, \underbrace{m_2,...,m_2}_{h(n-h)}\right] & \text{if} \quad a' \geq \widetilde{a}, \end{cases}$$

where $\widetilde{a} = (m'-h(n-h))m_1 + h(n-h)m_2$, $m_1 = \dfrac{1}{d_{h+1}} + \dfrac{1}{d_{h+2}}$ and $m_2 = \dfrac{1}{n-1} + \dfrac{1}{d_n}$.

For our purposes, in order to use (19), we need the minimal element of the set S_2 that can be easily written as:

$$\mathbf{x}_*(S_2) = \begin{cases} \left[\mathbf{x}_*(S'), \underbrace{\frac{2}{n-1},...,\frac{2}{n-1}}_{h(h-1)/2}\right] & \text{if} \quad a' < \widetilde{a} \\ \\ \left[\mathbf{x}_*(S'), \underbrace{\frac{2}{n-1},...,\frac{2}{n-1}}_{h(h-1)/2}\right] & \text{if} \quad a' \geq \widetilde{a}. \end{cases} \tag{28}$$

4 Numerical Examples

In this section we provide some numerical examples, using majorization in order to obtain bounds on $R_{-1}(G)$ and then we compare our results to those proposed in the literature.

To this aim we briefly recall the bounds we use for our analysis:

- (5): general bound given in [17];
- (7) and (8): bounds obtained by (2) and (3) via the inequality $R_{-1}(G) \geq \frac{n}{2d_1}$;
- (9): general bound for trees;
- (10): general bound for unicyclic graphs;
- (11) and (12): bounds for c-cyclic graphs;

- (20) and (21): bounds obtained by (2) and (3) via majorization technique.

4.1 Examples related to the first type of degree sequence

Example 1. Let us consider the family of trees $\mathcal{T}$ with 16 vertices, 10 pendent vertices and the degree sequence $\pi = (5,3,3,3,3,3,1,1,1,1,1,1,1,1,1,1)$. In this case $m = n-1 = 15$ (for more details see Section 4, Example i) in [3]).

The minimal element is

$$\mathbf{x}_*(\mathcal{T}) = \left[\underbrace{\frac{19}{15},\ldots,\frac{19}{15}}_{10},\underbrace{\frac{2}{3},\ldots,\frac{2}{3}}_{5}\right].$$

Replacing these values into (19) we obtain for any $T \in \mathcal{T}$:

$$R_{-1}(T) \geq 3.2 = L_2.$$

Since $L_2 > L_1 = 1$ we pick (21) that performs better than (20).

The results are summarized in Table 1:

Ref.	Bound
(21)	12
(9)	14.491

Table 1: Upper bounds for $ABC(T)$ for any $T \in \mathcal{T}$.

Example 2. We now deal with the family $\mathcal{U}$ of unicyclic graphs G, i.e. graphs for which $m = n$, with degree sequence $\pi = (3,3,3,3,2,2,2,2,2,2,1,1,1,1)$.

Since $\widetilde{a} > n$, the minimal element is:

$$\mathbf{x}_*(\mathcal{U}) = \left[\underbrace{\frac{4}{3},\ldots,\frac{4}{3}}_{4},\underbrace{\frac{23}{27},\ldots,\frac{23}{27}}_{9}\right].$$

Replacing these values into (19) we obtain for any $G \in \mathcal{U}$:

$$R_{-1}(G) \geq 2.904 = L_2$$

and because of $L_2 > L_1 = 0.926$ we choose inequality (21).

Furthermore, since condition (14) is not satisfied, bound (12) is better than (11).

The results are reported in Table 2:

Ref.	Bound
(21)	9.669
(12)	10.614
(10)	11.776
(5)	12.377

Table 2: Upper bounds for $ABC(G)$ for any $G \in \mathcal{U}$.

Example 3. Let us consider the family $\mathcal{B}$ of bicyclic graphs, i.e. those where $m = n+1$, with degree sequence $\pi = (3, 3, 3, 3, 2, 1, 1)$.

We have that $\widetilde{a} > n$ and the minimal vector is:

$$\mathbf{x}_*(G) = \left[\underbrace{\frac{4}{3}, \ldots, \frac{4}{3}}_{2}, \underbrace{\frac{13}{18} \cdots \frac{13}{18}}_{6} \right],$$

so that for $G \in \mathcal{B}$ we have

$$R_{-1}(G) \geq 1.425 = L_2.$$

Now, $L_2 > L_1 = 0.8$ and bound (21) is the best choice.

Moreover, condition (14) is not satisfied and bound (12) is preferable. The results are summed up in Table 3:

Ref.	Bound
(21)	5.762
(12)	6.110
(5)	6.768

Table 3: Upper bounds for $ABC(G)$ for any $G \in \mathcal{B}$.

4.2 Examples related to the second type of degree sequence

Example 1. Let us consider the family $\mathcal{G}$ of graphs with degree sequence:

$$\pi = (14, 14, 14, 14, 14, 14, 14, 14, 14, 14, 12, 11, 11, 10, 10)\,.$$

Notice that condition (26) is satisfied. We have $n = 15$, $m = 97$ and 45 summands of the type $\frac{1}{7}$.

Since $\widetilde{a} > a'$, because of (28), the minimal element is:

$$\mathbf{x}_*(\mathcal{G}) = \left[\underbrace{\frac{23}{132}, \ldots, \frac{23}{132}}_{2}, \underbrace{\frac{8223}{50000}, \ldots, \frac{8223}{50000}}_{50}, \underbrace{\frac{1}{7}, \ldots, \frac{1}{7}}_{45} \right],$$

so that we have for any $G \in \mathcal{G}$:

$$R_{-1}(G) \geq 0.576 = L_2,$$

by reason of $L_2 > L_1 = 0.5389$, we select bound (21). Now, in view of $d_1 = n - 1 = 14$ bound (7) is better than (8).

The results are summed up in Table 4:

Ref.	Bound
(21)	36.650
(5)	36.753
(7)	38.243

Table 4: Upper bounds for $ABC(G)$ for any $G \in \mathcal{G}$.

We can conclude that, for all the considered examples, bound (21) always performs better. It means that bound (3) modified with our methodology based on majorization technique is the best choice in these cases.

5 Final Remarks

The ABC index is one of the few chemical descriptors which passes the test of having a large correlation with the physicochemical properties it claims to describe (see [16]). It comes as no surprise, then, that both our upper bound (2) and the upper bound (3) of Horoldagva and Gutman are given in terms of the Randić index with $\alpha = -1$, which is also a highly correlated index, indeed the best among the general Randić indices R_α regarding this criterion.

The appeal of our bounds, such as those in Propositions 2 and 3, is of course their generality and simple proofs. Their weakness is that they do not produce, in general, optimal constants. In the case of our bound (2), this is probably due to the inequality

$$\frac{d_i + d_j - 2}{d_i d_j - 1} \leq R_{ij},$$

which becomes an equality only occasionally, for instance when $d_i = 1 \neq d_j$, that is, when i is a pendent vertex (and that is why our bounds produce the maximality of the star graph, where all its vertices are pendent). It also becomes an equality when all vertices other than i and j can be shorted (they have the same voltage) when a battery is placed between the neighbors i and j. This happens for every pair of vertices in the complete graph, and that is why our bounds achieve the maximality in this case.

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