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On a Relation Between Randić Index and Algebraic Connectivity

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Abstract

A conjecture of AutoGraphiX on the relation between the Randić index R and the algebraic connectivity a of a connected graph G is:

$$\frac{R}{a} \leq \left(\frac{n-3+2\sqrt{2}}{2}\right) / \left(2\left(1-\cos\frac{\pi}{n}\right)\right)$$

with equality if and only if G is P_n, which was proposed by Aouchiche et al. [M. Aouchiche, P. Hansen and M. Zheng, Variable neighborhood search for extremal graphs 19: further conjectures and results about the Randić index, *Match Commun. Math. Comput. Chem.* **58**(2007), 83–102.]. We prove that the conjecture holds for all trees and all connected graphs with edge connectivity $\kappa'(G) \geq 2$, and if $\kappa'(G) = 1$, the conjecture holds for sufficiently large n. The conjecture also holds for all connected graphs with diameter $D \leq \frac{2(n-3+2\sqrt{2})}{\pi^2}$ or minimum degree $\delta \geq \frac{n}{2}$. We also prove $R \cdot a \geq \frac{8\sqrt{n-1}}{nD^2}$ and $R \cdot a \geq \frac{n\delta(2\delta-n+2)}{2(n-1)}$, and then $R \cdot a$ is minimum for the path if $D \leq (n-1)^{1/4}$ or $\delta \geq \frac{n}{2}$.

1 Introduction

In 1975, Milan Randić [15] proposed a topological index R under the name "*branching index*", suitable for measuring the extent of branching of the carbon-atom skeleton of

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saturated hydrocarbons. For a graph $G = (V, E)$, the *Randić index* $R(G)$ of G was defined as the sum of $1/\sqrt{d(u)d(v)}$ over all edges uv of G, where $d(u)$ denotes the degree of a vertex u in G, i.e., $R(G) = \sum_{uv \in E(G)} \frac{1}{\sqrt{d(u)d(v)}}$. Later, in 1998 Bollobás and Erdös [4] generalized this index by replacing $-\frac{1}{2}$ with any real number α, which is called the general Randić index. Randić noticed that there is a good correlation between the Randić index R and several physico–chemical properties of alkanes: boiling points, chromatographic retention times, enthalpies of formation, parameters in the Antoine equation for vapor pressure, surface areas, etc. For a comprehensive survey of its mathematical properties, see the book of Li and Gutman [9] or the survey [10]. For terminology and notations not defined here, we refer the readers to [5].

Graffiti is a program designed to make conjectures about, but not limited to mathematics, in particular graph theory, which was written by Fajtlowicz from the mid-1980's. A numbered, annotated listing of several hundred of Graffiti's conjectures can be found in [2, 7]. Graffiti has correctly conjectured a number of new bounds for several well studied graph invariants. 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. The basic idea of the AGX approach is to view various problems in graph theory, i.e., finding graphs satisfying some given constraints; finding an extremal graph for some invariant; finding a conjecture which may be algebraic, i.e., a relation between graph invariants, or structural, i.e., a characterization of extremal graphs for some invariant; corroborating, refuting and/or strengthening or repairing a conjecture; and so on. AGX led to several hundred new conjectures, ranking from easy ones, proved automatically, to others requiring longer unassisted or partially assisted proofs, to open ones.

The Laplacian matrix of a graph G is $L(G) = D(G) - A(G)$, where $D(G)$ is the diagonal matrix of its vertex degrees and $A(G)$ is the adjacency matrix. Among all eigenvalues of the Laplacian matrix of G, one of the most popular is the second smallest, which was called the *algebraic connectivity* of a graph by Fiedler [8] in 1973, denoted by $a(G)$. Its importance is due to the fact that it is a good parameter to measure, to a certain extent, how well a graph is connected. For example, it is well-known that a graph is connected if and only if its algebraic connectivity is positive. There are several popular graphs for which their algebraic connectivity is known, such as $a(K_n) = n$, $a(P_n) = 2\left(1 - \cos\frac{\pi}{n}\right)$, $a(C_n) = 2\left(1 - \cos\frac{2\pi}{n}\right)$. Recently, there is an excellent survey on the algebraic connectivity of graphs written by de Abreu [1], for more details, see [6, 11, 12, 16].

In [3], the authors investigated the relation between Randić index and the algebraic connectivity of graphs, and proposed the following two conjectures.

Conjecture 1.1. *For any connected graph of order $n \geq 3$ with Randić index R and algebraic connectivity a, then*

$$\frac{R}{a} \leq \left(\frac{n-3+2\sqrt{2}}{2}\right) / \left(2\left(1 - \cos\frac{\pi}{n}\right)\right) \tag{1}$$

with equality if and only if G is P_n.

Conjecture 1.2. *For any connected graph on $n \geq 3$ vertices with Randić index R and algebraic connectivity a, then $R \cdot a$ is minimum for*

(1). *path if $n \leq 9$;*

(2). *a balanced double-comet (i.e., two equal sized stars joined by a path) if $n \geq 10$.*

In this paper, we prove that Conjecture 1.1 holds for all trees and all connected graphs with edge connectivity $\kappa'(G) \geq 2$, and if $\kappa'(G) = 1$, Conjecture 1.1 holds for sufficiently large n. Conjecture 1.1 also holds for all connected graphs with diameter $D \leq \frac{2(n-3+2\sqrt{2})}{\pi^2}$ or $\delta \geq \frac{n}{2}$. For the lower bound of $R \cdot a$, we show that $R \cdot a \geq \frac{8\sqrt{n-1}}{nD^2}$ and $R \cdot a \geq \frac{n\delta(2\delta-n+2)}{2(n-1)}$, and then $R \cdot a$ is minimum for the path if $D \leq (n-1)^{1/4}$ or $\delta \geq \frac{n}{2}$.

2 The Main Result

The following lemma due to [8] gives a lower bound of the algebraic connectivity, which is the main tool of our proof.

Lemma 2.1. *For a given connected graph G of order n with the algebraic connectivity a, then $a \geq 2\kappa'(G)\left(1 - \cos\frac{\pi}{n}\right)$ and $a \geq 2\delta(G) - n + 2$, where $\kappa'(G)$ and $\delta(G)$ denote the edge connectivity and the minimum degree of G, respectively.*

The other lower bound relates to the relationship of the algebraic connectivity and the diameter, which is from [13].

Lemma 2.2. *For a graph G of order n, its algebraic connectivity a imposes the upper bound on the diameter D of G: $D \geq \frac{4}{na}$.*

The following result comes from [14].

Lemma 2.3. *Fix a positive integer n. Then among all trees on n vertices the path has the smallest algebraic connectivity.*

The following bounds of the Randić index is well-known.

Lemma 2.4. *Among all connected graphs of order n, regular graphs have the maximum value of the Randić index, while the star has the minimum value of the Randić index. Among all trees with n vertices, the path has the maximum value of the Randić index.*

In [3], the authors gave the relation of Randić index and the minimum degree as follows.

Lemma 2.5. *For any connected graph on $n \geq 3$ vertices with Randić index R and minimum degree δ, then $\frac{n}{2(n-1)} \leq \frac{R}{\delta} \leq \frac{3n-7+\sqrt{6}+3\sqrt{2}}{6}$.*

Theorem 2.6. *For any connected graph of order $n \geq 3$ with Randić index R, algebraic connectivity a and diameter D, then*

(1). *the inequality (1) is strict holds for all graphs with edge connectivity $\kappa'(G) \geq 2$;*

(2). *the inequality (1) holds for all trees, with equality if and only if the tree is the path;*

(3). $\frac{R}{a} \leq \left(\frac{n}{2}\right) / \left(2\left(1-\cos\frac{\pi}{n}\right)\right)$ *holds for $\kappa'(G) = 1$, i.e., the inequality (1) holds for sufficiently large n.*

Proof. (1). By Lemma 2.1, if the edge connectivity $\kappa'(G) \geq 2$, then we directly obtain $a \geq 4\left(1-\cos\frac{\pi}{n}\right)$. By Lemma 2.4, we know that for any connected graph G, $R \leq \frac{n}{2}$. Therefore, we can easily to check that for $n \geq 3$,

$$\frac{R}{a} \leq \left(\frac{n}{2}\right) / \left(4\left(1-\cos\frac{\pi}{n}\right)\right) < \left(\frac{n-3+2\sqrt{2}}{2}\right) / \left(2\left(1-\cos\frac{\pi}{n}\right)\right).$$

Now in the following we assume $\kappa'(G) = 1$. Then by Lemma 2.1, we have $a \geq 2\left(1-\cos\frac{\pi}{n}\right)$.

(2). Suppose G is a tree. Since path P_n attains the maximum value of Randić index among all trees, we have $R \leq \frac{n-3+2\sqrt{2}}{2}$. By Lemma 2.3, $a(G) \leq a(P_n) = 2\left(1-\cos\frac{\pi}{n}\right)$. Then

$$\frac{R}{a} \leq \left(\frac{n-3+2\sqrt{2}}{2}\right) / \left(2\left(1-\cos\frac{\pi}{n}\right)\right),$$

with equality if and only if G is P_n.

(3). Similar as the proof of (1), we obtain $\frac{R}{a} \leq \left(\frac{n}{2}\right) / \left(2\left(1-\cos\frac{\pi}{n}\right)\right)$.

We complete the proof. ∎

Theorem 2.7. *For any connected graph of order $n \geq 3$ with diameter D and minimum degree δ, if $D \leq \frac{2(n-3+2\sqrt{2})}{\pi^2}$ or $\delta \geq \frac{n}{2}$, then inequality (1) holds.*

Proof. By Lemma 2.2, we have the lower bound $a \geq \frac{4}{nD}$. If $D \leq \frac{2(n-3+2\sqrt{2})}{\pi^2}$, then we can easily to check

$$\begin{aligned}\frac{R}{a} &\leq \left(\frac{n}{2}\right) / \left(\frac{4}{nD}\right) = \frac{n^2 D}{8} \leq \frac{n^2}{8} \cdot \frac{2(n-3+2\sqrt{2})}{\pi^2} \\ &< \left(\frac{n-3+2\sqrt{2}}{2}\right) / \left(2\left(1-\cos\frac{\pi}{n}\right)\right),\end{aligned}$$

since $1-\cos\frac{\pi}{n} < 1-\left(1-\frac{\pi^2}{n^2}\right) = \frac{\pi^2}{n^2}$.

By Lemmas 2.1 and 2.5, we know that $a \geq 2\delta - n + 2$ and $R \leq \frac{(3n-7+\sqrt{6}+3\sqrt{2})\delta}{6}$. Thus, we have $\frac{R}{a} \leq \frac{(3n-7+\sqrt{6}+3\sqrt{2})\delta}{6(2\delta-n+2)}$. If $\delta \geq \frac{n}{2}$, then we only need to verify that

$$\frac{(3n-7+\sqrt{6}+3\sqrt{2})\delta}{6(2\delta-n+2)} < \left(\frac{n-3+2\sqrt{2}}{2}\right) / \left(2\left(1-\cos\frac{\pi}{n}\right)\right).$$

For $3 \leq n \leq 8$ and $\delta \geq \frac{n}{2}$, we can directly check that the inequality holds. We assume that $n \geq 9$ in the following and observe that

$$\frac{(3n-7+\sqrt{6}+3\sqrt{2})\delta}{6(2\delta-n+2)} \leq \frac{(3n-7+\sqrt{6}+3\sqrt{2})(n-1)}{6(2\cdot\frac{n}{2}-n+2)} = \frac{(3n-7+\sqrt{6}+3\sqrt{2})(n-1)}{12}$$

and

$$\left(\frac{n-3+2\sqrt{2}}{2}\right) / \left(2\left(1-\cos\frac{\pi}{n}\right)\right) \geq \left(\frac{n-3+2\sqrt{2}}{2}\right) / \left(\frac{2\pi^2}{n^2}\right) = \frac{n^2(n-3+2\sqrt{2})}{4\pi^2}.$$

The result holds since $\frac{(3n-7+\sqrt{6}+3\sqrt{2})(n-1)}{12} < \frac{n^2(n-3+2\sqrt{2})}{4\pi^2}$ for $n \geq 9$. ∎

Theorem 2.8. *For any connected graph on $n \geq 3$ vertices with diameter D and minimum degree δ, then $R \cdot a \geq \frac{8\sqrt{n-1}}{nD^2}$, $R \cdot a \geq \frac{n\delta(2\delta-n+2)}{2(n-1)}$, and then $R \cdot a$ is minimum for the path if $D \leq (n-1)^{1/4}$ or $\delta \geq \frac{n}{2}$.*

Proof. By Lemma 2.4, the star has the minimum value of the Randić index among all graphs, then $R \geq \sqrt{n-1}$. Since $D \geq 2$, we have $R \cdot D \geq 2\sqrt{n-1}$, i.e., $R \geq \frac{2\sqrt{n-1}}{D}$. Then by Lemma 2.2, we obtain $R \cdot a \geq \frac{8\sqrt{n-1}}{nD^2}$. It is easy to check that if $D \leq (n-1)^{1/4}$, then $\frac{8\sqrt{n-1}}{nD^2} > (n-3+2\sqrt{2})\left(1-\cos\frac{\pi}{n}\right)$, i.e., $R \cdot a$ is minimum for the path if $D \leq (n-1)^{1/4}$. Actually, we have $\frac{8\sqrt{n-1}}{nD^2} \geq \frac{8\sqrt{n-1}}{n\sqrt{n-1}} = \frac{8}{n}$ and $\frac{8}{n} > (n-3+2\sqrt{2})\left(1-\cos\frac{\pi}{n}\right)$ for $n \geq 3$.

By Lemmas 2.1 and 2.5, we know that $a \geq 2\delta-n+2$ and $R \geq \frac{n\delta}{2(n-1)}$. And then $R \cdot a \geq \frac{n\delta(2\delta-n+2)}{2(n-1)}$. It is easy to verify that if $\delta \geq \frac{n}{2}-1$, then $\frac{n\delta(2\delta-n+2)}{2(n-1)} > (n-3+2\sqrt{2})\left(1-\cos\frac{\pi}{n}\right)$, i.e., $R \cdot a$ is minimum for the path if $\delta \geq \frac{n}{2}$. Actually, we have $\frac{n\delta(2\delta-n+2)}{2(n-1)} \geq \frac{n^2}{2(n-1)}$ and $\frac{n^2}{2(n-1)} > (n-3+2\sqrt{2})\left(1-\cos\frac{\pi}{n}\right)$ for $n \geq 3$. ∎

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