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On the Inequality between Radius and Randić Index for Graphs*

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Abstract

The Randić index $R(G)$ of a graph G is the sum of weights $(\deg(u)\deg(v))^{-0.5}$ over all edges uv of G, where $\deg(v)$ denotes the degree of a vertex v. Let $r(G)$ be the radius of G. We prove that for any connected graph G of maximum degree four which is not a path with even number of vertices, $R(G) \geq r(G)$. As a consequence, we resolve the conjecture $R(G) \geq r(G) - 1$ given by Fajtlowicz in 1988 for the case when G is a chemical graph.

1 Introduction

In chemical graph theory topological indices belong to the set of molecular descriptors that are calculated based on the molecular graph of a chemical compound. In 1975 Milan Randić [10] introduced the topological connectivity index $R(G)$ of a graph G defined as the sum of weights $(\deg(u)\deg(v))^{-0.5}$ over all edges uv of G, i.e.,

$$R(G) = \sum_{uv \in E(G)} \frac{1}{\sqrt{\deg(u)\deg(v)}},$$

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where $\deg(v)$ is the degree of a vertex v. Randić has shown that there exists a correlation of the Randić index with several physico-chemical properties of alkanes such as boiling points, chromatographic retention times, enthalpies of formation, parameters in the Antoine equation for vapor pressure, surface areas and others. More information about Randić index can be found in the survey [8] by Li and Shi or in the book [9] by Li and Gutman.

For the last two decades researchers are investigating extremal values and relations between topological indices. In 1988 Fajtlowicz [6] stated the following conjecture:

Conjecture 1.1. *For all connected graphs G, $R(G) \geq r(G) - 1$.*

Caporossi and Hansen [2] have shown that $R(T) \geq r(T) + \sqrt{2} - 3/2$ for all trees T. Liu and Gutman [11] verified Conjecture 1.1 for unicyclic graphs, bicyclic graphs and chemical graphs with cyclomatic number $c(G) \leq 5$. You and Liu [12] proved that the conjecture is true for biregular graphs, tricyclic graphs and connected graphs of order $n \leq 10$. More recent results related to extremal values of the Randić index can be found in [4, 5, 7, 13, 14].

Very recently Dvořák et al. [1] have shown that for every graph $R(G) \geq r(G)/2$. Their main idea was introducing a parameter $R'(G)$ defined as:

$$R'(G) = \sum_{uv \in E(G)} \frac{1}{\max(\deg(u), \deg(v))} .$$

It is easy to see that for every graph G we have $R(G) \geq R'(G)$. However $R'(G)$ proves to be very useful as it is much easier to follow during graph modifications than $R(G)$.

In this paper we investigate Conjecture 1.1 for the case when G is a chemical graph – a graph of maximum degree ≤ 4. The main result of this paper is the following theorem.

Theorem 1.2. *For all connected chemical graphs G the following inequality holds:*

$$R'(G) \geq r(G) - \frac{1}{2}.$$

As a consequence, we prove Conjecture 1.1 for the case when G is a graph of maximum degree four. Our proof uses the bound on the maximum degree of the graph only in one step. Therefore, it may be said that we develop a general framework for proving Conjecture 1.1, reducing the problem to a slightly stronger version regarding a very special type of a graph, which we call a bag (appropriate definitions can be found in section 4). This version appears to be quite easy in the chemical case; however the proof in the general case eluded us.

Finally, we strengthen our result to the version of Conjecture 1.1 stated in [2], also only for chemical graphs:

Theorem 1.3. *If a connected chemical graph G is not a path of odd length ≥ 3 then $R(G) \geq r(G)$.*

It is easy to verify that Theorem 1.3 is not valid for any path P of odd length ≥ 3 as in this case $R(P) = r(P) - \frac{3}{2} + \sqrt{2}$.

2 Preliminaries

Throughout this paper all graphs are simple and undirected. For a graph G by $V(G)$ we denote the set of vertices of the graph G, and by $E(G)$ the set of edges of the graph G. By a k-vertex we denote a vertex of degree exactly k.

Now, let us introduce some definitions and observations concerning bridges and the radius of a graph. An edge $e \in E(G)$ is called a *bridge* if removing e increases the number of connected components of G. A *centre* of a connected graph G is a vertex $v \in V(G)$ such that $d(v, w) \leq r(G)$ for all $w \in V(G)$. Intuitively, the centre of a graph is a vertex attaining minimum in the definition of the radius of the graph. Now we state a few simple bounds on the radius of a graph.

Lemma 2.1. *Let $G = (V, E)$ be a connected graph. Then $r(G) \leq \frac{|V|}{2}$. Moreover, if G contains a k-vertex for $k \geq 3$ then $r(G) \leq \frac{|V|-(k-2)}{2}$.*

Proof. Let us consider a spanning tree T of G. Obviously, $r(T) \geq r(G)$ as distances in G are not greater than in T. Now take the longest path P in T, consisting of d vertices. As T is a tree, the midpoint of P (or one of the midpoints if d is even) is distant by at most $\frac{d}{2}$ to all the vertices of T, by the maximality of P. Obviously $d \leq |V|$, so $r(G) \leq r(T) \leq \frac{d}{2} \leq \frac{|V|}{2}$. In order to obtain the second part of the claim let v be a k-vertex and let T be any spanning tree containing all the edges incident with the vertex v. Then the vertex v has degree k in the tree T, so the longest path P excludes at least $k-2$ neighbours of this vertex. Thus $r(G) \leq r(T) \leq \frac{d-(k-2)}{2} \leq \frac{|V|-(k-2)}{2}$. $\square$

A vertex $v \in V(G)$ is *locally minimal* (resp. *maximal*) if and only if $\deg(v) \leq \deg(w)$ (resp. $\deg(v) \geq \deg(w)$) for all $vw \in E(G)$. We use the following lemma from [1]. For the sake of completeness, we include its proof.

Lemma 2.2. *If G' is derived from G by removing an edge incident with a locally minimal vertex, then $R'(G') \leq R'(G)$.*

Proof. Let v be a locally minimal vertex and w be any of its neighbours. By G' we denote the graph G with the edge vw removed. Observe that since v is locally minimal, the only edges in G' which have a different contribution to $R'(G')$ comparing to their contribution to $R'(G)$ are those incident with w. Let d be the degree of the vertex w in G. The contribution of each of the $d-1$ edges incident with w in G' increases by at most $\frac{1}{d-1} - \frac{1}{d}$ and the contribution of the edge vw to $R'(G)$ was $\frac{1}{d}$. Hence, $R'(G') \leq R'(G) - \frac{1}{d} + (d-1)(\frac{1}{d-1} - \frac{1}{d}) = R'(G)$. $\square$

This immediately yields the following corollary:

Lemma 2.3. *If G' is derived from G by removing a locally minimal vertex, then $R'(G') \leq R'(G)$.*

Now we introduce two lemmas, which enable us to 'cut' larger parts of the graph.

Lemma 2.4. *Let H be a connected graph and $v \in V(H)$ be such a vertex, that after the removal of v the graph H becomes a union of connected components $H_1, H_2, \ldots, H_k$ where $k \geq 3$. Then there exists an index j that if H' is derived from H by removal of H_j then H' is connected and $r(H') = r(H)$.*

Proof. The fact that H' is connected is obvious — all the components of $H - v$ are adjacent to v and we remove one of them. For $1 \leq i \leq k$ let us denote

$$r_i = \max_{u \in V(H_i)} d_H(v, u)\,.$$

Let j be such an index $1 \leq j \leq k$ that r_j is minimal. Let H' be as in the lemma statement.

Observe that $r(H) \leq \max_{1 \leq i \leq k} r_i$ because we can take v as a centre. Let w be the centre of the graph H. By the definition of j there exists a vertex $u \in V(H) \backslash V(H_j)$ such that $d_H(v, u) = \max_{1 \leq i \leq k} r_i$. If $w \in V(H_j)$ then $d_H(w, u) = d_H(w, v) + d_H(v, u) > \max_{1 \leq i \leq k} r_i \geq r(H)$, which is not possible. Hence we have $w \in V(H')$. Consequently, for each vertex $x \in V(H')$ we have $d_{H'}(w, x) = d_H(w, x) \leq r(H)$, and so $r(H') \leq r(H)$.

Now we prove that the radius of the graph H' is not smaller than the radius of the graph H. Let w' be the centre of H'. We show that for each vertex $u \in V(H)$ there exists a vertex $u' \in V(H')$ such that $d_H(w', u) \leq d_{H'}(w', u')$, which proves that $r(H) \leq r(H')$ since w' is the centre of H'. Observe that for each $u \in V(H')$ we have $d_H(w', u) = d_{H'}(w', u)$, so for $u \in V(H')$ we set $u' = u$. Consider any vertex $u \in V(H_j)$. Since v is a cut vertex and every path between u and w' includes v we have

$$d_H(w', u) = d_H(w', v) + d_H(v, u) = d_{H'}(w', v) + d_H(v, u) \leq d_{H'}(w', v) + r_j \,.$$

As $k \geq 3$ there exists an index $j' \neq j$ such that $w' \notin V(H_{j'})$. Since r_j is minimal we have $r_{j'} \geq r_j$. Let u' be any vertex from $V(H_{j'})$ such that $d_H(v, u') = d_{H'}(v, u') = r_{j'}$. Finally we have

$$d_H(w', u) \leq d_{H'}(w', v) + r_j \leq d_{H'}(w', v) + d_{H'}(v, u') = d_{H'}(w', u') \,.$$

This establishes the lemma. $\square$

Lemma 2.5. *Let H be a connected graph and $v \in V(H)$ be such a vertex that after its removal the graph H becomes a union of connected components $H_1, H_2, \ldots, H_k$. Let H' be a graph derived from H by removal of some H_i. Then $R'(H') \leq R'(H)$.*

Proof. We consecutively remove vertices from $V(H_i)$ until the graph becomes H', each time ensuring that the value of R' does not increase. Note that possibly at some moments our graph is not connected. Let v_{min} be a vertex of minimum degree among the vertices still to be removed and v_{max} be a vertex of maximum degree. If $\deg(v_{min}) \leq \deg(v)$ then v_{min} is a locally minimal vertex and can be removed due to Lemma 2.3. Assume then that $\deg(v_{min}) > \deg(v)$, so $\deg(v_{max}) > \deg(v)$ as well. Thus v_{max} is a locally maximal vertex, so

$$1 = \sum_{v_{max}w \in E(H)} \frac{1}{\max(\deg(v_{max}), \deg(w))} \,.$$

We see that if one removes all the remaining vertices from H_i, then the value of R' will decrease by at least 1 due to removal of all the edges incident with v_{max} and it will increase by at most 1 — the only increase is due to the edges incident with v and not incident with H_i, and it can be at most 1, as in the end the whole sum $\sum_{vw \in E(H')} \frac{1}{\max(\deg_{H'}(v), \deg_{H'}(w))}$ is at most 1. Therefore, in this situation we can remove all the remaining vertices and the value of R' will not increase. $\square$

3 Decomposition

We shall prove Theorem 1.2 by contradiction. From now on we assume that $G_0 = (V_0, E_0)$ is the smallest counterexample to Theorem 1.2 regarding $|V_0| + |E_0|$. Let us introduce a few simple lemmas, which will enable us to characterize G_0. We begin with a simple observation concerning locally minimal vertices.

Lemma 3.1. *Suppose that v is locally minimal in G_0. Then all the edges incident with v are bridges.*

Proof. Suppose that vw is not a bridge. By Lemma 2.2 removal of the edge vw from the graph G_0 does not increase R'. Moreover, after its removal the graph remains connected and its radius cannot decrease (as all the distances can only be larger). Therefore, by removing the edge vw from the graph G_0 we obtain a smaller counterexample, a contradiction. $\square$

Observe that after removing all the bridges in a connected graph, it becomes a union of connected components of size at least 3 not containing bridges (called further *bridgeless components*) and isolated vertices. Let us introduce a notion of bridge decomposition: a graph is decomposed into a tree, where the set of nodes of the tree consists of bridgeless components connected by paths comprised of bridges. See Fig 1 for an illustration. For a graph $G = (V, E)$ let $E' \subseteq E$ be the set of bridges. Consider the graph $G' = (V, E \setminus E')$. By $\mathcal{H}(G) = \{H_1, \ldots, H_k\}$ we denote the set of connected components of the graph G' containing at least three vertices.

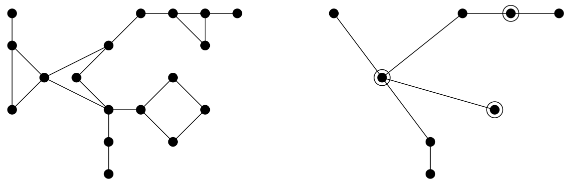

Figure 1: A connected graph G and a tree derived from G by identifying all components $H_i \in \mathcal{H}(G)$ into single vertices, which are presented as encircled nodes.

Lemma 3.2. *For any vertex v of the graph G_0 there are at most two bridges incident to the vertex v.*

Proof. Observe that if v is a cut-vertex of G_0, then removing v splits G_0 into exactly two connected components — otherwise by Lemmas 2.4 and 2.5 one of these components could be removed without decreasing radius and without increasing R', so we would obtain a smaller counterexample. Hence there are at most two bridges incident to the vertex v. $\square$

Let $E' \subseteq E$ be the set of bridges of G_0. Since we cannot have a cycle made of bridges, by Lemma 3.2 the edges E' form a set of paths. These paths end in the leaves of G_0 or in the bridgeless components $\mathcal{H}(G_0)$. Let us denote this set of paths by $\mathcal{B}(G_0)$. Lemmas 3.1,3.2 justify the following decomposition theorem.

Theorem 3.3. *Let $G_0 = (V_0, E_0)$ be a minimal counterexample to Theorem 1.2. Then:*

1. *G_0 is a tree of bridgeless components $H_i \in \mathcal{H}(G_0)$, connected by paths from the set $\mathcal{B}(G_0)$, and with possible additional paths from $\mathcal{B}(G_0)$ attached to them.*
2. *Every path from $\mathcal{B}(G_0)$ either connects two distinct components or is attached to one component.*
3. *The end-vertices of paths from $\mathcal{B}(G_0)$ leaving a given bridgeless component are distinct.*
4. *Removal of every edge that is not a bridge increases $R'(G_0)$.*

Proof. Let us decompose G_0 into bridgeless components $\mathcal{H}(G_0)$. By Lemma 3.2 the bridges of G_0 can form only a set of paths. Thus G_0 can be expressed as a set of bridgeless components connected by paths from $\mathcal{B}(G_0)$ and with paths from $\mathcal{B}(G_0)$ attached. Moreover, the end-vertices of paths from $\mathcal{B}(G_0)$ leaving a bridgeless component are distinct, because otherwise we would have a forbidden cut-vertex splitting the graph into at least 3 components.

To prove that removal of each edge that is not a bridge increases $R'(G_0)$, observe that otherwise after removal of such an edge the radius would not decrease, therefore we would obtain a smaller counterexample. □

4 Bridgeless components

Now we will resolve the case of a single bridgeless component from decomposition obtained in Theorem 3.3. Such a structure will be called a *bag*. We would be able to proceed with bags simply as subgraphs of G_0 induced by bridgeless components along with vertices at distance 1 from them, however we choose to introduce an abstract definition of a bag in order to establish a framework, which could be helpful in proving the general version of Conjecture 1.1.

Definition 4.1. *A connected graph H is a bag if:*

(1) *after removal of vertices of degree* 1 *it becomes a bridgeless component (denoted further by* $C(H)$*, the core of a bag),*

(2) *each vertex has at most one neighbour of degree* 1*,*

(3) *removal of each edge of* $C(H)$ *increases* $R'(H)$*.*

Firstly, let us observe the following properties of the bags:

Lemma 4.2. *If* H *is a bag then:*

(1) *no vertex of* $C(H)$ *is locally minimal,*

(2) H *does not contain* 2*-vertices,*

(3) *each* 3*-vertex has exactly one pendant neighbour,*

(4) 3*-vertices are not adjacent.*

Proof. To prove (1) observe that if $v \in V(C(H))$ is locally minimal, then all the edges incident with v would have to connect v with pendant vertices, due to property (3) of a bag and Lemma 2.2. So v would have to be the only vertex of $C(H)$, but it has at least 3 vertices.

In order to obtain (2) observe that a vertex v of degree 2 cannot have two pendant neighbours (then it would be the only vertex of $C(H)$) and it cannot have one pendant neighbour (then $C(H)$ would contain a bridge incident with v). So both of the edges incident with v connect it to other vertices of $C(H)$, having degree at least 2 by the definition of $C(H)$. Thus v is locally minimal, a contradiction.

To show (3) observe that if a 3-vertex has no pendant neighbour, then it is locally minimal as there are no 2-vertices in H. Moreover, each vertex has at most one neighbour of degree 1 by property (2) of a bag.

To verify (4) assume that $\deg(v) = \deg(w) = 3$ and $vw \in E(H)$. Obviously $vw \in E(C(H))$, so vw is not a bridge. Let us calculate the change of $R'(H)$ after the removal of vw:

- We have $-\frac{1}{3}$ due to the loss of the contribution of the edge vw.
- The contribution of remaining two edges incident with v can increase, but only from $\frac{1}{3}$ to $\frac{1}{2}$ if the corresponding neighbour had degree at most 2. But there are no 2-vertices, so only the contribution of edges connecting v to pendants can increase. Both remaining

neighbours of v cannot be pendants at the same time, because in this situation vw would be a bridge in $C(H)$. So the increase of the contribution of these edges can be at most $\frac{1}{2} - \frac{1}{3} = \frac{1}{6}$.

- Analogously, the increase of the contribution of the remaining two edges incident with w can be at most $\frac{1}{6}$.

Therefore, after the removal of vw, the change of R' is at most $-\frac{1}{3} + \frac{1}{6} + \frac{1}{6} = 0$, which is a contradiction with property (3) of a bag. $\square$

Now we are ready to prove that for chemical bags (namely bags with maximum degree at most 4) even stronger form of Theorem 1.2 holds. This stronger form will be crucial in the general case. As in the further proof we do not use the bound on the maximum degree of the graph, the following lemma stated for general bags would imply Conjecture 1.1 in full generality.

Proposition 4.3. *If H is a chemical bag, then $R'(H) \geq r(C(H)) + 1$.*

Proof. Denote by v_i the number of i-vertices in H. By (2) of Lemma 4.2 we know that $v_1 + v_3 + v_4 = |V(H)|$ and $v_3 + v_4 = |V(C(H))|$. Observe that H has exactly $\frac{v_1+3v_3+4v_4}{2}$ edges. Let $e_{i,j}$ be the number of edges in H with one end-vertex of degree i and the other of degree j. By further use of Lemma 4.2, we infer that:

- $e_{1,3} = v_3$,
- $e_{1,4} = v_1 - v_3$,
- $e_{3,4} + e_{4,4} = \frac{v_1+3v_3+4v_4}{2} - v_1$.

The contribution to R' of each edge is either $\frac{1}{3}$ or $\frac{1}{4}$. Thus

$$R'(H) = \frac{v_3}{3} + \frac{1}{4}\left(v_1 - v_3 + \frac{v_1 + 3v_3 + 4v_4}{2} - v_1\right) = \frac{v_3}{12} + \frac{v_1 + 3v_3 + 4v_4}{8} = \\ = \frac{v_3 + v_4}{2} + \frac{v_1 - v_3}{8} + \frac{v_3}{12}.$$

Observe that by Lemma 4.2(3) the number $v_1 - v_3$ is always nonnegative, as every 3-vertex has exactly one pendant neighbour. Thus $R'(H) \geq \frac{v_3+v_4}{2}$.

Suppose that there is a 4-vertex which does not have a pendant neighbour. Then it has degree 4 in $C(H)$ and from Lemma 2.1, we conclude that $r(C(H)) \leq \frac{v_3+v_4-2}{2}$. Thus

$$R'(H) = \frac{v_3 + v_4}{2} + \frac{v_1 - v_3}{8} + \frac{v_3}{12} \geq \frac{v_3 + v_4}{2} = \frac{v_3 + v_4 - 2}{2} + 1 \geq r(C(H)) + 1,$$

and we are done.

We are left with the case when all the vertices of the core have pendant neighbours. That means that $v_1 = v_3 + v_4$ and in $C(H)$ all the vertices are of degrees 2 or 3. Note that as the core has at least three vertices and 3-vertices in H (2-vertices in $C(H)$) are not connected, there must be at least one 4-vertex in H (which is a 3-vertex in $C(H)$). The sum of degrees of vertices of a graph is always even, so there must be at least two of them. Obviously, the number of vertices in $C(H)$ is at least 4, because we have a 3-vertex in $C(H)$. Observe that if there exists a vertex in $C(H)$ connected to all the other vertices, then $r(C(H)) = 1$ and thus $R'(H) \geq \frac{v_3+v_4}{2} \geq 2 = r(C(H)) + 1$ — we are done. Now we assume that every vertex of $C(H)$ is not connected to all the other vertices. In this situation there are at least 5 vertices in $C(H)$, because we have a 3-vertex, three its neighbours and at least one other vertex. At least two of these vertices are of degree 3 in $C(H)$, so $v_3 + v_4 \geq 5$ and $v_4 \geq 2$. Therefore,

$$\frac{v_1 - v_3}{8} + \frac{v_3}{12} = \frac{v_4}{8} + \frac{v_3}{12} = \frac{v_4}{24} + \frac{v_3 + v_4}{12} \geq \frac{2}{24} + \frac{5}{12} = \frac{1}{2}.$$

By Lemma 2.1, we conclude that $r(C(H)) \leq \frac{v_3+v_4-1}{2}$ as there is at least one 3-vertex in $C(H)$, so

$$R'(H) = \frac{v_3 + v_4}{2} + \frac{v_1 - v_3}{8} + \frac{v_3}{12} \geq \frac{v_3 + v_4}{2} + \frac{1}{2} = \frac{v_3 + v_4 - 1}{2} + 1 \geq r(C(H)) + 1.$$

Thus we are done in this case as well. □

5 The general case

Now using the decomposition from Theorem 3.3, we construct a tree T containing all the important information about the graph G_0.

Let $B \in \mathcal{H}(G_0)$ be a bridgeless component and let r_B be its radius. Moreover, let $V' \subseteq V(B)$ be the set of vertices of B that are incident with bridges in G_0. Remove all the vertices from the set $V(B) \setminus V'$ and add a central vertex v_B. Connect the central vertex v_B to each vertex $v \in V'$ be a path of length r_B. Additionally, attach two paths of length $r_B + 1$ to the central

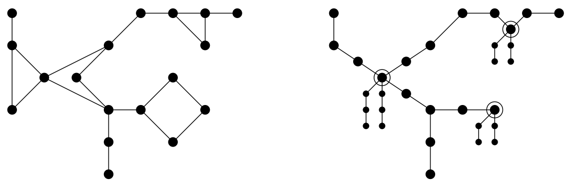

Figure 2: A graph G and its derived tree T with components of G replaced by star-like graphs. Centers of the star-like subgraphs are encircled. Vertices on the additional paths of length r_B+1 are smaller.

vertex v_B. See Fig 2 for an illustration. Theorem 3.3 assures that graph T constructed in this manner will be indeed a tree.

Lemma 5.1. *The following inequality holds:* $r(T) \geq r(G_0)$.

Proof. Let v_T be the centre of the tree T. Observe that as during the construction there were two paths of equal length attached to every central vertex, if v_T is on these attached paths it means that $v_T = v_B$ for some B. We choose a vertex $v \in V_0$ as follows:

- if $v_T \in V_0$ then let $v = v_T$,
- if v_T lies on a path added for some bridgeless component B connecting v_B with u — the end-vertex of some outgoing path from $\mathcal{B}(G_0)$, then let w be the centre of the component B. We know that $d_{G_0}(u, w) \leq r_B$ so one can choose a shortest path between u and w and take v from it such that $d_{G_0}(u, v) \leq d_T(u, v_T)$ and $d_{G_0}(v, w) \leq d_T(v_T, v_B)$. In particular, we let $v = w$, if $v_T = v_B$.

Now take any vertex $u \in V_0$. We shall prove that one can find a path between u and v in G_0 that is not longer than $r(T)$. We choose u_T in $V(T)$ as follows:

- if $u \in V(T)$ then let $u_T = u$,
- if u lies in a bridgeless component B then let u_T be a vertex on one of the two additional paths attached to v_B, in the same distance from v_B as u was from the centre of B.

To prove the lemma it is enough to show, that we can transform the shortest path between v_T and u_T in the tree T into a walk between v and u in the graph G_0 of non greater length. Indeed, in such a situation we would have that $r(T) \geq d_T(v_T, u_T) \geq d_{G_0}(v, u)$ and, as u was arbitrarily chosen, this would prove that $r(T) \geq r(G_0)$.

Let P be the shortest path from v_T to u_T in the tree T. We construct a walk P' in the graph G_0. Consider the first edge of the path P.

- If the first edge of the path P corresponds to a bridge in G_0, which means that it belongs to some path in $\mathcal{B}(G_0)$, in the walk P' we use the corresponding bridge.
- Now we consider the maximal prefix of the path P, which does not use an edge of the tree T which corresponds to a bridge in G_0. Observe that the path P ends either in a vertex belonging to both sets $V_0, V(T)$ or belonging to an attached path of length $r_B + 1$. In both cases we can construct a corresponding fragment of the walk P' going through the centre of the bridgeless component B, which will be of non greater length.

We continue in this manner with the following edges of the path P: each time we either use a bridge in the graph G_0 or replace a maximal fragment not using bridges from G_0 with a walk going through the centre of the bridgeless component. In the end we obtain the desired walk P', which concludes the proof. □

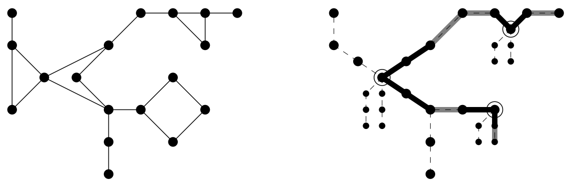

Figure 3: A graph G and its derived tree T with components of G replaced by star-like graphs together with a marked longest path in T. For the marked longest path in T we have $d_0 = 1, r_1 = 1, d_1 = 1, r_1 = 2, d_2 = 2, r_2 = 1, d_3 = 1$.

Now we are ready to finish the proof of Theorem 1.2. Take the longest path in T and denote it by P. This path consists of alternately paths from $\mathcal{B}(G_0)$ connecting bridgeless components in G_0 (or attached to bridgeless components) and joined pairs of radii connecting central vertices of stars (replacing bridgeless components) with their boundaries. We denote the lengths of paths originated in G_0 by $d_0, d_1, \ldots, d_k$ (in order of the appearance on P) and the radii of the bridgeless components by $r_1, r_2, \ldots, r_k$. Denote these bridgeless components by $B_1, B_2, \ldots, B_k$. If the path P starts (resp. ends) with an attached path of length $r_B + 1$ for some B, we simply assume that $d_0 = 1$ (resp. $d_k = 1$). Thus the length of P is equal to $l = \sum_{i=0}^{k} d_i + \sum_{i=1}^{k} 2r_i$ (see Fig 3).

If $k = 0$ then the whole graph G_0 is a path of length d_0 with $R'(G_0) = \frac{d_0}{2}$ if $d_0 > 1$ and $R'(G_0) = 1$ if $d_0 = 1$. In this situation $r(G_0) = \lceil \frac{d_0}{2} \rceil$ so we are done. From now assume that $k > 0$.

For every $1 \leq i \leq k$ with B_i we associate a chemical bag H_i: H_i is a graph induced in G_0 by $V(B_i)$ and vertices in distance 1 from B_i. Let us formally check that the graphs H_i are chemical bags, using Theorem 3.3:

(1) The only pendants in H_i are vertices in distance 1 from B_i, so $C(H_i) = B_i$ is a bridgeless component.

(2) The end-vertices of paths outgoing from B_i are distinct, so every vertex has at most one pendant neighbour.

(3) Removal of every edge vw from B_i increases $R'(G_0)$. The degrees of v, w are the same in G_0 and in H_i so the losses of contribution from vw to $R'(G_0)$ and to $R'(H_i)$ are equal. However, the neighbours of v and w have non greater degree in H_i than in G_0 so the increase of the contributions from the edges incident with v and w will be larger in H_i than in G_0. Therefore, removal of vw increases $R'(H_i)$ as well.

(4) H_i are induced subgraphs of a chemical graphs, so they are chemical as well.

By Proposition 4.3 we conclude that $R'(H_i) \geq r(B_i) + 1 = r_i + 1$. Thus

$$l \leq \sum_{i=0}^{k} d_i + \sum_{i=1}^{k} 2(R'(H_i) - 1) = (d_0 - 1) + \sum_{i=1}^{k-1} (d_i - 2) + (d_k - 1) + \sum_{i=1}^{k} 2R'(H_i).$$

Now we construct G' from G_0 by cutting out all the irrelevant parts of the graph: we cut out everything apart from bags H_i and parts of path P originated in the graph G_0. Note that these cuts can be expressed as applications of Lemma 2.5 to vertices in distance 1 from components B_i. Therefore $R'(G') \leq R'(G_0)$.

Now let us calculate $R'(G')$. Observe that $R'(G')$ consists of contributions of all H_i's and paths connecting them (plus the first and the last attached paths). Assume that $d_i \geq 2$ for some $1 \leq i \leq k-1$. Then the contributions of the first and last edge of the i-th path to $R'(G')$ is the same as the contributions to $R'(H_i)$ and $R'(H_{i+1})$, respectively. The contributions to $R'(G')$ of all $d_i - 2$ remaining edges are equal to $\frac{1}{2}$. Similarly, if $i = 0$ or $i = k$ then the contribution to $R'(G')$ of the last or first edge, respectively, is equal to its contribution to $R'(H_1)$ or $R'(H_k)$, respectively, and all the remaining $d_i - 1$ edges have contributions equal to $\frac{1}{2}$.

The only left case is when $d_i = 1$ for some $1 \le i \le k-1$. In this case subgraphs H_i and H_{i+1} share this edge and its contribution to the $R'(G')$ is equal to its contribution to $R'(H_i)$ or $R'(H_{i+1})$, depending which end-vertex of the edge has larger degree. However, both the contributions of this edge to $R'(H_i)$ or $R'(H_{i+1})$ are at most $\frac{1}{2}$, so the contribution to $R'(G')$ is not smaller than the sum of contributions to $R'(H_i)$ and $R'(H_{i+1})$ plus $-\frac{1}{2} = \frac{d_i-2}{2}$.

From this we conclude that

$$R'(G') \ge \frac{d_0-1}{2} + \sum_{i=1}^{k-1} \frac{d_i-2}{2} + \frac{d_k-1}{2} + \sum_{i=1}^{k} R'(H_i) \ge \frac{l}{2}.$$

As $r(T) = \lceil \frac{l}{2} \rceil$ and l is an integer, $r(T) \le \frac{l}{2} + \frac{1}{2}$. Therefore

$$R'(G_0) \ge R'(G') \ge \frac{l}{2} \ge r(T) - \frac{1}{2} \ge r(G_0) - \frac{1}{2},$$

which finishes the proof of Theorem 1.2.

□

6 From R' to Randić Index R

As for every graph G it holds $R'(G) \le R(G)$, we have proven that for chemical graphs $R(G) \ge r(G) - \frac{1}{2}$. We can slightly strengthen this result to prove Theorem 1.3, i.e. if a connected chemical graph G is not a path of odd length greater than 2 then $R(G) \ge r(G)$.

Proof of Theorem 1.3 Observe that for all $a \in \{1,2,3,4\}$ and $b \in \{1,2,3,4\}$ the following inequality holds:

$$\left(\frac{1}{\sqrt{a}} - \frac{1}{\sqrt{b}}\right)^2 \le \frac{1}{\sqrt{ab}} - \frac{1}{\max(a,b)}. \tag{6.1}$$

Obviously, the equality holds for $a = b$. Simple calculations of all 6 relevant cases (without losing generality $a < b$) show that the term RHS − LHS, which is right hand side minus left hand side of (6.1), is always positive:

a	1	1	1	2	2	3
b	2	3	4	3	4	4
RHS − LHS ≥	0.1213	0.0653	0.0000	0.0580	0.0606	0.0326

Observe that if $|V| = 1$, then $r(G) = R(G) = 0$ so the theorem holds.

Now suppose that all the vertices of G have degrees 1 or 2. As G is connected it is a cycle or a path. We will use an alternative formula introduced by Caporossi et al. [3] for the Randić

Index of a connected graph on at least two vertices:

$$R(G) = \frac{|V(G)|}{2} - \frac{1}{2} \sum_{vw \in E(G)} \left(\frac{1}{\sqrt{\deg(v)}} - \frac{1}{\sqrt{\deg(w)}} \right)^2 . \tag{6.2}$$

If G is a cycle then it is a regular graph, so $R(G) = \frac{|V(G)|}{2} \geq r(G)$ due to Lemma 2.1. If G is a path of length 1 then $r(G) = 1 = R(G)$. If G is a path of even length ≥ 2 then $r(G) = \frac{|V(G)|-1}{2}$ and $R(G) = \frac{|V(G)|}{2} - \left(1 - \frac{1}{\sqrt{2}}\right)^2 \geq \frac{|V(G)|}{2} - \left(\frac{1}{2}\right)^2 \geq r(G)$.

We are left with the case in which there exists at least one vertex of degree ≥ 3. By Lemma 2.1 we know that $r(G) \leq \frac{|V(G)|-1}{2}$. Applying inequality (6.1) to $a = \deg(v)$ and $b = \deg(w)$ for all edges $vw \in E(G)$ and using equation (6.2) we conclude that

$$\begin{aligned} R(G) &= \frac{|V(G)|}{2} - \frac{1}{2} \sum_{vw \in E(G)} \left(\frac{1}{\sqrt{\deg(v)}} - \frac{1}{\sqrt{\deg(w)}} \right)^2 \\ &\geq \frac{|V(G)|}{2} - \frac{1}{2} \sum_{vw \in E(G)} \left(\frac{1}{\sqrt{\deg(v)\deg(w)}} - \frac{1}{\max(\deg(v), \deg(w))} \right) \\ &= \frac{|V(G)|}{2} - \frac{R(G)}{2} + \frac{R'(G)}{2}. \end{aligned}$$

Therefore

$$2\left(\frac{|V(G)|}{2} - R(G)\right) \leq R(G) - R'(G).$$

If $\frac{|V(G)|}{2} - R(G) \leq \frac{1}{2}$ then, by Lemma 2.1, $R(G) \geq \frac{|V(G)|-1}{2} \geq r(G)$ and we are done. However if $\frac{|V(G)|}{2} - R(G) > \frac{1}{2}$ then $R(G) > R'(G) + 1 \geq r(G) - \frac{1}{2} + 1 > r(G)$ due to Theorem 1.2, and we are done as well. This establishes the theorem. $\square$

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