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Variable Neighborhood Search for Extremal Graphs.18. Conjectures and Results about the Randić Index

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Abstract: Using the AutoGraphiX 2 system (AGX2), we study 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 among matching number μ and the index (or the maximum eigenvalue) λ_1, $\oplus$ denotes one of the four operations $+, -, \times, /$, while 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). Conjectures are obtained in 14 out of 16 cases, 6 of which are proved automatically, 7 are proved by hand and one remains open.

1 Introduction

Let $G = (V, E)$ denote a graph with vertex set $V = \{v_1, v_2, \ldots v_n\}$, edge set $E = \{e_1, e_2, \ldots e_m\}$ and vertex degrees $d_1, d_2, \ldots d_n$. The number of vertices of G, $n = |V|$, is called the *order* of G. Similarly, the number of edges, $m = |E|$, is the *size* of G. The Randić index [27] is defined as follows:

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

i.e., as the sum over the edges of weights equal to the inverse of the geometric mean of the vertices degrees.

Since 1975, when Milan Randić [27] proposed this index (initially called the connectivity index, and viewed as a measure of molecular branching) it was very extensively studied, extended and applied in over 1300 papers and books (*e.g.* [14, 15, 28, 21, 22]). For a comprehensive survey of its mathematical properties see the recent book of Li and Gutman on *Mathematical Aspects of Randic-Type Molecular Structure Descriptors* [24].
The AutoGraphiX 1 and 2 systems (AGX 1 and AGX 2) for computer-assisted as well as, for some functions, fully automated graph theory were developed at GERAD, Montréal, since 1997. AGX 1 is described in [8, 9] and AGX 2 in [2]. References to many applications of AGX 1 and AGX 2 in mathematics and chemistry are given in the short survey [4]. For more general surveys, discussions and references about discovery systems in graph theory, one may consult chapters [10, 11, 16, 17] in the recent book *Graphs and Discovery* [12], edited by Fajtlowicz, Fowler, Hansen, Janowitz and Roberts. The basic idea of the AGX approach is to view various problems in graph theory - *i.e.*, finding a graph satisfying given constraints, finding an extremal graph for some invariant, corroborating, strengthening, refuting or repairing conjectures, finding conjectures and proofs or ideas of proofs - as optimization problems on an infinite parametric family of graphs (the members of moderate size of which are mainly studied) to be solved by a *generic* heuristic. The heuristic used is an application of Variable Neighborhood Search metaheuristic [25, 19]. Results are analyzed using tools from data mining, linear programming and graph theory.
AGX 1 was already applied to the study of the Randić index in two papers: (a) in [6] chemical trees with maximum and minimum Randić index were determined (see also [29, 14, 7] for proofs that the path has maximum Randić index for trees). This approach and a new way to use linear 0-1 programming to prove relations which can be deduced from the graphs found led to many extensions, e.g. [15, 26]; (b) in [18] interactive use of AGX led to improve relations between R and the ramification index obtained by Araujo and de la Peña [5]. In the thesis [1] a systematic comparison of 20 graph theoretic invariants was made. 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 $-, +, /, \times$, while 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. Moreover, 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 of the results of that study, which 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 $G = (V, E)$, $i \in \{\mu, \lambda_1\}$, μ denotes the *matching number* of G (*i.e.*, the largest number of edges without common vertices in a set)

and λ_1 denotes *the index* of G (*i.e.*, the largest eigenvalue of the adjacency matrix of the graph).
These indices are considered in turn in the next two 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.

G for lb_n	lb_n	Inv.	ub_n	G for ub_n
S_n	$\sqrt{n-1}$	R	$\frac{n}{2}$	G regular (K_n, C_n ...)
P_n	$2cos(\frac{\pi}{n+1})$	λ_1	$n-1$	K_n
S_n	1	μ	$\lfloor\frac{n}{2}\rfloor$	K_n, P_n, C_n, ...

Table 1: Bounds on the invariants and associated extremal graphs.

2 The Randić index and the matching number

AGX 2 led to results in 6 cases out of 8; in the 2 remaining cases, the extremal graphs obtained did not present enough regularity in their structure to deduce conjectures. The results obtained are presented next.

Observation 1 : *For any connected graph on $n \geq 3$ vertices with Randic index R and matching number μ,*

$$1+\sqrt{n-1} \leq R+\mu \leq \frac{n}{2}+\left\lfloor\frac{n}{2}\right\rfloor$$

$$\sqrt{n-1} \leq R\cdot\mu \leq \frac{n}{2}\cdot\left\lfloor\frac{n}{2}\right\rfloor.$$

The lower (resp. upper) bounds are attained for stars (resp. regular graphs with $\mu=\lfloor\frac{n}{2}\rfloor$).

The bounds in the above Observation are proved automatically by AGX 2 using the information presented in Table 1.

Theorem 1 : *For any connected graph on $n \geq 4$ vertices with Randic index R and matching number μ,*

$$\frac{R}{\mu} \leq \sqrt{n-1},$$

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

Theorem 1 (an AGX 2 conjecture) is a corollary of the following lemma, which is also of interest in its own right.

Lemma 1 : *For any connected graph on $n \geq 4$ vertices with Randic index R, matching number μ and maximum degree Δ,*

$$R \leq \mu\sqrt{\Delta}.$$

Proof of the lemma:
Let us compute a maximal matching of G in the following way

1. Let V_1 denote the set of vertices of degree 1 and $N(V_1)$ the set of vertices which are adjacent to some vertex in V_1. Let G_1 be the subgraph of G formed by the edges between V_1 and $N(V_1)$. let M_1 be a maximum matching of G_1. Let C be the set of end vertices of M_1 which are not in V_1. Then C covers all edges of G_1 and has the same cardinality as M_1.

2. Let $G' = G - V(G_1)$. Let V_{23} be the set of vertices of degree 2 or 3 of G which also belong to G'. Let G_{23} be the subgraph of G' which is induced by V_{23}. Let M_2 be a maximum matching of G_{23}. Let C' be the set of vertices of M_2 and $E[C']$ the set of edges covered by C'.

3. Let $G'' = G' - C'$ and $V'_{23} = V_{23} \cap G''$. Then there are no edges of G'' among V'_{23} (since M_2 is maximum in G_{23}). Let $N(V'_{23})$ be the set of neighboring vertices of V'_{23} in G''. Let M_3 be a maximum matching of the bipartite graph B which consists of the edges between V'_{23} and $N(V'_{23})$. By König's Theorem [23], which states that the size of a maximum matching of a bipartite graph is equal to the size of a minimum vertex covering of the graph, there will be a minimum covering set of B, denoted by C'', which has the same size as M_3.

4. Let $G''' = G'' - V'_{23} - C''$. Note that all the vertices in G''' have degree greater than 3 in G. Let M_4 be a maximal matching of G'''. Let C^* be the vertex set of M_4. For each edge of G''', both end vertices have at least degree 4.

Note that M_1, M_2, M_3 and M_4 together form a (maximal) matching of G. Also C, C', C'' and C^* together form a cover of all edges of G.

Thus

$$R \leq \sum_{\substack{i \in C \\ (i,j) \in E}} \frac{1}{\sqrt{d_i d_j}} + \sum_{(i,j) \in E[C']} \frac{1}{\sqrt{d_i d_j}} + \sum_{\substack{i \in C'' \\ j \in V(G'') \\ (i,j) \in E}} \frac{1}{\sqrt{d_i d_j}} + \sum_{\substack{i \in C^* \\ j \in V(G''') \\ (i,j) \in E}} \frac{1}{\sqrt{d_i d_j}}$$

We have:

$$\sum_{\substack{i \in C \\ (i,j) \in E}} \frac{1}{\sqrt{d_i d_j}} \leq \sum_{i \in C} \sqrt{d_i} \leq |C|\sqrt{\Delta} = |M_1|\sqrt{\Delta} \qquad (1)$$

$$\sum_{\substack{i \in C'' \\ (i,j) \in E}} \frac{1}{\sqrt{d_i d_j}} \leq \sum_{i \in C''} \sqrt{d_i} \leq |C''|\sqrt{\Delta} = |M_3|\sqrt{\Delta} \qquad (2)$$

$$\sum_{\substack{i \in C^* \\ j \in V(G''') \\ (i,j) \in E}} \frac{1}{\sqrt{d_i d_j}} \le \sum_{\substack{i \in C^* \\ j \in V(G''') \\ (i,j) \in E}} \frac{1}{\sqrt{4d_i}} \le \sum_{i \in C^*} \frac{\sqrt{d_i}}{2} \le \frac{|C^*|\sqrt{\Delta}}{2} = |M_4|\sqrt{\Delta} \tag{3}$$

Let us compute

$$R[C'] = \sum_{(i,j) \in E[C']} \frac{1}{\sqrt{d_i d_j}}.$$

For each edge e in M_2, let $N(e)$ denote the set of edges of G adjacent to e (including e itself). Let

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

Then

$$R[C'] = \sum_{(i,j) \in E[C']} \frac{1}{\sqrt{d_i d_j}} \le \sum R(e).$$

There are two cases:
Case 1. $\Delta \ge 4$

(a) If both end vertices of e have degree 2. Then $R(e) \le 1.5 \le \sqrt{3}$.

(b) If one end vertex of e has degree 2 and the other one has degree 3. Then $R(e) \le \frac{3}{\sqrt{2 \times 3}} + \frac{1}{2} \le \sqrt{3}$.

(c) If both end vertices of e have degree 3. Then $R(e) \le \frac{4}{\sqrt{2 \times 3}} + \frac{1}{3} \le \sqrt{4}$.

Thus

$$\sum_{\substack{i \in C' \\ (i,j) \in E}} \frac{1}{\sqrt{d_i d_j}} \le \sum_{e \in M_2} R(e) \le |M_2|\sqrt{4} \le |M_2|\sqrt{\Delta}. \tag{4}$$

Using (1), (2), (3) and (4), we have

$$R \le \left(\sum_{i=1}^{4} |M_i| \right) \sqrt{\Delta},$$

and then Lemma 1 holds.
Case 2. $\Delta \in \{1, 2, 3\}$.
When $\Delta = 1$ or $\Delta = 2$, we can verify easily that Lemma 1 holds.
When $\Delta = 3$, G''' is empty.

(a) If both end vertices of e have degree 2. Then at least one of the two edges in $N(e)$ other than e belongs to another $N(e')$. Otherwise M_2 will not be a maximum matching of G_{23}. Thus there is at least one edge in $N(e)$ which is counted twice in $\sum R(e)$. If we only count half the weight of the doubly counted edges, then the contribution to $R[C']$ from the edges in $N(e)$ is at most $R(e) - 1/4 < 1/2 + 1/2 + 1/2 = 1.5$.

(b) If one end vertex of e has degree 2 and the other one has degree 3. By the same reasoning as in (a) above, at least one edge in $N(e)$ is counted twice in $N(e)$. If we only count half the weight of the doubly counted edges, then the contribution to $R[C']$ from the edges in $N(e)$ is at most $R(e) - 1/6 < 3/\sqrt{2 \times 3} + 1/2 - 1/6 \leq \sqrt{3}$.

(c) If both end vertices of e have degree 3. Then at least two edges in $N(e)$ other then e, are covered by the end vertices of edges in M_2 (not equal to e). Otherwise M_2 can be augmented by removing e and add a perfect matching of $N(e)$. This will contradict to that M_2 is a maximum matching of G_{23}. So there are at least two edges in $N(e)$ which are counted twice in $\sum R(e)$. Thus the contribution from these edges in $N(e)$ to $R[C']$ is at most $R(e) - 1/3 \leq 4/\sqrt{2 \times 3} + 1/3 - 1/3 < \sqrt{3}$.

By (a), (b) and (c)

$$R[C'] = \sum_{(i,j)\,\in\, E[C']} \frac{1}{\sqrt{d_i d_j}} \leq |M_2|\sqrt{3}. \tag{5}$$

Using (1), (2), (3) and (5), we have

$$R \leq \left(\sum_{i=1}^{4} |M_i|\right)\sqrt{\Delta},$$

and then Lemma 1 holds. □

Theorem 1 follows immediately from the lemma and the relation $\Delta \leq n-1$. Unicity follows from the fact that the star S_n is the only graph for which $R = \sqrt{n-1}$ and $\mu = 1$.

The following conjecture, obtained in a straightforward way from the extremal graphs found by AGX 2, is open.

Conjecture 1 : *For any connected graph on $n \geq 3$ vertices with Randic index R and matching number μ,*

$$R - \mu \leq \sqrt{\left\lfloor \frac{n+4}{7} \right\rfloor \left\lfloor \frac{6n+2}{7} \right\rfloor} - \left\lfloor \frac{n+4}{7} \right\rfloor,$$

with equality if and only if G is a complete bipartite graphs $K_{p,q}$ with $p = \mu = \left\lfloor \frac{n+4}{7} \right\rfloor$.

3 The Randić index and the index

Using the upper bounds on the index λ_1 and on the Randić index (see Table 1), AutoGraphiX proves the following observation.

Observation 2 : *For any connected graph on $n \geq 3$ vertices with Randić index R and index λ_1,*

$$R + \lambda_1 \leq \frac{3n-2}{2} \quad \textit{and} \quad R \cdot \lambda_1 \leq \frac{n(n-1)}{2}$$

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

To prove the next propostion we need to recall the following theorem due to Favaron, Mahéo and Saclé [13].

Theorem 2 [13] : *For any connected graph G of size m, Randić index R and index λ_1,*

$$\lambda_1 \geq \frac{m}{R} \tag{6}$$

with equality if and only if G is a bipartite biregular graph (i.e., a bipartite graph in which vertices of the same independent set have the same degree).

Proposition 3.1 : *For any connected graph on $n \geq 3$ vertices with Randić index R and index λ_1,*

$$R + \lambda_1 \geq 2\sqrt{n-1} \quad \textit{and} \quad R \cdot \lambda_1 \geq n-1,$$

with equality for both formulae if and only if G is the star S_n.

Proof:
The lower bound on $R \cdot \lambda_1$ follows from (6), and equality holds if and only if G is a bipartite biregular graph of size $m = n-1$, *i.e.*, G is S_n.
For the lower bound on $R + \lambda_1$, using the corresponding bound on $R \cdot \lambda_1$, we have

$$R + \lambda_1 \geq R + \frac{n-1}{R} = \frac{R^2 + n - 1}{R}.$$

The latest bound reaches its minimum if and only if $R = \sqrt{n-1}$ and the corresponding graph is S_n. □

The bounds given in the following Proposition 3.2 were obtained in an assisted way. First, the AGX optimization component found the extremal graphs associated to the upper bounds on $R - \lambda_1$ and R/λ_1 (paths if $n \leq 9$ in the case of the difference and if $n \leq 26$ in the case of the ratio, and cycles if $n \geq 10$ in the case of the difference and if $n \geq 27$ in the case of the ratio). Then using the *algebraic attributes* of the extremal graphs, namely, if P_n and C_n are, respectively, a path and a cycle on n vertices

$$R(P_n) = \frac{n-3+2\sqrt{2}}{2} \quad \text{and} \quad \lambda_1(P_n) = 2cos(\frac{\pi}{n+1}),$$
$$R(C_n) = \frac{n}{2} \quad \text{and} \quad \lambda_1(C_n) = 2,$$

we formulated the expressions of the bounds. This way of deriving conjectures is called *algebraic method of conjecture making* [1, 2, 9].

Before stating and proving the next proposition, let us recall the following theorem due to Hong [20].

Theorem 3 [20] : *For any connected graph G of order n, size m and index λ_1,*

$$\lambda_1 \leq \sqrt{2m - n + 1} \tag{7}$$

with equality if and only if G is either K_n or S_n.

Proposition 3.2 : *For any connected graph on $n \geq 3$ vertices with Randić index R and index λ_1,*

$$\frac{2-n}{2} \leq R - \lambda_1 \leq \begin{cases} \frac{n-3+2\sqrt{2}}{2} - 2cos(\frac{\pi}{n+1}) & if\, n \leq 9, \\ \frac{n-4}{2} & if\, n \geq 10. \end{cases}$$

The lower bound is attained if and only if G is K_n, and the upper bound is attained if and only if G is P_n for $n \leq 9$ or G is C_n for $n \geq 10$. Moreover

$$\frac{n}{2n-2} \leq \frac{R}{\lambda_1} \leq \begin{cases} \frac{n-3+2\sqrt{2}}{4cos(\frac{\pi}{n+1})} & if\, n \leq 26, \\ \frac{n}{4} & if\, n \geq 27 \end{cases}$$

The lower bound is attained if and only if G is K_n, and the upper bound is attained if and only if G is P_n for $n \leq 26$ or G is C_n for $n \geq 27$.

Proof:
Lower bounds:
Using (6) and (7), we have

$$R - \lambda_1 \geq \frac{m}{\lambda_1} - \lambda_1 = \frac{m}{\sqrt{2m-n+1}} - \sqrt{2m-n+1} = \frac{n-1-m}{\sqrt{2m-n+1}}.$$

The derivative of the latest expression is

$$\frac{-m}{(2m-n+1)^{\frac{3}{2}}} < 0.$$

Thus the expression decreases and reaches its unique minimum for the maximum value of m, namely

$$m = \frac{n(n-1)}{2},$$

which leads to the lower bound on $R - \lambda_1$ and the corresponding extremal graph is K_n. In a similar way, we prove the lower bound on R/λ_1.

Upper bounds:
If G is a tree, λ_1 is minimum and R is maximum for a path and we have

$$R - \lambda_1 \leq \frac{n-3+2\sqrt{2}}{2} - 2cos(\frac{\pi}{n+1}). \tag{8}$$

If G is not a tree, the cycle C_n minimizes λ_1 and maximizes R simultaneously, then we have

$$R - \lambda_1 \leq \frac{n}{2} - 2. \tag{9}$$

A comparison between the bounds given in (8) and (9) leads to the results. □

4 Conclusion

The comparison of the Randić index R with the matching number μ and the index λ_1 implies 16 (lower or upper) bounds. AGX 2 found complete results, *i.e.* the best possible bounding functions together with a characterization of the associated extremal graphs, in 11 cases; structural conjectures in three cases, for which algebraic formulae were found by hand; no result in the remaining two cases. Automated proofs were found in 6 cases, 7 conjectures are proved by hand and one remains open.

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