About a Conjecture on the Randić Index of Graphs

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Abstract. For an edge uv of a graph G, the weight of the edge $e = uv$ is defined by $w(e) = 1/\sqrt{d(u)d(v)}$. Then

$$R(G) = \sum_{uv \in E(G)} 1/\sqrt{d(u)d(v)} = \sum_{e \in E(G)} w(e)$$

is called the Randić index of G. If G is a connected graph, then

$$\mathrm{rad}(G) = \min_x \max_y d(x, y)$$

is called the radius of G, where $d(x, y)$ is the distance between two vertices x, y. In 2000, Caporossi and Hansen conjectured that for all connected graphs except the even paths, $R(G) \geq r(G)$. They proved the conjecture holds for all trees except the even paths. In this paper, it is proved that the conjecture holds for all unicyclic graphs, bicyclic graphs and some class of chemical graphs.

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1. Introduction

In this paper, all graphs $G = (V, E)$ will be finite, undirected and simple. The degree and the neighborhood of a vertex $u \in V$ will be denoted by $d(u)$ and $N(u)$, respectively. The graph that arises from G by deleting the edge $uv \in E$ will be denoted by $G - uv$. For $x \in R$, $\lfloor x \rfloor$ denotes the greatest integer not exceeding x and $\lceil x \rceil$ the least integer not less than x. The other notions and denotations are same in [10].

Around the middle of the last century theoretical chemists recognized that useful information on the dependence of various properties of (mainly) organic substances on molecular structure can be obtained by examining pertinently constructed invariants of the underlying molecular graph. Eventually, graph invariants that are useful for chemical purposes, were named "topological indices" or, less confusing, "molecular structure-descriptors". Their main use is for designing so called *quantitative structure − property relations*, QSPR and *quantitative structure − activity relations*, QSAR.

In 1975 the Croatian scientist Milan Randić (who then lived in US) was aiming at constructing a mathematical model suitable for describing the extent of branching of organic moleculars, especially of the carbon-atom skeleton of alkanes. For this purpose conceived a so-called "branching index" [12] that is denoted by $R(G)$ and called *connectivity index* or *Randić (connectivity) index*. Here G stands for a molecular graph, that is a graph representation of the carbon-atoms skeleton of underlying hydrocarbon. Latter, Bollobás and Erdös [1, 2] generalized the concept and stimulated many other colleagues to study the *Randić index* and the *general Randić index*.

The Randić index $R(G)$ of a graph $G = (V, E)$ is defined as the sum of $1/\sqrt{d(u)d(v)}$ over all edges $uv \in E$, i.e.,

$$R(G) = \sum_{uv \in E(G)} 1/\sqrt{d(u)d(v)}.$$

The term $1/\sqrt{d(u)d(v)}$ will be called the weight of the edge $uv \in E$, and denoted by $w(uv)$.

Randić proposed this index in order to "quantitatively characterize the degree of molecular branching". According to him, the "degree of branching of the molecular skeleton is a critical factor" for some molecular properties such as "boiling points of hydrocarbons and the retention volumes and the retention times obtained from chromatographic studies" [12].

Already in 1947, Wiener [13, 14] proposed the *average distance* of a graph for the same purpose. This parameter is somehow easier to handle theoretically and it is received far more attention than the *Randić* index. For results and further references the reader may refer to the recent survey article [5].

The eccentricity $\varepsilon(v)$ of a vertex v in a connected graph G is the maximum graph distance between v and any other vertex u of G. For a disconnected graph, all vertices are defined to have infinite eccentricity.

The maximum eccentricity is the graph diameter. The minimum graph eccentricity is called the graph radius and denoted by $\text{rad}(G)$ or simplified by $r(G)$, i.e.,

$$\text{rad}(G) = r(G) = \min_x \max_y d(x, y),$$

where $d(x, y)$ is the distance between two vertices x, y. It should be obvious that $\text{diam}(G) \leq 2r(G)$. The center of a graph is the set of vertices of the graph that eccentricity equal to the graph radius, i.e., $\text{center}(G) = \{v \in V(G) : \varepsilon(v) = \text{rad}(G)\}$.

A tree T has $|\text{center}(T)| = 1$ or $|\text{center}(T)| = 2$. If $|\text{center}(T)| = 1$, the tree is called central, and if $|\text{center}(T)| = 2$, the tree is called bicentral. For any graph G, the diameter is at least the radius and at most twice the radius. For a tree T, $\text{diam}(T) = 2\text{rad}(T) - 1$ if T is bicentral, and $\text{diam}(T) = 2\text{rad}(T)$ if T is central. Hence, $\text{rad}(T) = \lceil \text{diam}(T)/2 \rceil$ for any tree T.

The *Randić* index of a graph G and its average distance $u(G)$ and other parameters are probably not independent for each other (see [3, 4, 6, 7, 8]). It is conjectured [6, Conjecture 3] that they satisfy the inequality $R(G) \geq u(G)$ for every graph G. In [3], Caporossi and Hansen proposed a stronger conjecture.

Conjecture 1.1. [3] *For all connected graphs G except even paths, $R(G) \geq r(G)$.*

They proved the conjecture holds for all trees except even paths.

In [11], it was obtained that $R(G) \geq r(G) - 1$ for all unicyclic graphs, all bicyclic graphs, and some class of chemical graphs. In [15], it was shown that $R(G) \geq r(G) - 1$ for biregular graphs, connected graphs with order $n \leq 10$ and tricyclic graphs.

In this paper, it is obtained that Conjecture 1.1 holds for all unicyclic graphs, all bicyclic graphs, and some class of chemical graphs.

2. Unicyclic graphs

Theorem 2.1. *For any unicyclic graph G, we have $R(G) \geq r(G)$.*

For the proof of Theorem 2.1, we need the following lemmas.

Lemma 2.1. [3]
  (1) *For all trees T, $R(T) - r(T) \geq \sqrt{2} - 3/2$;*
  (2) *For all trees T, except even paths, $R(T) \geq r(T)$.*

Lemma 2.2. [9] *Let T be a tree of order $n \geq 4$ with n_1 pendent vertices. Then if $n_1 < n - 1$,*

$$R(T) \geq \sqrt{n_1} + \left(1/\sqrt{2} - 1\right)/\sqrt{n_1} + (n - n_1 - 2)/2 + 1/\sqrt{2}$$

with equality if and only if T is the comet T_{n,n_1} (i.e.,a tree formed by a path P_{n-n_1} of which one end vertex coincides with a pendent vertex of a star S_{n_1+1} of order $n_1 + 1$)

Lemma 2.3. *Let T be a tree of order $n \geq 4$ with $n_1 \geq 3$ pendent vertices. Then $r(T) \leq \lceil (n - n_1 + 1)/2 \rceil$.*

Proof. Suppose that v_0 is a central point of T, i.e., $\text{rad}(T) = \max_y d(v_0, y)$. Then there are two pendent vertices v_1, v_2 of T such that $r(T) - 1 \leq d(v_i, v_0) \leq r(T)$ and $\max_i d(v_i, v_0) = r(T)$. Hence the $v_1 - v_0 - v_2$ path is a diameter of T and then

$$r(T) = \lceil \text{diam}(T)/2 \rceil \leq \lceil (n - (n_1 - 2) - 1)/2 \rceil = \lceil (n - n_1 + 1)/2 \rceil. \qquad \blacksquare$$

Lemma 2.4. *For every connected graph G with at least one cycle, if there is a $(2,2)$-edge $e_1 = u_1v_1$ in a cycle, then $R(G) - R(G - e_1) \geq 3/2 - \sqrt{2}$.*

Proof. Suppose that $N_G(u_1) = \{x_1, v_1\}, N_G(v_1) = \{y_1, u_1\}$. Then

$$R(G) - R(G - e_1)$$
$$= 1/2 + 1/\sqrt{2d_G(x_1)} - 1/\sqrt{d_G(x_1)} + 1/\sqrt{2d_G(y_1)} - 1/\sqrt{d_G(y_1)}$$
$$= 1/2 + 1/\sqrt{d_G(x_1)}\left(1/\sqrt{2} - 1\right) + 1/\sqrt{d_G(y_1)}\left(1/\sqrt{2} - 1\right)$$
$$\geq 1/2 + 1/\sqrt{2}\left(1/\sqrt{2} - 1\right) + 1/\sqrt{2}\left(1/\sqrt{2} - 1\right) = \frac{3}{2} - \sqrt{2} > 0. \qquad \blacksquare$$

Lemma 2.5. *For every connected graph G, if there is a $(2,3)$-edge $e = uv$ on a cycle but no $(2,2)$-edge on this cycle, then $R(G) - R(G - e) \geq 0.0176$.*

Proof. Without lose of generality, suppose that $d(u) = 2$ and $d(v) = 3$. Clearly, e is the edge with the maximum weight in the cycle, and the degree of another neighbor of u is at least 3.

Let $S_1 = \sum_{uy \in E \setminus \{uv\}} w(uy)$ and $S_2 = \sum_{vy \in E \setminus \{uv\}} w(vy)$. Then $S_1 \leq 1/\sqrt{6}$ and $S_2 \leq 1/\sqrt{6} + 1/\sqrt{3}$ since there is no $(2,2)$-edge on this cycle. Hence, we have

$$R(G) - R(G - e)$$

$$= 1/\sqrt{6} + S_1\left(1 - \sqrt{2}\right) + S_2\left(1 - \sqrt{3/2}\right)$$

$$\geq 1/\sqrt{6} + 1/\sqrt{6}\left(1 - \sqrt{2}\right) + \left(1/\sqrt{6} + 1/\sqrt{3}\right)\left(1 - \sqrt{3/2}\right) \approx 0.0176. \qquad \blacksquare$$

Lemma 2.6. *For any unicyclic graph G with n vertices, if there is no vertex of degree 2 on the cycle, then we have $r(G) \leq \lceil (n-3)/2 \rceil$; if there is at least one pendent path of length larger than 1 with every vertex on the cycle, then $r(G) \leq \lceil (n-4)/2 \rceil$.*

Proof. It is need only to prove the former case. It is obvious that the number of the pendent vertices > 2. Let v_0 denote a central point of G, then there are vertices $v_1, v_2 \in V(G)$, such that $r(G) - 1 \leq d(v_0, v_i) \leq r(G)$ and $\max\{d(v_0, v_1), d(v_0, v_2)\} = r(G)$. Then there are at least two vertices of G that are not on the path $v_1 - v_0 - v_2$. Hence $r(G) \leq \lceil (n-3)/2 \rceil$.

Similarly, $r(G) \leq \lceil (n-4)/2 \rceil$ if there is at least one pendent path of length larger than 1 for every vertex on the cycle. $\qquad \blacksquare$

Lemma 2.7. *Let e be any edge on the cycle of a connected graph G, then we have*

$$R(G) - R(G - e) \geq -1/4.$$

Proof. Suppose that $e = uv$ and $d(u) = d_1$ and $d(v) = d_2$. It is obvious that $S_1 = \sum_{uy \in E \setminus \{uv\}} w(uy) \leq (d_1 - 1)/\sqrt{d_1}$ and $S_2 = \sum_{vy \in E \setminus \{uv\}} w(vy) \leq (d_2 - 1)/\sqrt{d_2}$. Hence we have

$$R(G) - R(G - e)$$

$$\geq 1/\sqrt{d_1 d_2} + (d_1 - 1)/\sqrt{d_1}\left(1 - \sqrt{d_1/(d_1 - 1)}\right) + (d_2 - 1)/\sqrt{d_2}\left(1 - \sqrt{d_2/(d_2 - 1)}\right)$$

$$= 1/\left(\sqrt{d_1} + \sqrt{d_1 - 1}\right) + 1/\left(\sqrt{d_2} + \sqrt{d_2 - 1}\right) + 1/\sqrt{d_1 d_2} - 1/\sqrt{d_1} - 1/\sqrt{d_2}$$

$$> 1/\left(2\sqrt{d_1}\right) + 1/\left(2\sqrt{d_2}\right) + 1/\sqrt{d_1 d_2} - 1/\sqrt{d_1} - 1/\sqrt{d_2}$$

$$= f(d_1, d_2) \geq f(4, 4) = -1/4$$

because $\partial f/\partial d_1 = 1/\left(2\sqrt{d_1^3}\right)\left(1/2 - 1/\sqrt{d_2}\right)$, $\partial f/\partial d_2 = 1/\left(2\sqrt{d_2^3}\right)\left(1/2 - 1/\sqrt{d_1}\right)$,

and $\partial^2 f/(\partial d_1 \partial d_2) = 1/\left(4\sqrt{d_1^3 d_2^3}\right) > 0$. $\qquad \blacksquare$

We close this section with a proof of Theorem 2.1.

Proof of Theorem 2.1. Let G be an unicyclic graph. Then a tree T is obtained by deleting an edge on the cycle of G.

Case 1. If $G = S_n^+$ (i.e., G is the graph obtained from a star S_n by adding an edge which joins two pendent vertices), then $r(G) = 1$ and

$$R(G) = \begin{cases} 3/2, & n = 3, \\ 2/\sqrt{6} + 1/\sqrt{3} + 1/2 \approx 1.8938, & n = 4, \\ (n-3)/\sqrt{n-1} + \sqrt{2}/\sqrt{n-1} + 1/2 \geq \sqrt{2}/\sqrt{3} + 1/2 \approx 1.3165, & n > 4. \end{cases}$$

In the following, suppose that $G \neq S_n^+$. Then the tree T which is obtained by deleting any edge on the cycle has less than $n - 1$ pendent vertices.

Case 2. If there is a $(2,2)$-edge $e_1 = u_1 v_1$ on the cycle, then $R(G) - R(G - e_1) \geq 3/2 - \sqrt{2}$ by Lemma 2.4 and $R(G - e_1) - r(G - e_1) \geq \sqrt{2} - 3/2$ by Lemma 2.1. Hence $R(G) \geq R(G - e_1) + 3/2 - \sqrt{2} \geq r(G - e_1) \geq r(G)$.

Suppose that there is no $(2,2)$-edge on the cycle below. Then there are at least two pendent vertices in G.

Case 3. Suppose that the maximum weight edge on the cycle is a $(2,3)$-edge $e = uv$.

Then $G - e$ is not a path. By Lemmas 2.5 and 2.1, we have $R(G) > R(G - e) \geq r(G - e) \geq r(G)$.

In the following, suppose that there is neither $(2,2)$-edge nor $(2,3)$-edge on the cycle. Then there are at least 3 pendent vertices in G.

$(2,2)$-edge $(2,3)$-edge

Case 2   Case 3

Case 4

Case 5
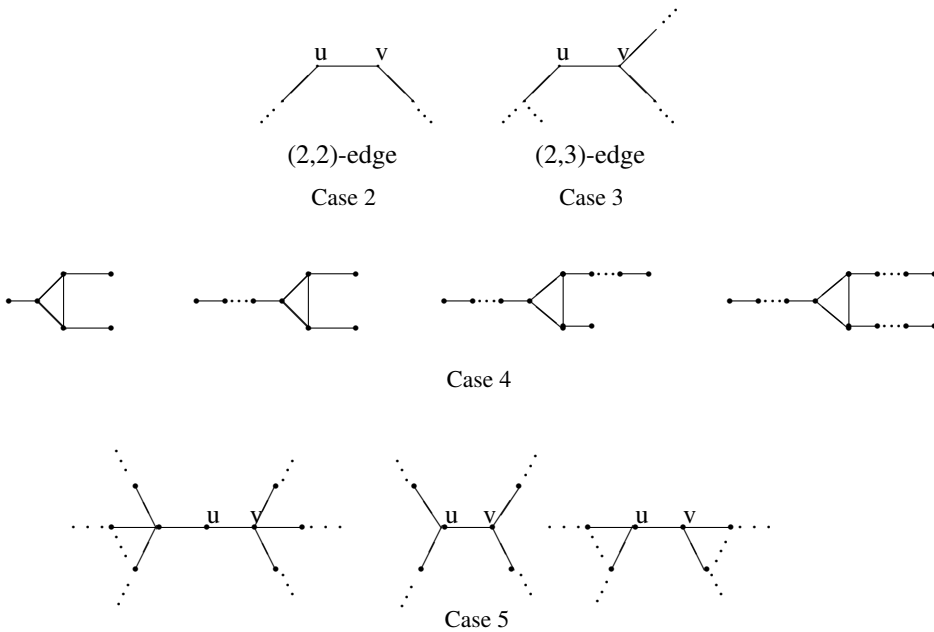
Figure 1. All subcases of Cases 2–5.

Case 4. Suppose that G has exactly 3 pendent vertices.

Then the cycle is a triangle and all edges on the cycle are $(3,3)$-edges (see Figure 1).

Suppose that the cycle is the triangle $v_1 v_2 v_3 v_1$ and $N(v_i) \setminus \{v_1, v_2, v_3\} = \{u_i\}$ with $d(u_i) \in \{1, 2\}$.

If $d(u_i) = 1$ for all $i = 1, 2, 3$, then $n = 6$ and $R(G) = \sqrt{3} + 1 > 2 = r(G)$.

If there is exactly one 2 in the multiset $\{d(u_1), d(u_2), d(u_3)\}$, then, by Lemma 2.6,

$$R(G) = 1 + 1/\sqrt{6} + 2/\sqrt{3} + 1/\sqrt{2} + (n - 7)/2 \approx n/2 - 0.23 > \lceil (n - 3)/2 \rceil \geq r(G).$$

If there is exactly one 1 in the multiset $\{d(u_1), d(u_2), d(u_3)\}$, then, by Lemma 2.6,

$$R(G) = 1 + 2/\sqrt{6} + 1/\sqrt{3} + \sqrt{2} + (n - 8)/2 \approx n/2 - 0.192 > \lceil (n - 3)/2 \rceil \geq r(G).$$

If $d(u_i) = 2$ for all $i = 1, 2, 3$, then, by Lemma 2.6,

$$R(G) = 1 + 3/\sqrt{6} + 3/\sqrt{2} + (n-9)/2 \approx n/2 - 0.154 > \lceil (n-4)/2 \rceil \geq r(G).$$

Case 5. Suppose that G has $n_1 \geq 4$ pendent vertices.

We will deal with it in three subcases.

Subcase 5.1. Assume that the maximum weight edge on the cycle is a $(2,4)$-edge $e = uv$, $d(u) = 2$, $d(v) = 4$, $N(u)\backslash v = \{x\}$ and $N(v)\backslash u = \{y_1, y_2, y_3\}$.

Then the degree of x is at least 4 and $G - e$ has just $n_2 = n_1 + 1 \geq 5$ pendent vertices. It is obvious that $S_1 = \sum_{uy \in E\backslash\{uv\}} w(uy) \leq 1/\left(2\sqrt{2}\right)$ and $S_2 = \sum_{vy \in E\backslash\{uv\}} w(vy) \leq 1 + 1/\left(2\sqrt{2}\right)$. Therefore, we have

$$R(G) - R(G-e)$$
$$= 1/\left(2\sqrt{2}\right) + S_1\left(1 - \sqrt{2}\right) + S_2\left(1 - \sqrt{4/3}\right)$$
$$\geq 1/\left(2\sqrt{2}\right) + 1/\left(2\sqrt{2}\right)\left(1 - \sqrt{2}\right) + \left(1 + 1/\left(2\sqrt{2}\right)\right)\left(1 - 2/\sqrt{3}\right)$$
$$\approx -0.0023.$$

Hence, by Lemma 2.2,

$$R(G) \geq R(G-e) - 0.0023$$
$$\geq \sqrt{n_2} + \left(1/\sqrt{2} - 1\right)/\sqrt{n_2} + (n - n_2 - 2)/2 + 1/\sqrt{2} - 0.0023$$
$$\geq \sqrt{5} + 1/\sqrt{10} - 1/\sqrt{5} + 1/\sqrt{2} + (n - n_2 - 2)/2 - 0.0023$$
$$= 2.8099 + (n - n_2 - 2)/2$$
$$\geq \lceil (n - n_2 + 1)/2 \rceil + 0.8099$$
(2.1) $\qquad > \lceil (n - n_2 + 1)/2 \rceil \geq r(G-e) \geq r(G).$

Subcase 5.2. Suppose that the maximum weight edge on the cycle is a $(3,3)$-edge e.

Then $G - e$ has just n_1 pendent vertices, and we may assume that $N(u) = \{v, y_1, y_2\}$ and $N(v) = \{u, x_1, x_2\}$. Clearly, there exist $d(y_i) \geq 3$ for some $i \in \{1, 2\}$ and $d(x_j) \geq 3$ for some $j \in \{1, 2\}$. Hence $S_1 = \sum_{uy \in E\backslash\{uv\}} w(uy) \leq 1/3 + 1/\sqrt{3} \approx 0.9107$ and $S_2 = \sum_{vy \in E\backslash\{uv\}} w(vy) \leq 1/3 + 1/\sqrt{3} \approx 0.9107$. Then we obtain that

$$R(G) - R(G-e) \geq 1/3 + 2 \times 0.9107\left(1 - \sqrt{3/2}\right) \approx -0.0760.$$

Hence, by Lemma 2.2, we have

$$R(G) \geq R(G-e) - 0.0760$$
$$\geq \sqrt{n_1} + \left(1/\sqrt{2} - 1\right)/\sqrt{n_1} + (n - n_1 - 2)/2 + 1/\sqrt{2} - 0.0760$$
$$\geq 2 + \left(1/\sqrt{2} - 1\right)/2 + (n - n_1 - 2)/2 + 1/\sqrt{2} - 0.0760$$
$$\approx 2.4847 + (n - n_1 - 2)/2$$
$$\geq \lceil (n - n_1 + 1)/2 \rceil + 0.4847 > \lceil (n - n_1 + 1)/2 \rceil$$

(2.2) $\qquad \geq r(G-e) \geq r(G).$

Subcase 5.3. Suppose that the maximum weight edge in the cycle is a (d_1,d_2)-edge e with $d_1 \geq 2, d_2 \geq 2$ and $d_1 + d_2 \geq 7$.

Clearly, $n_1 \geq 5$ in this case. Then $G - e$ has $n_2 \geq n_1$ pendent vertices. By Lemmas 2.7 and 2.2, we have

$$R(G) \geq R(G-e) - 1/4$$

$$\geq \sqrt{n_2} + \left(1/\sqrt{2} - 1\right)/\sqrt{n_2} + (n - n_2 - 2)/2 + 1/\sqrt{2} - 1/4$$

$$\geq \sqrt{5} + \left(1/\sqrt{2} - 1\right)/\sqrt{5} + (n - n_2 + 1)/2 - 3/2 + 1/\sqrt{2} - 1/4$$

$$= 8.8929/\sqrt{10} - 1.75 + (n - n_2 + 1)/2$$

$$> 1 + (n - n_2 + 1)/2 \geq \lceil (n - n_2 + 1)/2 \rceil + 0.5$$

(2.3) $\qquad > \lceil (n - n_2 + 1)/2 \rceil \geq r(G - e) \geq r(G).$

In a word, we have shown that $R(G) \geq r(G)$ for all unicyclic graphs. ∎

3. Bicyclic graphs

Recall that the cyclomatic number $g(G)$ of a graph G is the dimension of the cycle space of G, that is, the cyclomatic number of a graph G with $\kappa(G)$ components is $g(G) = \kappa(G) - |V(G)| + |E(G)|$. Clearly, the cyclomatic number of any connected graph G is $g(G) = 1 - |V(G)| + |E(G)|$. Now we consider the graphs with $g(G) = 2$, i.e., the bicyclic graphs.

Let x_1x_2 be an edge of the maximum weight in a graph G. In [1], it was obtained that $R(G) > R(G - x_1x_2)$. We shall have the following result with the same proof as in [1].

Lemma 3.1. *If $e = x_1x_2$ is the maximum edge in all edges that are incident to x_1 or x_2, then $R(G) - R(G - e) \geq 0$.*

Theorem 3.1. *For any bicyclic graph G, we have $R(G) \geq r(G)$.*

Proof. If there is a $(2,2)$-edge or a $(2,3)$-edge e in cycles of G, then the theorem holds by Lemmas 2.4 and 2.5 and Theorem 2.1.

Suppose that the maximum weight edge e in all cycles of G is a (d_1,d_2)-edge with $d_1 + d_2 \geq 6$ hereafter. We will inspect all cases of $\{d(u), d(v)\}$.

Case 1. $d(u) = d_1 = 2$ and $d(v) = d_2 = 4$. Then the degree of another neighbor of u is at least 4. It is evident that $S_1 = \sum_{uy \in E \setminus \{uv\}} w(uy) \leq 1/\sqrt{8}$ and $S_2 = \sum_{vy \in E \setminus \{uv\}} w(vy) \leq (d_2 - 2)/\sqrt{d_2} + 1/\sqrt{2d_2} = 1 + 1/\left(2\sqrt{2}\right)$ by the hypothesis.

Hence we have

$$R(G) - R(G-e)$$

$$\geq 1/\sqrt{8} + 1/\sqrt{8}\left(1 - \sqrt{2}\right) + \left(1 + 1/\left(2\sqrt{2}\right)\right)\left(1 - 2/\sqrt{3}\right)$$

$$= 3/\left(2\sqrt{2}\right) + 3/4 - 2/\sqrt{3} - 1/\sqrt{6} \geq 0.2477.$$

By Theorem 2.1, we have $R(G) \geq r(G)$.

Case 2. $d(u) = d(v) = 3$ and the maximum weight edge in the cycle of $G - e$ is a (d_1', d_2')-edge with $d_1' + d_2' = 5$.

Without loss of generality, assume that $d_1' = d_{(G-e)}(u) = 2$. Then every neighbor of u is in the cycles and its degree ≥ 3, and $S_1 \leq 2/3 \approx 0.6667$. Thus

$$R(G) - R(G - e) \geq 1/3 + 0.6667 \left(1 - \sqrt{3/2}\right) + 0.9107 \left(1 - \sqrt{3/2}\right)$$

$$\approx -0.0212.$$

Clearly, G has at least 2 pendent vertices and the two cycles have common vertices.

Subcase 2.1. G has two pendent vertices.

If G has exactly 2 pendent vertices, then G would be the one of graphs in Figure 2. Now we can chose e as the common edge of two cycles and then e is the maximum weight edge in all edges that incident to u, v, and so the result holds by Lemma 3.1 and Theorem 2.1. (In fact, it is straightforward to prove that the theorem holds in each case of the Figure 2.)

$R \approx 2.8214 > 2 = r$ $R \approx \frac{n}{2} - 0.1407 > \lceil \frac{n-2}{2} \rceil = r$ $R \approx \frac{n}{2} - 0.1026 \geq \lceil \frac{n-2}{2} \rceil \geq r$
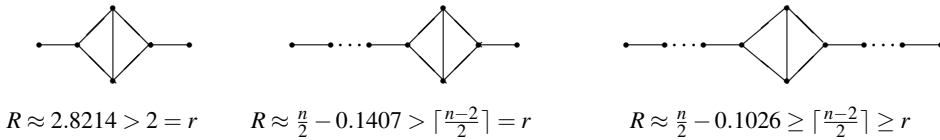
Figure 2. All cases of the graph with two pendent vertices.

Subcase 2.2. G has three pendent vertices.

If G has exactly 3 pendent vertices, then G would be the one of graphs in the Figure 3. It is straightforward to prove that the result holds in all of cases.

Subcase 2.3. G has at least 4 pendent vertices.

Then $G - e - e_1$ has at least 5 pendent vertices in this subcase. Therefore we have $R(G) \geq r(G)$ by Lemma 2.5 and the proof of Case 5 in Theorem 2.1.

Case 3. $d(u) = d(v) = 3$ and the maximum weight edge in the cycle of $G - e$ is a (d_1', d_2')-edge with $d_1' + d_2' \geq 6$.

By the hypothesis, we have $S_i \leq 1/3 + 1/\sqrt{3} \approx 0.9107$ for $i \in \{1, 2\}$. Hence

$$R(G) - R(G - e) \geq 1/3 + 2 \times 0.9107 \left(1 - \sqrt{3/2}\right)$$

$$\geq -0.0760.$$

Moreover, G has at least 4 pendent vertices, and the theorem holds by Lemma 2.5 and the proof of the Cases 4 and 5 in Theorem 2.1.
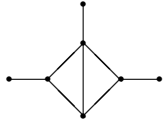
$R \approx 3.1874 > 2 = r$
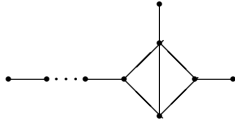
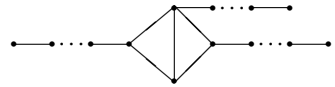$R \approx \frac{n}{2} - 0.2746 > \lceil \frac{n-3}{2} \rceil \geq r$
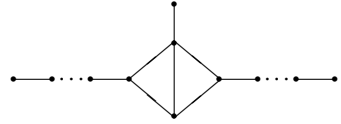
$R \approx \frac{n}{2} - 0.2366 \geq \lceil \frac{n-3}{2} \rceil \geq r$
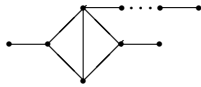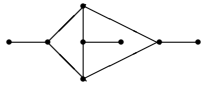
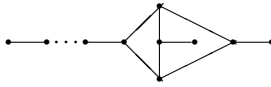$R \approx \frac{n}{2} - 0.2520 > \lceil \frac{n-4}{2} \rceil \geq r$
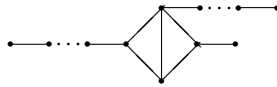
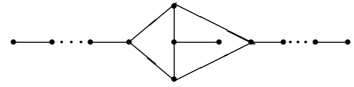$R \approx \frac{n}{2} - 0.2139 > \lceil \frac{n-4}{2} \rceil \geq r$

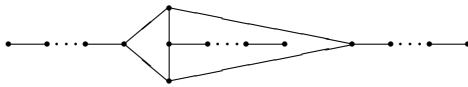$R \approx \frac{n}{2} - 0.1759 \geq \lceil \frac{n-4}{2} \rceil \geq r$
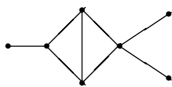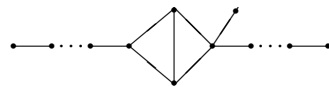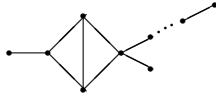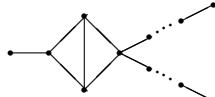
$R \approx 3.7321 > 2 = r$

$R \approx \frac{n}{2} - 0.23 > \lceil \frac{n-4}{2} \rceil \geq r$

$R \approx \frac{n}{2} - 0.1919 \geq \lceil \frac{n-4}{2} \rceil \geq r$

$R \approx n/2 - 0.154 > \lceil (n-5)/2 \rceil \geq r$

$R \approx 2.6547 > 2 = r$
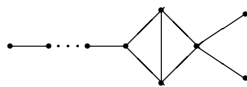
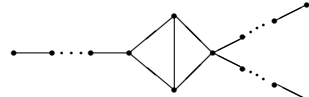$R \approx \frac{n}{2} - 0.3072 > \lceil \frac{n-3}{2} \rceil \geq r$

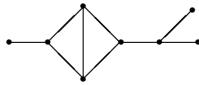$R \approx \frac{n}{2} - 0.2466 > \lceil \frac{n-3}{2} \rceil \geq r$

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$$R \approx \frac{n}{2} - 0.2846 > \lceil \frac{n-3}{2} \rceil \geq r$$
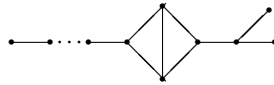
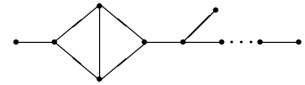$$R \approx \frac{n}{2} - 0.2240 > \lceil \frac{n-4}{2} \rceil \geq r$$

$$R \approx \frac{n}{2} - 0.1860 \geq \lceil \frac{n-4}{2} \rceil \geq r$$
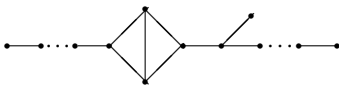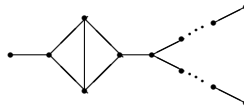
$$R \approx 3.7321 > 3 = r$$

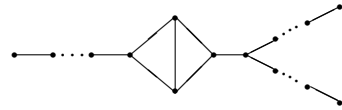$$R \approx \frac{n}{2} - 0.2300 > \lceil \frac{n-3}{2} \rceil \geq r$$

$$R \approx \frac{n}{2} - 0.2300 \geq \lceil \frac{n-3}{2} \rceil \geq r$$

$$R \approx \frac{n}{2} - 0.1919 > \lceil \frac{n-3}{2} \rceil \geq r$$

$$R \approx \frac{n}{2} - 0.1919 > \lceil \frac{n-4}{2} \rceil \geq r$$

$$R \approx \frac{n}{2} - 0.1539 \geq \lceil \frac{n-4}{2} \rceil \geq r$$

$$R \approx \frac{n}{2} - 0.2848 > \lceil \frac{n-3}{2} \rceil \geq r$$

$$R \approx \frac{n}{2} - 0.2468 \geq \lceil \frac{n-3}{2} \rceil \geq r$$

$$R \approx \frac{n}{2} - 0.2468 > \lceil \frac{n-3}{2} \rceil \geq r$$

$$R \approx \frac{n}{2} - 0.2088 > \lceil \frac{n-3}{2} \rceil \geq r$$

$$R \approx \frac{n}{2} - 0.2088 > \lceil \frac{n-4}{2} \rceil \geq r$$

$$R \approx \frac{n}{2} - 0.1708 \geq \lceil \frac{n-4}{2} \rceil \geq r$$

$R \approx 3.7320 > 3 = r$ $R \approx \frac{n}{2} - 0.23 > \lceil \frac{n-4}{2} \rceil \geq r$ $R \approx \frac{n}{2} - 0.23 \geq \lceil \frac{n-4}{2} \rceil \geq r$
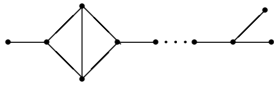

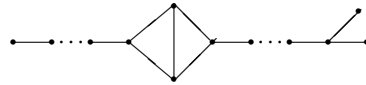$R \approx \frac{n}{2} - 0.1919 > \lceil \frac{n-4}{2} \rceil \geq r$ $R \approx \frac{n}{2} - 0.1919 > \lceil \frac{n-4}{2} \rceil \geq r$ $R \approx \frac{n}{2} - 0.1540 \geq \lceil \frac{n-5}{2} \rceil \geq r$
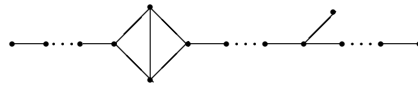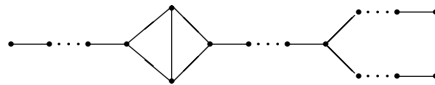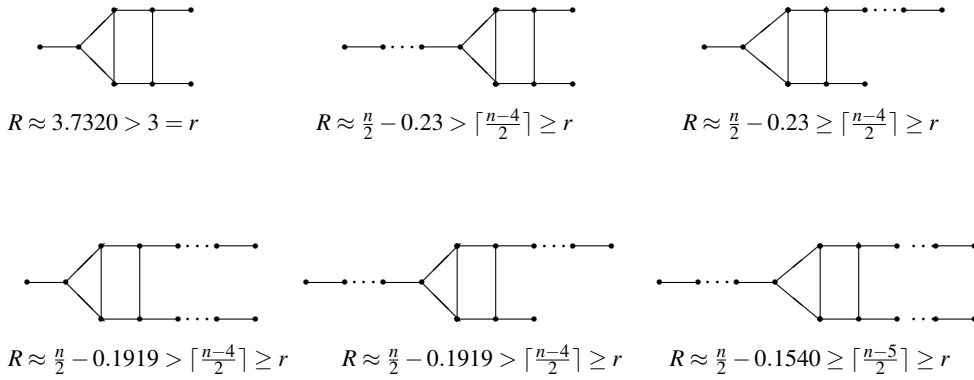
Figure 3. All cases of the graph with three pendent vertices.

Case 4. $d_1 = 3$ and $d_2 = 4$.

By the hypothesis, the degree of each neighbor of u in cycles is at least 4, and the degree of every neighbor of v in cycles is at least 3. It is obvious that $S_1 = \sum_{uy \in E \setminus \{uv\}} w(uy) \leq 1/(2\sqrt{3}) + 1/\sqrt{3}$ and $S_2 = \sum_{vy \in E \setminus \{uv\}} w(vy) \leq 1/(2\sqrt{3}) + 1$. Hence

$$R(G) - R(G - e)$$
$$\geq 1/(2\sqrt{3}) + \left(1/(2\sqrt{3}) + 1/\sqrt{3}\right)\left(1 - \sqrt{3/2}\right) + \left(1/(2\sqrt{3}) + 1\right)\left(1 - \sqrt{4/3}\right)$$
$$= \sqrt{3}/6 + 2/3 - \left(3\sqrt{2}\right)/4 \approx -0.1053.$$

Clearly, $G - e$ is a unicyclic graph which the maximum weight edge e_1 is a (d_1', d_2')-edge with $d_1' + d_2' \geq 6$.

Subcase 4.1. $d_1' = 2$ and $d_2' = 4$.

Then the neighbors of u are all in the cycles, and $S_1 = \sum_{uy \in E \setminus \{uv\}} w(uy) \leq 1/\sqrt{3}$ and $S_2 = \sum_{vy \in E \setminus \{uv\}} w(vy) \leq 1/(2\sqrt{3}) + 1$. Thus

$$R(G) - R(G - e)$$
$$\geq 1/(2\sqrt{3}) + 1/\sqrt{3}\left(1 - \sqrt{3/2}\right) + \left(1/(2\sqrt{3}) + 1\right)\left(1 - \sqrt{4/3}\right)$$
$$= 2/3 - 1/\sqrt{2} \approx -0.0404.$$

Clearly, $G - e$ has $n_1 \geq 4$ pendent vertices, and by the proof of Subcase 5.1 in Theorem 2.1, we have the result.

Subcase 4.2. $d_1' = d_2' = 3$.

Then $R(G) \geq r(G)$ by the proof of Cases 4 and 5 in Theorem 2.1.

Subcase 4.3. $d_1' + d_2' \geq 7$.

The result is obvious by the proof of Case 5 in Theorem 2.1.

Case 5. $d(u) = 2$ and $d(v) = 5$.

In this case, the degree of another neighbor x of u is at least 5. Hence, $G - e$ has at least $n_1 \geq 5$ pendent vertices, and thus $R(G) \geq R(G - e) - 1/4 \geq r(G)$ by Lemma 2.7 and formulas $(2.1),(2.2)$ and (2.3) in the Case 5 of the proof of Theorem 2.1.

Case 6. $d_1 + d_2 \geq 8$.

The result is obtained by Lemma 2.7 and the proof of Case 5 in Theorem 2.1.   ∎

4. Chemical graphs

Recall that a chemical graph is a connected graph which degree of every vertex is not larger than 4. Clearly, $g(G) \leq n + 1$ for any n-vertex chemical graph G.

Lemma 4.1. [3] *Let T be a chemical tree of order n with $n_1 \geq 5$ pendent vertices. Then*

$$R(T) \geq \frac{n}{2} + \frac{n_1}{2}\left(\frac{1}{\sqrt{2}} - 1\right) + \frac{3}{2} - \sqrt{2}$$

with equality if and only if n_1 is even and T is isomorphic to $L_e(n, n_1)$.
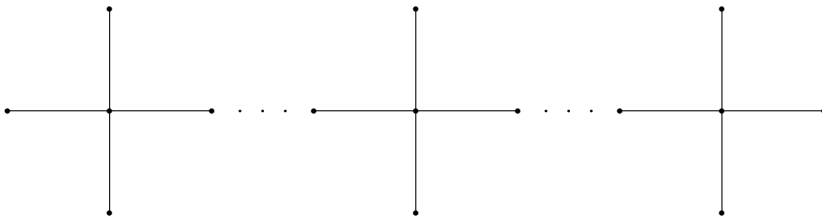

Figure 4. $L_e(n, n_1)$

Lemma 4.2. *Let $e = uv$ be the maximum weight edge on all cycles of a chemical graph G with $d_1 = d(u)$, $d_2 = d(v)$ and $d_1 + d_2 \geq 6$. Then we have $R(G) - R(G - e) \geq -0.1368$.*

Proof. We inspect all the possible cases for $d_1, d_2 \in \{2, 3, 4\}$.

Case 1. $d_1 = 2$ and $d_2 = 4$.

Then the degree of another neighbor vertex of u is 4. It is evident that $S_1 = \sum_{uy \in E \setminus \{uv\}} w(uy) = 1/\sqrt{8}$ and

$$S_2 = \sum_{vy \in E \setminus \{uv\}} w(vy) \leq \frac{d_2 - 2}{\sqrt{d_2}} + \frac{1}{\sqrt{2d_2}} = 1 + \frac{1}{2\sqrt{2}}$$

by the hypothesis. Hence we have

$$R(G) - R(G - e)$$
$$\geq \frac{1}{\sqrt{8}} + \frac{1}{\sqrt{8}}\left(1 - \sqrt{2}\right) + \left(1 + \frac{1}{2\sqrt{2}}\right)\left(1 - \frac{2}{\sqrt{3}}\right) \geq -0.0023.$$

Case 2. $d_1 = d_2 = 3$.

By the hypothesis, we have $S_i \leq 1/3 + 1/\sqrt{3} \approx 0.9107$ for $i \in \{1, 2\}$. Then

$$R(G) - R(G - e) \geq \frac{1}{3} + 2\left(1 - \sqrt{\frac{3}{2}}\right)$$

$$\geq 1/3 + (S_1 + S_2)\left(1 - \sqrt{3/2}\right)$$

$$\geq 1/3 + \left(2/3 + 2/\sqrt{3}\right)\left(1 - \sqrt{3/2}\right) \geq 0.0760.$$

Case 3. $d_1 = 3$ and $d_2 = 4$.

It is obvious that

$$S_1 = \sum_{uy \in E \setminus \{uv\}} w(uy) \leq \frac{1}{2\sqrt{3}} + \frac{1}{\sqrt{3}}$$

and

$$S_2 = \sum_{vy \in E \setminus \{uv\}} w(vy) \leq \frac{1}{2\sqrt{3}} + 1$$

by the hypothesis. Then

$$R(G) - R(G - e)$$

$$\geq \frac{1}{2\sqrt{3}} + \left(\frac{1}{2\sqrt{3}} + \frac{1}{\sqrt{3}}\right)\left(1 - \sqrt{\frac{3}{2}}\right) + \left(\frac{1}{2\sqrt{3}} + 1\right)\left(1 - \sqrt{\frac{4}{3}}\right)$$

$$\approx -0.1053$$

Case 4. $d_1 = d_2 = 4$.

By the hypothesis, we have $S_i \leq (1/4) + 1 = 1.25$ for $i \in \{1, 2\}$. Then

$$R(G) - R(G - e) \geq \frac{1}{4} + 2.5\left(1 - \sqrt{\frac{4}{3}}\right) \approx -0.1368 \qquad \blacksquare$$

In the following, suppose that G is a chemical graph with the cyclomatic number $g(G)$ and n_1 pendent vertices.

Theorem 4.1. *For any chemical graph G with $n_1 \geq 7$ pendent vertices and cyclomatic number $g(G) < (3/2)n_1$, we have $R(G) \geq r(G)$.*

Proof. By induction on the cyclomatic number $g(G)$ of G. Clearly, the theorem holds for $g(G) \in \{0, 1, 2\}$ by Lemma 2.1, Theorems 2.1 and 3.1.

Assume that the theorem holds for any chemical graph with $n_1 \geq 7$ pendent vertices and cyclomatic number $g = k \geq 2$, and let G be a chemical graph with $n_1 \geq 7$ pendent vertices and $g(G) = k + 1 < \frac{3}{2}n_1$. In the following, we show that the result holds for G.

Let T be the tree of G by a series of deleting the maximum weight edge on cycles. If there is a $(2,2)$- or $(2,3)$-edge $e = uv$ in some cycle of G, then the theorem holds by the induction hypothesis and Lemmas 2.4 and 2.5. Suppose that the maximum weight edge in all cycles of G is a (d_1, d_2)-edge with $d_1 + d_2 \geq 6$ and T has n_1 pendent vertices.

Since $n_1 \geq 7$, by Lemma 4.1, we have

$$R(G) \geq R(T) - 0.1368(g(G))$$

$$\geq \frac{n}{2} + \frac{n_1}{2}\left(\frac{1}{\sqrt{2}} - 1\right) + \frac{3}{2} - \sqrt{2} - 0.1368(g(G))$$

$$\geq \frac{n}{2} - 0.1465n_1 - 0.1368(g(G))$$

$$\geq \frac{n - n_1}{2} + 0.1483n_1 \geq \left\lceil \frac{n - n_1 + 1}{2} \right\rceil \geq r(G).$$

Hence the result holds. $\qquad \blacksquare$

Remark 4.1. Now it has been proved that the conjecture of Caporossi and Hansen is true for all unicyclic graphs, all bicyclic graphs and some class of chemical graphs. But we still do not know how to prove it for any connected graph. The case may be much more complicated.

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