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Randić Index and Energy

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Abstract

In this paper, we construct families of graphs that satisfy the conjecture for the Randić energy $RE(G)$ proposed by Gutman, Furtula and Bozkurt [8] based on the Randić index $R_{-1}(G)$. More specifically, we provide upper bounds for the energy and we show how to add edges to TB-graphs that maintain the energy bounded.

1 Introduction

Let $G = (V, E)$ be an undirected graph with vertex set V and edge set E. In 1975 Milan Randić [11] proposed a molecular structure descriptor under the name "branching index" defined as

$$R_{-1}(G) = \sum_{\{u,v\}\in E(G)} \frac{1}{\deg(u)\cdot\deg(v)},$$

where $\deg(v)$ denotes the degree of v. Nowadays this parameter is known as *Randić index*. Like other chemical indices, the Randić index has received considerable attention from mathematicians, see for example [4, 6, 9, 10]. Connected to $R_{-1}(G)$ we have the *Randić matrix* $R = [r_{ij}]$ of G defined [3, 7, 8] as

$$r_{ij} = \begin{cases} \frac{1}{\sqrt{\deg(u)\cdot\deg(v)}} & \text{if } \{u,v\} \in E, \\ 0 & \text{otherwise.} \end{cases}$$

Denote the eigenvalues of R by $\lambda_1, \ldots, \lambda_n$. The multiset $\sigma_R = \{\lambda_1, \ldots, \lambda_n\}$ is called the *R-spectrum* of the graph G.

The *Randić energy* $RE(G)$ of a graph G is

$$\sum_{i=1}^{n} |\lambda_i|.$$

The normalized Laplacian matrix, defined by Chung [5], can be written using the Randić matrix as

$$\mathcal{L} = I_n - R,$$

where I_n is the identity matrix of order n. Thus, the eigenvalues of $\mathcal{L}$ are given by

$$\mu_i = 1 - \lambda_i$$

for $i = 1, \ldots, n$. For graphs without isolated vertices Cavers [4] defined the normalized Laplacian energy as

$$E_{\mathcal{L}}(G) = \sum_{i=1}^{n} |\mu_i - 1|.$$

An interesting fact about $E_{\mathcal{L}}(G)$, see [8], is that if G does not have isolated vertices then

$$RE(G) = E_{\mathcal{L}}(G).$$

Thus, results in this paper on Randić energy apply also to the normalized Laplacian energy.

In [8] Gutman, Furtula and Bozkurt conjectured that the graphs called *sun*, denoted by S^p, and *double sun*, denoted by $DS^{p,q}$, have the largest Randić energy depending on the parity of n. For each $p \geq 0$, the *p-sun*, S^p, is the tree of order $n = 2p + 1$ formed by taking the star on $p + 1$ vertices and subdividing each edge.

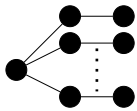

Figure 1. Sun.

For $p, q \geq 0$ the (p, q)-*double sun*, denoted $D^{p,q}$, is the tree of order $n = 2(p + q + 1)$ obtained by connecting the centers of S^p and S^q with an edge. Without loss of generality we assume $p \geq q$. When $p - q \leq 1$ the double sun is called *balanced*.

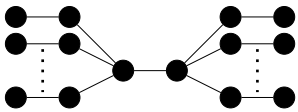

Figure 2. Double Sun.

More precisely, they stated the following conjecture.

Conjecture 1 *Let G be a connected graph on n vertices. Then*

$$RE(G) \leq \begin{cases} RE(S^p) & \text{if } n = 2p+1 \text{ is odd,} \\ RE(DS^{p,q}) & \text{if } n = 2p+2q+2 \text{ is even and } q \leq p \leq q+1 \ . \end{cases}$$

In [1] the authors computed the Randić energy of the sun and the double sun. The energy of the sun is $RE(S^p) = (n-3)\frac{\sqrt{2}}{2} + 2$ with $n = 2p+1$. The energy of the double sun depends on whether $q = p$ or $q = p-1$. If $p = q$ then

$$RE(D^{p,p}) = \frac{\sqrt{2}(n^2 - 4n - 12) + 4\sqrt{n^2 + 4n + 20}}{2(n+2)}.$$

If $q = p-1$ then

$$RE(D^{p,p-1}) = \frac{\sqrt{2}}{2n(n+4)}(n^3 - 2n^2 - 24 + 2\sqrt{n(n+4)(n^2 + 8 + \sqrt{-64n + n^4 + 64})} + 2\sqrt{n(n+4)(n^2 + 8 - \sqrt{-64n + n^4 + 64})}).$$

Cavers *et al.* [4] showed that $R_{-1}(G) = \frac{1}{2}\mathrm{tr}(R^2)$ and $RE(G) \leq \sqrt{n \cdot tr(R^2)}$, which implies that the parameters $R_{-1}(G)$ and $RE(G)$ are related by the following inequality

$$RE(G) \leq \sqrt{2 \cdot n \cdot R_{-1}(G)}. \tag{1}$$

Motivated by (1), in this work we compute bounds for the Randić index. We also give bounds for R_{-1} of graphs obtained from *TB-graphs* by adding edges. A *TB-graph* (see [1]) is a bipartite graph with bipartition A, B, such that $\deg(b) \leq 2$ for every $b \in B$. As an application, we construct families of graphs that respect the conjecture for graphs of odd order.

The paper is organized as follows. In section 2, we present upper bounds for the Randić index. In section 3, we give an upper bound for the R_{-1} of *ATB-graphs*, which are graphs obtained from TB-graphs by adding edges between vertices in A and edges between a vertex in A and a vertex in B. In section 4, we provide upper bounds for the Randić energy and we show that some families of graphs satisfy the conjecture proposed in [8].

2 Upper bound for the Randić index

The Randić index of a graph G, $R_{-1}(G)$, can also be defined as

$$R_{-1}(G) = \sum_{\{v,w\} \in E(G)} \frac{1}{\deg(v)\deg(w)} = \frac{1}{2} \sum_{v \in V(G)} \sum_{w \in N(v)} \frac{1}{\deg(v)\deg(w)},$$

where $N(v)$ is the neighbourhood of v, i.e., the set of the vertices of G that are adjacent to v. Given a vertex $v \in G$, we define *the Randić index of* v, $r_{-1}(v)$, as

$$r_{-1}(v) = \sum_{w \in N(v)} \frac{1}{\deg(v)\deg(w)}.$$

Thus,

$$R_{-1}(G) = \frac{1}{2} \sum_{v \in V(G)} r_{-1}(v).$$

An independent vertex set of a graph G is a subset of vertices such that no two vertices of G are adjacent.

Lemma 2.1 *If B is an independent set of G and $A = V(G) \setminus B$, then*

$$\sum_{b \in B} r_{-1}(b) \leq \sum_{a \in A} r_{-1}(a).$$

Proof: Notice that

$$\sum_{b \in B} r_{-1}(b) = \sum_{b \in B} \sum_{a \in N(b)} \frac{1}{\deg(b)\deg(a)}.$$

Since B is an independent set, $N(b) \subseteq A$. Thus,

$$\begin{aligned}
\sum_{b \in B} \sum_{a \in N(b)} \frac{1}{\deg(b)\deg(a)} &= \sum_{b \in B} \sum_{a \in N(b) \cap A} \frac{1}{\deg(b)\deg(a)} \\
&= \sum_{a \in A} \sum_{b \in N(a) \cap B} \frac{1}{\deg(b)\deg(a)} \\
&\leq \sum_{a \in A} \sum_{v \in N(a)} \frac{1}{\deg(v)\deg(a)} \\
&= \sum_{a \in A} r_{-1}(a).
\end{aligned}$$

■

Lemma 2.2 *If B is an independent set of G and $A = V(G) \setminus B$, then*

$$R_{-1}(G) \leq \sum_{a \in A} r_{-1}(a).$$

Proof: Since A and B is a partition of the vertices of G, we have that

$$R_{-1}(G) = \frac{1}{2} \sum_{v \in V(G)} r_{-1}(v) = \frac{1}{2} \sum_{a \in A} r_{-1}(a) + \frac{1}{2} \sum_{b \in B} r_{-1}(b).$$

Applying Lemma 2.1 we obtain

$$\begin{aligned} R_{-1}(G) =& \frac{1}{2}\sum_{a\in A} r_{-1}(a) + \frac{1}{2}\sum_{b\in B} r_{-1}(b) \\ \leq& \frac{1}{2}\sum_{a\in A} r_{-1}(a) + \frac{1}{2}\sum_{a\in A} r_{-1}(a) \\ =& \sum_{a\in A} r_{-1}(a). \end{aligned}$$

■

A dominant set for a graph $G = (V, E)$ is a subset B of V such that every vertex in $V \setminus B$ is adjacent to at least one vertex of B.

Lemma 2.3 *Let G be a connected graph of order $n \geq 3$, B a dominant independent set of G, B_1 the set of vertices in B of degree 1, $B_{\geq 2}$ the set of vertices in B with degree greater or equal to 2, and A the set of vertices of G that are not in B. Then for every $a \in A$,*

$$r_{-1}(a) \leq \frac{1}{2} + \frac{1}{4}|N(a) \cap B_1|,$$

where $N(a)$ is the neighbourhood of a.

Proof: Let $a \in A$. Consider the vertices of degree 1 in $N(a)$. As B is a dominant set, any such vertex must be in B. This means that b is a neighbour of a with $\deg(b) = 1$ if and only if $b \in B_1$. In other words, every vertex in $N(a) \cap (B_{\geq 2} \cup A)$ has degree at least 2.

If $\deg(a) \geq 2$, then

$$\begin{aligned} r_{-1}(a) &= \sum_{b\in N(a)} \frac{1}{\deg(b)\deg(a)} \\ &= \sum_{b\in N(a)\cap B_1} \frac{1}{\deg(a)} + \sum_{b\in N(a)\cap(B_{\geq 2}\cup A)} \frac{1}{\deg(b)\deg(a)} \\ &\leq \sum_{b\in N(a)\cap B_1} \frac{1}{\deg(a)} + \sum_{b\in N(a)\cap(B_{\geq 2}\cup A)} \frac{1}{2\deg(a)} \\ &= \sum_{b\in N(a)\cap B_1} \frac{2}{2\deg(a)} + \sum_{b\in N(a)\cap(B_{\geq 2}\cup A)} \frac{1}{2\deg(a)} \\ &= \sum_{b\in N(a)\cap B_1} \frac{1}{2\deg(a)} + \sum_{b\in N(a)\cap B_1} \frac{1}{2\deg(a)} + \sum_{b\in N(a)\cap(B_{\geq 2}\cup A)} \frac{1}{2\deg(a)} \end{aligned}$$

$$
\begin{aligned}
&= \sum_{b\in N(a)\cap B_1} \frac{1}{2\deg(a)} + \sum_{b\in N(a)} \frac{1}{2\deg(a)} \\
&= |N(a)\cap B_1| \frac{1}{2\deg(a)} + \deg(a)\frac{1}{2\deg(a)} \\
&= |N(a)\cap B_1| \frac{1}{2\deg(a)} + \frac{1}{2} \\
&\leq |N(a)\cap B_1| \frac{1}{4} + \frac{1}{2}.
\end{aligned}
$$

If $\deg(a) = 1$, let b be the only neighbour of a. Since G is a connected graph of order $n \geq 3$, $\deg(b) \geq 2$, and so $N(a) \cap B_1 = \emptyset$. Hence,

$$r_{-1}(a) = \frac{1}{\deg(b)} \leq \frac{1}{2} = |N(a)\cap B_1|\frac{1}{4} + \frac{1}{2}.$$

■

Combining Lemma 2.2 with Lemma 2.3 we obtain an upper bound for $R_{-1}(G)$ in terms of $|A|$ and $|B_{\geq 2}|$.

Lemma 2.4 *Let G be a connected graph of order $n \geq 3$, B a dominant independent set of G, B_1 the set of vertices in B of degree 1, $B_{\geq 2}$ the set of vertices in B with degree greater or equal than 2, and A the set of vertices of G that are not in B. Then*

$$R_{-1}(G) \leq \frac{n + |A| - |B_{\geq 2}|}{4}.$$

Proof: By Lemma 2.2,

$$R_{-1}(G) \leq \sum_{a\in A} r_{-1}(a).$$

By Lemma 2.3

$$
\begin{aligned}
\sum_{a\in A} r_{-1}(a) &\leq \sum_{a\in A} \left(|N(a)\cap B_1|\frac{1}{4} + \frac{1}{2} \right) \\
&= \sum_{a\in A} |N(a)\cap B_1|\frac{1}{4} + \sum_{a\in A}\frac{1}{2} \\
&= \sum_{a\in A} |N(a)\cap B_1|\frac{1}{4} + \frac{|A|}{2}.
\end{aligned}
$$

Since the vertices in B_1 have degree 1, each vertex $b \in B_1$ appears in exactly one subset $N(a) \cap B_1$, for $a \in A$. Hence

$$\sum_{a\in A} \frac{1}{4}|N(a)\cap B_1| = \sum_{b\in B_1} \frac{1}{4} = \frac{|B_1|}{4}.$$

Then

$$\begin{aligned} R_{-1}(G) \leq & \frac{|A|}{2} + \frac{|B_1|}{4} \\ = & \frac{2|A|}{4} + \frac{|B_1|}{4} \\ = & \frac{|A| + |A| + |B_1|}{4}. \end{aligned}$$

Since $n = |A| + |B_{\geq 2}| + |B_1|$, we have

$$R_{-1}(G) \leq \frac{n + |A| - |B_{\geq 2}|}{4}.$$

■

3 Adding edges to TB graphs

A TB-graph (see [1]) is a bipartite graph with bipartition A, B, such that $\deg(b) \leq 2$ for every $b \in B$.

In [1], while studying the Randić energy of TB-graphs, the authors showed that if G is a TB-graph of order n, then

$$R_{-1}(G) \leq \frac{n+1}{4}.$$

To do this, they partitioned B into B_1 and B_2, where B_1 is the set of the vertices in B of degree 1 and B_2 is the set of the vertices in B of degree 2. Then, they showed that

$$R_{-1}(G) \leq \frac{2|A| + |B_1|}{4} \text{ and } |A| \leq |B_2| + 1.$$

And, as an application they obtained the following result. We denote $\mathit{null}(R)$ the nullity of the matrix R.

Theorem 3.1 *[1, Theorem 5.5] Let G be a connected TB graph. Then*

$$RE(G) \leq \sqrt{n-2}\sqrt{n-3}\frac{\sqrt{2}}{2} + 2.$$

Even more, if $\mathit{null}(R) \geq 1$, then

$$RE(G) \leq (n-3)\frac{\sqrt{2}}{2} + 2.$$

In this section we study graphs obtained from TB-graphs by adding edges.

Let G be a TB-graph. Let G' be a graph obtained from G by adding edges between vertices in A or adding edges between a vertex in A and a vertex in B. That is, $V(G') =$

$V(G)$, $E(G) \subset E(G')$ and if $e \in E(G') \setminus E(G)$, then $|e \cap B| \leq 1$. If G' can be obtained in such way from a TB-graph G, we say that G' is an *ATB-graph* (*Augmented TB-graph*) of G, and in general we say that G' is an *ATB-graph*.

Denoting by $B_{\geq 2}(G)$ the set of the vertices in B whose degree is at least 2, since G is a TB-graph and G' is an ATB-graph of G, then $B_2(G) = B_{\geq 2}(G) \subset B_{\geq 2}(G')$. Applying Lemma 2.4, we have

$$R_{-1}(G') \leq \frac{n + |A| - |B_{\geq 2}(G')|}{4}.$$

Using that $|A| \leq |B_2(G)| + 1 \leq |B_{\geq 2}(G')| + 1$,

$$R_{-1}(G') \leq \frac{n+1}{4}.$$

Hence, we have the following result.

Theorem 3.2 *If G is a connected ATB-graph with order $n \geq 3$, then*

$$R_{-1}(G) \leq \frac{n+1}{4}.$$

4 Applications to Randić energy

In [1], the authors provided bounds for the Randić energy in terms of the number of vertices, the nullity of the graph and the Randić index as follows.

Theorem 4.1 *[1, Corollary 3.4] If G is a graph of order n, then*

$$RE(G) \leq \sqrt{(n - 1 - \mathit{null}(R))(2R_{-1}(G) - 1)} + 1.$$

Furthermore, if G is bipartite, then

$$RE(G) \leq \sqrt{(n - 2 - \mathit{null}(R))(2R_{-1}(G) - 2)} + 2.$$

Theorem 4.1 and Theorem 3.2 yield the following result.

Theorem 4.2 *If G is an ATB connected graph with $n \geq 3$, then*

$$RE(G) \leq \sqrt{(n - 1 - \mathit{null}(R))\left(\frac{n+1}{2} - 1\right)} + 1,$$

and

$$RE(G) \leq \sqrt{(n - 2 - \mathit{null}(R))\left(\frac{n+1}{2} - 2\right)} + 2$$

if G is bipartite.

In particular, if G is bipartite and has an odd number of vertices, then $null(R) \geq 1$.

Corollary 4.3 *If G is a connected bipartite ATB-graph with an odd number of vertices $n \geq 3$, then*

$$RE(G) \leq \sqrt{(n-3)\frac{n-3}{2}} + 2 = (n-3)\frac{\sqrt{2}}{2} + 2.$$

For ATB-graphs in general we can obtain a similar upper bound when $null(R) \geq 2$, using that $(n-3)(n-1) < (n-2)^2$ and that $\frac{\sqrt{2}}{2} < 1$.

Corollary 4.4 *If G is a connected ATB-graph with $n \geq 3$ vertices and $null(R) \geq 2$, then*

$$RE(G) < (n-3)\frac{\sqrt{2}}{2} + 2.$$

Proof: Since $null(R) \geq 2$,

$$\begin{aligned} RE(G) \leq & \sqrt{(n-1-null(R))\left(\frac{n+1}{2}-1\right)} + 1 \\ \leq & \sqrt{(n-3)\left(\frac{n-1}{2}\right)} + 1. \end{aligned}$$

Notice that $(n-3)(n-1) = n^2 - 4n + 3 < (n-2)^2$. Hence,

$$\begin{aligned} RE(G) < & \sqrt{\frac{(n-2)^2}{2}} + 1 \\ = & (n-2)\frac{\sqrt{2}}{2} + 1 \\ = & (n-3)\frac{\sqrt{2}}{2} + \frac{\sqrt{2}}{2} + 1 \\ < & (n-3)\frac{\sqrt{2}}{2} + 2. \end{aligned}$$

■

5 Examples

In this section, we give examples of families of graphs that satisfy Conjecture 1.

Example 1 *A starlike is a tree that has exactly one vertex of degree greater than 2. As an example, consider the starlike G in Figure 3. Notice that G is a TB-graph where $B = \{2,4,5,7\}$, $B_1 = \{4,7\}$, $B_2 = \{2,5\}$ and $A = \{1,3,6\}$. Since $n = 7$ is odd, by Theorem 3.1, we have that $RE(G) \leq RE(S^3)$.*

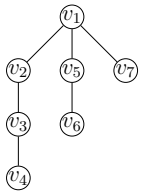

Figure 3. Starlike G.

Notice that, we can add edges to G from A to B, as shown in Figure 4, to generate bipartite ATB-graphs. From Corollary 4.3, we have that $RE(G^{'}) \leq RE(S^3)$ for each possible ATB-graph G' of G. Notice that this process can be done for any starlike of odd order.

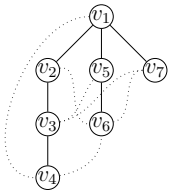

Figure 4. ATB-graph of G.

Example 2 *Consider now a connected bipartite TB-graph G with bipartition $A = \{a_1, \ldots, a_t\}$ and $B = \{b_1, \ldots, b_s\}$, with $s \geq t$ and $n = s + t$ odd. The edges of G are $\{a_i, b_i\}$, for $i = 1, \ldots, t$, $\{b_{i-1}, a_i\}$, for $i = 2, \ldots, t$ and $\{b_i, a_t\}$, for $i = t+1, \ldots, s$. Figure 5 illustrates such graph. Using Theorem 3.1, we know that $RE(G) \leq RE(S^p)$ with $n = 2p + 1$. We can add edges from A to B until we have the complete bipartite graph $K_{s,t}$. According to Corollary 4.3, $RE(G^{'}) \leq RE(S^p)$ for any ATB-graph $G^{'}$ of G.*

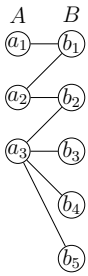

Figure 5. TB-graph.

Example 3 *A Threshold graph on n vertices is defined by a binary sequence of length n, where a vertex v_i, for $i = 1, ..., n$, corresponds to digit 0, if an isolated vertex v_i is added and v_i corresponds to digit 1 if v_i is added as a dominating vertex (see for example [2] for more details). If G is a Threshold graph with binary sequence $0^{t_1}1^{s_1}0^{t_2}1^{s_2}\dots 0^{t_w}1^{s_w}$, then $null(G) = (t_1 - 1) + \cdots + (t_w - 1)$ [2, Theorem 3]. We show that any connected Threshold graph G with binary sequence $0^{s_1}1^{s_1}0^{s_2}1^{s_2}\dots 0^{s_w}1^{s_w}$ where $s_i \geq 3$ for some $1 \leq i \leq w$ or where exist s_i, $s_j \geq 2$ for some $1 \leq i < j \leq w$ is an ATB-graph and $RE(G) < (n-3)\frac{\sqrt{2}}{2} + 2$, where $n = 2\sum_{i=1}^{w} s_i$.*

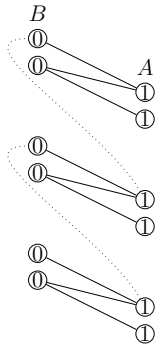

Figure 6. TB-graph.

For instance, consider the TB-graph G depicted in Figure 6. G is a connected bipartite graph with bipartition A, B, where the vertices in B are labeled with digit 0 and the vertices in A are labeled with digit 1. Now, we can add edges to G from A to A and from A to B until we construct the Threshold graph G' with binary sequence $0^2 1^2 0^2 1^2 0^2 1^2$. Since $null(R(G')) = 3$ and G' is an ATB-graph, then, by Corollary 4.4, $RE(G') < (n-3)\frac{\sqrt{2}}{2} + 2$ where $n = 12$. Following the argument above, we see that any Threshold graph with binary sequence $0^{s_1}1^{s_1}0^{s_2}1^{s_2}\dots 0^{s_w}1^{s_w}$ is an ATB-graph, since this graph can be obtained adding edges to a TB-graph in the same way as it was done for the graph of Figure 6. In addition, the fact that $s_i \geq 3$ for some $1 \leq i \leq w$ or s_i, $s_j \geq 2$ for some $1 \leq i < j \leq w$ implies that $null(R(0^{s_1}1^{s_1}0^{s_2}1^{s_2}\dots 0^{s_w}1^{s_w})) \geq 2$. Thus, in this case, by Corollary 4.4, we have that $RE(0^{s_1}1^{s_1}0^{s_2}1^{s_2}\dots 0^{s_w}1^{s_w}) < (n-3)\frac{\sqrt{2}}{2} + 2$, where $n = 2\sum_{i=1}^{w} s_i$.

Using the same argument above, we see that any connected Threshold graph with binary sequence $0^{s_1}1^{s_1}0^{s_2}1^{s_2}\dots 0^{s_w}1^{s_w-1}$ is an ATB-graph with odd order $n = 2(\sum_{i=1}^{w} s_i) - 1$. By Corollary 4.3, $RE(0^{s_1}1^{s_1}0^{s_2}1^{s_2}\dots 0^{s_w}1^{s_w-1}) \leq RE(S^p)$, where $p = (\sum_{i=1}^{w} s_i) - 1$ and $n = 2p + 1$.

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