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Variable Neighborhood Search for Extremal Graphs. 19. Further Conjectures and Results about the Randić Index

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Abstract

Using the AutoGraphiX 2 system (AGX2), we study further relations between graph invariants of the form

 $lb_n \leq R \oplus i \leq ub_n$

where R denotes the Randić index of a graph G = (V, E), *i* another invariant, \oplus denotes one of the four operations $+, -, \times, /, lb_n$ and ub_n lower and upper bounding functions of the order n of the graph considered which are tight for all n (except possibly very small values due to border effects). Here *i* is in turn maximum, minimum and average degree, Δ , δ and \overline{d} , diameter D, girth g, algebraic and node connectivity, a and ν , Conjectures are obtained in 51 out of 56 cases, 28 of which are proved automatically, 19 are proved by hand, 7 remain open and only one is refuted.

1 Introduction

Let G = (V, E) denote a graph, where V is the set of its vertices and E the set of its edges. For a vertex v_i of G, $d_i = d(v_i)$ is the degree of v_i , *i.e.*, the number of its adjacent vertices. Let δ , \overline{d} and Δ be respectively the minimum, average and maximum degree of G.

G is a tree if it is connected and has no cycles. A leaf of a tree, also called a pending vertex, is a vertex of degree 1. Any non-trivial tree has at least two leaves. An inner vertex of a tree is a non-leaf vertex.

For a subset S of vertices of G, G - S denotes the graph obtained from G by removing all vertices in S and incident edges.

The Randić index [23] of G is defined as follows:

$$R = \sum_{(i,j)\in E} \frac{1}{\sqrt{d_i d_j}}$$

and $\frac{1}{\sqrt{d_i d_j}}$ is called the weight of edge (i, j).

Since 1975, when Milan Randić proposed this index (initially called connectivity index, and viewed as a measure of molecular branching) it was very extensively studied, extended and applied in over 1400 papers and books (*e.g.* [15, 16, 19, 20, 24]). For a comprehensive survey of its mathematical properties see the recent book of Li and Gutman on *Mathematical Aspects of Randić-Type Molecular Structure Descriptors* [21].

The AutoGraphiX system (AGX) [2, 11, 12] for computer-assisted and, for some of its functions, automated graph theory has been developed at GERAD, Montreal since 1997. This system leads to, among other features, automated generation of conjectures and automated proof of the easiest among them. Over two dozen papers have been written on AGX and its applications to mathematical and chemical graph theory. References can be found in a short recent survey paper [4]. The two successive versions AGX 1 and AGX 2 were already applied to the study of the Randić index in five papers: (a) in [9] chemical trees with maximum and minimum Randić index were determined (see also [10, 15, 25] for proofs that the path has maximum Randić index for trees). This approach, and a new way to use integer linear programming to obtain relations which can be deduced from the graphs found, led to many extensions, e.g. [16, 22]; (b) in [17] interactive use of AGX led to improve relations between R and the ramification index obtained by Araujo and de la Peña [7]; (c) in [6] relations between the Randić index R and the matching number μ or the index λ_1 are studied in a similar way as done below for other invariants, (d) in [5] a conjecture of Delorme, Favaron and Rautenbach [14] on graphs with given order n, minimum degree δ and minimum Randić index R is refuted by AGX 2 and a new conjecture is proposed, (e) in [18] the same was done for the Randić index R and the chromatic number χ . Moreover, in the thesis [1] a systematic comparison was made on relations between pairs selected from a set of 20 graph invariants, including the Randić index. The general form of these relations is

$$lb_n \leq i_1 \oplus i_2 \leq ub_n$$

where i_1 and i_2 are graph invariants, \oplus denotes one of the four operations $-, +, /, \times, lb_n$ and ub_n lower and upper bounding functions for $i_1 \oplus i_2$ depending on the order n (or number of vertices) of the graphs under consideration. These bounding functions are requested to be best possible in the strong sense, *i.e.*, for all n (except possibly for very small values due to border effects) there is a graph such that the lower (upper) bound is attained.

In this paper, we focus on some further results of that study, which as in [6, 18] concern the Randić index. More precisely we study relations of the form

$$lb_n \leq R \oplus i \leq ub_n$$

where R denotes the Randić index of a graph G = (V, E), $i \in \{\delta, \overline{d}, \Delta, D, g, a, \nu\}$ and δ, \overline{d} and Δ denote, respectively, the *minimum, average and maximum degree,* D denotes the diameter (*i.e.*, the maximum distance between two vertices), g denotes the girth (*i.e.*, the length of the shortest cycle), a denotes the *algebraic connectivity* of G (*i.e.*, the second smallest eigenvalue of

G for \underline{b}_n	\underline{b}_n	Inv.	\overline{b}_n	G for \overline{b}_n
S_n	$\sqrt{n-1}$	Ra	$\frac{n}{2}$	G regular: $K_n, C_n \ldots$
P_n, S_n, \ldots	1	δ	n-1	K_n
Tree: P_n, S_n, \ldots	$2 - \frac{2}{n}$	\overline{d}	n-1	K_n
P_n, K_n	2	Δ	n-1	K_n, S_n, \ldots
K_n	1	D	n-1	P_n
K_n, \ldots	3	g	n	C_n
P_n	$2(1-\cos\frac{\pi}{n})$	a	n	K_n
P_n, S_n, \ldots	1	ν	n-1	K_n

Table 1: Bounds and associated extremal graphs on the invariants

the Laplacian matrix L of G, where $L_{ij} = 1$ if $ij \in E$, $L_{ij} = 0$ if $ij \notin E$ and $i \neq j$, and $L_{ii} = -d_i$) and ν denotes the node connectivity of G (*i.e.*, the minimum number of vertices whose removal disconnects the graph or reduces it to a single vertex).

These indices are considered in turn in the next seven sections. Brief conclusions are drawn in the last section.

In order to prove automatically some easy relations, we need the best possible bounding functions for the individual invariants as well as the lists of families of extremal graphs for which they are attained. This information is gathered in Table 1.

2 The minimum degree

The lower and upper bounds on $R+\delta$ and $R\cdot\delta$ are obtained and proved automatically by AGX 2 using the information summarized in Table 1.

Observation 1 For any connected graph G on $n \ge 3$ vertices with Randić index R and minimum degree δ ,

$$1+\sqrt{n-1} \leq R+\delta \leq \frac{3n-2}{2} \qquad and \qquad \sqrt{n-1} \leq R\cdot\delta \leq \frac{n(n-1)}{2}.$$

The lower bounds are attained if and only if G is the star S_n , and the upper bounds if and only if G is the complete graph K_n . To prove the next proposition (an AGX 2 automated conjecture) we need to use the following formula, due to Caporossi et al. [9], for the Randić index of a connected graph G = (V, E) on n vertices and with degree sequence $d_1, d_2, \dots d_n$:

$$R = \frac{n}{2} - \frac{1}{2} \sum_{ij \in E} \left(\frac{1}{\sqrt{d_i}} - \frac{1}{\sqrt{d_j}} \right)^2.$$
 (2.1)

We need also the following lemma, which may be of interest in its own right.

Lemma 1 For any connected graph G on n vertices with minimum degree δ , maximum degree Δ and Randić index R, we have

$$R \ge \frac{\delta n}{\delta + \Delta}.\tag{2.2}$$

Proof

Using the formula (2.1) for the Randić index and assuming, without loss of generality, that for an edge ij, $d_j \ge d_i$ and thus $d_j = d_i + t_{ij}$ with $t_{ij} \ge 0$, we have

$$\begin{split} R &= \frac{n}{2} - \frac{1}{2} \sum_{ij \in E} \left(\frac{1}{\sqrt{d_i}} - \frac{1}{\sqrt{d_j}} \right)^2 = \frac{n}{2} - \frac{1}{2} \sum_{ij \in E} \left(\frac{\sqrt{d_i} - \sqrt{d_j}}{\sqrt{d_i d_j}} \right)^2 \\ &= \frac{n}{2} - \frac{1}{2} \sum_{ij \in E} \frac{d_i + d_j - 2\sqrt{d_i d_j}}{d_i d_j} = \frac{n}{2} - \frac{1}{2} \sum_{ij \in E} \frac{2d_i + t_{ij} - 2\sqrt{d_i (d_i + t_{ij})}}{d_i d_j} \\ &\geq \frac{n}{2} - \frac{1}{2} \sum_{ij \in E} \frac{2d_i + t_{ij} - 2d_i}{d_i d_j} = \frac{n}{2} - \frac{1}{2} \sum_{ij \in E} \frac{t_{ij}}{d_i d_j} \\ &\geq \frac{n}{2} - \frac{1}{2} \sum_{ij \in E} \frac{\Delta - \delta}{d_i d_j} = \frac{n}{2} - \frac{\Delta - \delta}{2} \sum_{ij \in E} \frac{1}{\sqrt{d_i d_j}\sqrt{d_i d_j}} \\ &\geq \frac{n}{2} - \frac{\Delta - \delta}{2\delta} \sum_{ij \in E} \frac{1}{\sqrt{d_i d_j}} = \frac{n}{2} - \frac{\Delta - \delta}{2\delta} R. \end{split}$$

 \mathbf{So}

$$\frac{\Delta+\delta}{2\delta}R \ge \frac{n}{2}$$

and

$$R \ge \frac{\delta n}{\Delta + \delta},$$

which proves the lemma.

Proposition 1 For any connected graph G on $n \ge 7$ vertices with Randić index R and minimum degree δ .

$$\frac{2-n}{2} \le R - \delta \le \frac{3n - 13 + \sqrt{6} + 3\sqrt{2}}{6},\tag{2.3}$$

$$\frac{n}{2n-2} \le \frac{R}{\delta} \le \frac{3n-7+\sqrt{6}+3\sqrt{2}}{6}$$
(2.4)

The lower (resp. upper) bounds are attained for complete graphs (resp. a graph composed of one edge with endvertices of degree 1 and 2, one edge with endvertices of degree 2 and 3, possibly edges with endvertices of degree 2, and edges with endvertices of degree 3).

Proof

Lower bound of (2.3):

Using (2.2), we have

$$R - \delta \ge \frac{\delta n}{\delta + \Delta} - \delta \ge \frac{\delta n}{\delta + n - 1} - \delta$$

This last bound reaches its minimum for and only for $\delta = n - 1$. Then the lower bound follows and is reached if and only if G is the complete graph K_n .

Similarly, we prove the lower bound of (2.4).

Upper bound of (2.3):

If $\delta \geq 2$, we have

$$R - \delta \le \frac{n}{2} - 2 < \frac{3n - 13 + \sqrt{6} + 3\sqrt{2}}{6}.$$

So, necessarily the bound is reached for graphs with $\delta = 1$ and $\Delta \ge 3$ (if $\Delta = 2$, G is a path for which the bound is not attained). Let G be such a graph and uv a pending edge of G with d(u) = 1 and $d(v) = d \ge 2$ (G is a connected graph on at least 3 vertices).

If $d \ge 3$, then using (2.1), we get

$$R - \delta = \frac{n}{2} - \frac{1}{2} \sum_{ij \in E} \left(\frac{1}{\sqrt{d_i}} - \frac{1}{\sqrt{d_j}} \right)^2 - 1 \le \frac{n}{2} - \frac{1}{2} \left(1 - \frac{1}{\sqrt{d}} \right)^2 - 1$$

$$\leq \frac{n}{2} - \frac{1}{2} \left(1 - \frac{1}{\sqrt{3}} \right)^2 - 1 = \frac{3n - 10 + 2\sqrt{3}}{6}$$
$$< \frac{3n - 13 + \sqrt{6} + 3\sqrt{2}}{6}.$$

Thus, the upper bound is reached for a graph with d = 2. In this case, there exists a vertex w with $d(w) \ge 3$ (due to $\Delta \ge 3$) with a neighbor of degree 2 (due to the connectedness). So

$$\begin{aligned} R - \delta &= \frac{n}{2} - \frac{1}{2} \sum_{ij \in E} \left(\frac{1}{\sqrt{d_i}} - \frac{1}{\sqrt{d_j}} \right)^2 - 1 \\ &\leq \frac{n}{2} - \frac{1}{2} \left(1 - \frac{1}{\sqrt{2}} \right)^2 - \frac{1}{2} \left(\frac{1}{\sqrt{2}} - \frac{1}{\sqrt{3}} \right)^2 - 1 \\ &= \frac{3n - 13 + \sqrt{6} + 3\sqrt{2}}{6}. \end{aligned}$$

Thus the bound is proved. The corresponding extremal graph is composed of one edge with endvertices of degree 1 and 2, one edge with endvertices of degree 2 and 3, possibly edges with endvertices of degree 2 and edges with endvertices of degree 3 (see Figure 1 for an example of such a graph). A graph satisfying such conditions always exists for $n \ge 7$: consider a 3-regular graph H on k vertices, $4 \le k \le n-4$, and a path on n-k vertices; delete an edge, say uv, from H; add two edges from u and v to the same endpoint from the path.

Similarly, we prove the upper bound of (2.4).



Figure 1: An extremal graph for the upper bounds of (2.3) and (2.4)

3 The average degree

Again using the information in Table 1, AGX 2 proves automatically the lower and upper bounds on $R + \overline{d}$ and $R \cdot \overline{d}$, which are given in the following observation.

Observation 2 For any connected graph G on $n \ge 3$ vertices with Randić index R and average degree \overline{d} .

$$2+\sqrt{n-1}-\frac{2}{n} \leq R+\overline{d} \leq \frac{3n-2}{2} \quad and \quad \frac{2n-2}{n}\sqrt{n-1} \leq R\cdot\overline{d} \leq \frac{n^2-n}{2}$$

The lower bounds are attained if and only if G is the star S_n , and the upper bounds if and only if G is the complete graph K_n .

In the four other cases conjectures are obtained by AGX 2 and proved by hand. They are as follows.

Proposition 2 For any connected graph G on $n \ge 3$ vertices with Randić index R and average degree \overline{d} .

$$\frac{2-n}{2} \le R - \overline{d} \le \begin{cases} \frac{n-7+2\sqrt{2}}{2} + \frac{2}{n} & \text{if } n \le 23, \\ \\ \frac{n-4}{2} & \text{if } n \ge 24. \end{cases}$$

The lower bound is attained if and only if G is K_n and the upper bound if and only if G is P_n for $n \leq 23$, and if and only if G is C_n for $n \geq 24$.

$$\frac{n}{2n-2} \le \frac{R}{\overline{d}} \le \frac{n-3+2\sqrt{2}}{n-1} \cdot \frac{n}{4}.$$

The lower bound is attained if and only if G is K_n and the upper bound if and only if G is P_n .

Proof

Lower bounds:

According to [6], we have

$$R - \lambda_1 \ge \frac{2-n}{2}$$
 and $\frac{R}{\lambda_1} \ge \frac{n}{2n-2}$,

where λ_1 denotes the index of G, *i.e.* the largest eigenvalue of the adjacency matrix of G. Then using the inequality [13] $\overline{d} \leq \lambda_1$, the bounds follow.

Upper bound on the difference:

If G is a tree, the Randić index is maximum for a path [25], so

$$R - \overline{d} \le \frac{n - 7 + 2\sqrt{2}}{2} + \frac{2}{n},\tag{3.1}$$

with equality if and only if G is the path P_n . If G is not a tree, the Randić index R is maximum for a regular graph and the average degree \overline{d} is minimum for a unicyclic graph, so

$$R - \overline{d} \le \frac{n-4}{2},\tag{3.2}$$

with equality if and only if G is the cycle C_n (the only regular unicyclic graph).

Comparing bounds (3.1) and (3.2) gives the bound on $R - \overline{d}$.

Upper bound on the ratio:

If G is a tree, as in the case of the difference, we have the bound.

If G is not a tree, we have

$$\frac{R}{\overline{d}} \le \frac{n}{4} < \frac{n-3+2\sqrt{2}}{n-1} \cdot \frac{n}{4}$$

and the result follows.

4 The maximum degree

In this section, we discuss results obtained using AGX 2 when comparing the Randić index Rand the maximum degree Δ of a connected graph. Using the fact that the star S_n simultaneously minimizes R and maximizes Δ , AGX 2 proves automatically the lower bounds on $R - \Delta$ and on R/Δ . Similarly, using the fact that the cycle C_n maximizes R and minimizes Δ , we get upper bounds on $R - \Delta$ and on R/Δ . The upper bounds on $R + \Delta$ and on $R \cdot \Delta$ are due to the fact that the complete graph K_n maximizes both R and Δ . All these results are summarized in the following observation.

Observation 3 For any connected graph G on $n \ge 3$ vertices with Randić index R and maximum degree Δ ,

$$1 - n + \sqrt{n - 1} \le R - \Delta \le \frac{n - 4}{2} \qquad and \qquad \frac{1}{\sqrt{n - 1}} \le \frac{R}{\Delta} \le \frac{n}{4}.$$

The lower bounds are attained if and only if G is the star S_n , and the upper bounds if and only if G is the cycle C_n .

$$R + \Delta \leq rac{3n-2}{2}$$
 and $R \cdot \Delta \leq rac{n(n-1)}{2}$,

with equalities if and only if G is the complete graph K_n .

The following conjecture was obtained automatically by AGX 2 and refuted by hand.

Conjecture 1 For any connected graph G on $n \ge 3$ vertices with Randić index R and maximum degree Δ ,

$$R + \Delta \ge \frac{n + 1 + 2\sqrt{2}}{2},$$

with equality if and only if G is P_n .

There is a family of counter-examples for this conjecture. Indeed, a *comb* on at least 23 vertices is a counter-example (see Figure 2). Larger similar counter-examples are easily obtained.



Figure 2: A counter-example for Conjecture 1 on 23 vertices

The following proposition was first obtained automatically by AGX 2 as a conjecture and then proved by hand. **Proposition 3** For any connected graph on $n \ge 3$ vertices with Randić index R and maximum degree Δ ,

$$R \cdot \Delta \ge n - 3 + 2\sqrt{2}$$

with equality if and only if G is P_n .

Proof

If $\Delta = 2$, G is either a path or a cycle, and the minimum value of $R \cdot \Delta$ corresponds to a path. If $\Delta \geq 3$ and G a tree, with n_1 pending vertices, then $n_1 \geq \Delta$. It follows that

$$R \cdot \Delta \ge (\frac{n-1-n_1}{\Delta} + \frac{n_1}{\sqrt{\Delta}}) \cdot \Delta \ge n-1 + \Delta(\sqrt{\Delta}-1) > n-3 + 2\sqrt{2}.$$

If $\Delta \geq 3$ and G contains a cycle, then $m \geq n$. Hence

$$R \cdot \Delta \ge \frac{m}{\Delta} \cdot \Delta \ge n > n - 3 + 2\sqrt{2},$$

so the result holds.

5 The diameter

In this section we report on the comparison between the Randić index R and the diameter D. AGX 2 proves automatically four bounds (Observation 4) and generates conjectures on the other four bounds (Proposition 4 and Conjecture 2). The upper bounds on R-D and R/D are proved using the information of Table 1, exploiting the intersection based technique [1, 2]. The lower bounds on R+D and $R \cdot D$ are proved using the second value based technique [1, 2]. Application of this last technique can be summarized as follows. The diameter is minimum, D = 1, if and only if G is the complete graph K_n , a graph for which R is maximum (and large). Thus, the minimum of R+D is attained for some graph with $D \ge 2$. So, if any graph H minimizes R and has a diameter with the second smallest value D = 2, then H minimizes R+D and $R \cdot D$. This is true for a star. We therefore have:

Observation 4 For any connected graph on $n \ge 3$ vertices with Randić index R and diameter D,

$$R-D \le \frac{n-2}{2}$$
 and $\frac{R}{D} \le \frac{n}{2}$,

with equality if and only if G is the complete graph K_n .

$$R+D \ge 2+\sqrt{n-1}$$
 and $R \cdot D \ge 2\sqrt{n-1}$

with equalities if and only if G is the star S_n .

The following proposition is obtained by AGX 2 as a conjecture and then proved by hand.

Proposition 4 For any connected graph on $n \ge 3$ vertices with Randić index R and diameter D,

$$R + D \le \frac{3n - 5 + 2\sqrt{2}}{2}$$
 and $R \cdot D \le \frac{(n - 1)(n - 3 + 2\sqrt{2})}{2}$

with equality if and only if G is the path P_n .

Proof

If D = n - 1, then G is P_n and we have the bound in both cases.

If $D \leq n-2$, we have

$$R + D \le \frac{n}{2} + n - 2 = \frac{3n - 4}{2} < \frac{3n - 5 + 2\sqrt{2}}{2},$$
$$R \cdot D \le \frac{n}{2} \cdot n - 2 = \frac{n^2 - 2n}{2} < (n - 1)\frac{n - 3 + 2\sqrt{2}}{2}$$

This proves the result.

The following conjecture remains open.

Conjecture 2 For any connected graph on $n \ge 3$ vertices with Randić index R and diameter D,

$$R - D \ge \sqrt{2} - \frac{n+1}{2}$$
 and $\frac{R}{D} \ge \frac{n-3+2\sqrt{2}}{2n-2}$,

with equalities if and only if G is the path P_n .

6 The girth

When comparing the Randić index R and the girth g, AGX 2 proves easily the upper bounds on R - g, R/g, R + g and $R \cdot g$ which are given in the following observation.

Observation 5 For any connected graph on $n \ge 3$ vertices with Randić index R and girth g,

$$R-g \leq \frac{n}{2}-3$$
 and $\frac{R}{g} \leq \frac{n}{6}$,

with equality in both formulae if and only if G is a regular graph with a triangle.

$$R+g \leq \frac{3n}{2}$$
 and $R \cdot g \leq \frac{n^2}{2}$,

with equalities if and only if G is C_n .

In the four other cases, AGX 2 failed to find automated proofs, but generated conjectures. Two of them are proved by hand in Proposition 5. The two others remain open and are given in Conjecture 3 below.

Proposition 5 For any connected graph on $n \ge 3$ vertices with Randić index R and girth g,

$$R-g \ge -\frac{n}{2}$$
 and $\frac{R}{g} \ge \frac{1}{2}$,

with equality in both formulae if and only if G is C_n .

Proof

If G is C_n , the bounds are true.

Assume that G is not C_n and let uv be the edge of maximum weight in G. Delete this edge. Thus [8]

$$R(G - uv) \le R(G).$$

Iterating this operation leads to a cycle or a forest. (i) If G - uv contains at least a cycle

$$g(G - uv) \ge g(G).$$

If the successive deletions of an edge of maximum weight lead to a cycle, then by induction

$$g(G) \le g(G - uv) \le 2R(G - uv) \le 2R(G). \tag{6.1}$$

(*ii*) If G - uv contains no cycle, then G is a unicyclic graph. Then instead of removing an edge of maximum weight, we remove a pending edge. According to [8], this operation decreases the Randić index, thus

$$g(G) = g(G - uv) \le 2R(G - uv) < 2R(G).$$
(6.2)

At the end of the sequence of edge removals (edges of maximum weight and then pending edges) we get a cycle and from (6.1) and (6.2) we have

$$g(G) \le 2R(G). \tag{6.3}$$

From (6.3) we have

$$R-g \ge -\frac{g}{2} \ge -\frac{n}{2}$$
 and $\frac{R}{g} \ge \frac{1}{2}$.

with equality in both formulae if and only if G is C_n .

Conjecture 3 For any connected graph on $n \ge 3$ vertices with Randić index R and girth g,

$$R+g \geq \frac{n-3+\sqrt{2}}{\sqrt{n-1}} + \frac{7}{2} \quad and \quad R \cdot g \geq \frac{3n-9+3\sqrt{2}}{\sqrt{n-1}} + \frac{3}{2},$$

with equalities if and only if G is S_n^+ , i.e., a star plus one additional edge (see Figure 3).

7 The algebraic connectivity

The automated results, which are deduced from the bounds listed in Table 1, obtained from the comparison between the Randić index R and the algebraic connectivity a are given in the following observation.



Figure 3: S_{11}^+ , an extremal graph in Conjecture 3

Observation 6 For any connected graph on $n \ge 3$ vertices with Randić index R and algebraic connectivity a.

$$R+a \le \frac{3n}{2}$$
 and $R \cdot a \le \frac{n^2}{2}$

with equality in both formulae if and only if G is the complete graph K_n .

The bounds given in the following proposition are obtained as conjectures by AGX 2 and then proved by hand.

Proposition 6 For any connected graph on $n \ge 3$ vertices with Randić index R and algebraic connectivity a,

$$R-a \ge -\frac{n}{2}$$
 and $\frac{R}{a} \ge \frac{1}{2}$

with equality in both formulae if and only if G is the complete graph K_n .

Proof

If G is K_n , we have the bounds.

If G is not K_n , according to Proposition 1,

$$R - a \ge R - \delta \ge \frac{2 - n}{2} > -\frac{n}{2},$$

and

$$\frac{R}{a} \ge \frac{R}{\delta} \ge \frac{n}{2n-2} > \frac{1}{2}.$$

Thus the proof is done.

In three cases, the conjectures obtained by AGX 2 remain open. They are summarized as follows.

Conjecture 4 For any connected graph on $n \ge 3$ vertices with Randić index R and algebraic connectivity a:

R + a is minimum for a comet, i.e., a star with a appended path.

 $R \cdot a$ is minimum for a path if $n \leq 9$ and for a balanced double-comet (i.e., two equal sized stars joined by a path) if $n \geq 10$.

$$\frac{R}{a} \leq \begin{cases} \left(\frac{n-3+2\sqrt{2}}{2}\right) / \left(2(1-\cos\frac{\pi}{n})\right) & \text{if } n \text{ is odd} \\ \left(\frac{n-3+2\sqrt{2}}{2}\right) / \left(2(1-\cos\frac{\pi}{n})\right) & \text{if } n \text{ is even} \end{cases}$$

with equality if and only if G is P_n .

No result was obtained about the upper bound on R - a. The graphs obtained by AGX 2 are not regular enough to derive any algebraic formula or conjecture about the graphs structure.

8 The node connectivity

Finally, AGX 2 found and proved automatically conjectures about the Randić index R and the node connectivity ν in four cases. These results are summarized next.

Observation 7 For any connected graph on $n \ge 10$ vertices with Randić index R and node connectivity ν ,

$$1 + \sqrt{n-1} \le R + \nu \le \frac{3n-2}{2}$$
 and $2\sqrt{n-1} \le R \cdot \nu \le \frac{n(n-1)}{2}$

The lower (resp. upper) bounds are attained for stars S_n (resp. complete graphs K_n).

Conjectures were also obtained in the four remaining cases, and proved by hand.

Proposition 7 For any connected graph on $n \ge 3$ vertices with Randić index R and node connectivity ν .

$$\frac{2-n}{2} \le R-\nu \le \frac{n-2}{2} \quad and \quad \frac{n}{2n-2} \le \frac{R}{\nu} \le \frac{n}{2}$$

The lower (resp. upper) bounds are attained for complete graphs K_n (resp. regular graphs with $\nu = 1$).

Proof

The lower bounds follow from Propositon 1 and the fact that $\nu \leq \delta$.

The upper bounds follow from $R \le n/2$ and $\nu \ge 1$. It is trivial that the bounds are reached if and only if R = n/2 and $\nu = 1$, *i.e.*, G is a regular graph with $\nu = 1$.

Now, let us construct a family of graphs for which the upper bounds are attained, *i.e.*, regular graphs with $\nu = 1$.

- If n = 2k + 1 for k integer, let $V = \{w\} \cup V_1 \cup V_2$ where $V_1 = \{u_1, u_2, \dots u_k\}$ and $V_2 = \{v_1, v_2, \dots v_k\}$. Consider a 4-regular graph on each vertex subset V_1 and V_2 (this implies $k \ge 5$, *i.e.*, $n \ge 11$). Delete an edge from each graph, say u_1u_2 and v_1v_2 and add edges wu_1, wu_2, wv_1 and wv_2 . The whole graph so obtained is 4-regular in which w is a cut vertex (*i.e.*, a vertex whose deletion disconnects the graph).
- If n = 2k and k is odd, let V = V₁ ∪ V₂ where V₁ = {u₁, u₂, ... u_k} and V₂ = {v₁, v₂, ... v_k}. Consider a cycle, which is not a triangle, on each vertex subset V₁ and V₂ (this implies k ≥ 5, *i.e.*, n ≥ 10). Add ⌊k/2⌋ disjoint edges to each cycle. Each of the two graphs contains exactly one vertex of degree 2, say u₁ and v₁ and the remaining vertices are of

degree 3. Add the edge u_1v_1 . The whole graph so obtained is a 3-regular graph in which u_1 (and v_1) is a cut vertex.

• If n = 2k and k is even, let $V = \{w\} \cup V_1 \cup V_2$ where $V_1 = \{u_1, u_2, \cdots u_k\}$ and $V_2 = \{v_1, v_2, \cdots v_k\}$. Consider a 4-regular graph on each vertex subset V_1 and V_2 , say $u_i u_j$ (resp. $v_i v_j$ is an edge if and only if $j = i + 1 \mod(k)$ or $j = i + 2 \mod(k)$ (this implies $k \ge 6$, *i.e.*, $n \ge 12$). Delete the edges $u_1 u_2$, $v_1 v_3$ and $v_1 v_k$ and add the edges $u_1 v_1$, $u_2 v_1$ and $v_3 v_k$. The graph so obtained is 4-regular with v_1 as a cut vertex.

9 Conclusion

The comparison of the Randić index R with δ , \overline{d} , Δ , D, g, a and ν implies 56 (lower or upper) bounds. AutoGraphiX found complete results, *i.e.* the best possible bounding functions together with a characterization of the associated extremal graphs, in 51 cases; structural conjectures in 4 cases, for 2 of which algebraic formulae were found by hand; no result was obtained in only 1 case. Automated proofs were found in 28 cases, 19 conjectures were proved by hand (with proofs ranging from the very easy to the somewhat more difficult), 7 remain open and only 1 was refuted.

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