Bounds for the Sum-Balaban index and (revised) Szeged index of regular graphs

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Abstract

Mathematical properties of many topological indices are investigated. Knor et al. gave an upper bound for the Balaban index of r-regular graphs on n vertices and a better upper bound for fullerene graphs. They also suggested exploring similar bounds for other topological indices. In this paper, we consider the Sum-Balaban index and the (revised) Szeged index, and give upper and lower bounds for these three indices of r-regular graphs, and also the cubic graphs and fullerene graphs, respectively.

Keywords: Sum-Balaban index; the (revised) Szeged index; regular graph; fullerene graph

1. Introduction

Thousands of topological indices are introduced to characterize the physical-chemical properties of molecules [57]. We can divide these topological indices into three types according the definitions: degree-based indices, distance-based indices and spectrum-based indices. Degree-based indices contain (general) Randić index [47], (general) zeroth order Randić index [47, 34, 35, 55], Zagreb index [29, 26, 3, 5, 20, 58], connective eccentricity index [62, 63] and so on. Distance-based indices [61, 15] include Balaban index [7, 8, 4], Wiener index [51, 50, 41, 22, 25, 33], Wiener polarity index [19, 52], Szeged index [2], Kirchhoff index [23, 24], the ABC index [32, 54], and the Harary index [1, 6], and so on. Eigenvalues of graphs [64], various of graph energies [10, 11, 36, 37, 43, 48, 38, 49,

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27, 13, 15, 30, 53], the Estrada index [39], and HOMO-LUMO index [46] belong to spectrum-based indices. Actually, there are also some topological indices defined based on both degrees and distances [60], such as degree distance [21]. From mathematical aspect, one direction to studying properties of each index is to determine the extremal values of the index among a given classes of graphs. In this paper, we focus on the bound for the Sum-Balaban index and the (revised) Szeged index.

Let $G = (V,E)$ be a simple graph. The distance between vertices u and v is denoted by $d_G(u,v)$. Let $w(u) = \sum_{a\in V} d_G(u,a)$. The *Balaban index* of G is defined as

$$J(G) = \frac{m}{m-n+2} \sum_{e=uv\in E} \frac{1}{\sqrt{w(u)\cdot w(v)}},$$

which was proposed by Balaban [7, 8] in 1982. It is also called the *average distance-sum connectivity index* or *Balaban J index*. Furthermore, Balaban et al. [9] proposed the concept of the *Sum-Balaban index* for a connected graph G, namely,

$$SJ(G) = \frac{m}{m-n+2} \sum_{e=uv\in E} \frac{1}{\sqrt{w(u)+w(v)}}.$$

We emphasize that many mathematical properties and results on the Balaban index and the Sum-Balaban index have been achieved, see [12, 16, 17, 45, 59, 65].

As a topological index, the Sum-Balaban index was widely used in QSAR/QSPR modeling. And several approaches have been presented for the calculation of Sum-Balaban index by taking into account the chemical nature of elements. However, many mathematical properties of Sum-Balaban index are still not studied extensively. For example, we have known that the complete graph K_n has the maximum Sum-Balaban index and

$$SJ(K_n) = \frac{\binom{n}{2}}{\binom{n}{2}-n+2}\binom{n}{2}\frac{1}{\sqrt{2(n-1)}}.$$

However, the minimum value among n-vertex graphs is not known.

Let $e = uv \in E$. Define three sets as follows:

$$N_u(e) = \{w \in V(G) : d_G(u,w) < d_G(v,w)\},$$

$$N_v(e) = \{w \in V(G) : d_G(v,w) < d_G(u,w)\},$$

$$N_0(e) = \{w \in V(G) : d_G(u,w) = d_G(v,w)\}.$$

Obviously, $N_u(e), N_v(e), N_0(e)$ constitutes a partition of $V(G)$. And set $|N_u(e)| = n_u(e)$, $|N_v(e)| = n_v(e)$ and $|N_0(e)| = n_0(e)$. Gutman [28] presented a graph invariant named as *Szeged index*, defined by

$$S_z = \sum_{e=uv\in E} n_u(e)n_v(e).$$

The above index is based on counting of vertices of the underlying graph. Also the edge-invariant is considered, say "edge-Szeged index" [18, 44]. Randić [56] found the Szeged index does not count the contributions of the vertices at equal distances to the two endpoints of an edge and then proposed the *revised Szeged index* as follows

$$S_z^* = \sum_{e=uv\in E} \left(n_u(e) + \frac{n_0(e)}{2}\right)\left(n_v(e) + \frac{n_0(e)}{2}\right).$$

In [7], Aouchiche and Hansen proved the upper bound of the connected graph with n vertices and m edges is $\frac{n^2m}{4}$. Then Xing and Zhou [57] determined the maximum and minimum revised Szeged index of unicyclic graphs with $n \geq 5$ and the unicyclic graph with the unique cycle is of length $r(3 \leq r \leq n)$. Several properties and applications of two indices have been presented in [8, 16, 17].

Denote by K_n, P_n and C_n the complete graph, path graph and cycle graph with n vertices, respectively. Among graphs on n vertices, Balaban index attains its maximum for the complete graph K_n and $J(K_n) = \frac{n^3-n^2}{2(n^2-3n+2)}$, which is slightly more than $n/2$. However, its minimum value among n-vertex graphs is not known. Recently, Knor et al. [42] prove that if G is an n-vertex r-regular graph, then $J(G)$ tends to 0 as n tends to ∞. In other words, zero is also an accumulation point for Balaban index.

Theorem 1. *Let G be an r-regular graph on n vertices with $r \geq 3$. Then*

$$J(G) \leq \frac{r^2(r-1)^2}{2(r-2)^2\left\lfloor \log_{r-1}\frac{(r-2)n+2}{r}\right\rfloor},$$

which implies that $\lim_{n\to\infty} J(G) = 0$.

The upper bound of fullerene graphs was also determined. Fullerenes [40] are polyhedral molecules made of carbon atoms arranged in pentagonal and hexagonal faces, and their corresponding graphs, fullerene graphs, are 3-connected, cubic planar graphs with only pentagonal and hexagonal faces.

Theorem 2. *Let G be a fullerene graph on $n \geq 60$ vertices. Then $J(G) \leq \frac{25}{\sqrt{n}}$.*

At the end of [42], Knor et al. suggested exploring similar bounds for other indices. In this paper, we consider the Sum-Balaban index and the (revised) Szeged index. Following the result of Knor et al., we will give bounds for the Sum-Balaban index and the (revised) Szeged index of r-regular graphs, and also the cubic graphs and fullerene graphs, respectively.

2. Regular graphs

In this section, we will concentrate the bounds on r-regular graphs.

Theorem 3. *Let G be an r-regular graph on n vertices with $r \geq 3$. Then*

$$SJ(G) \leq \frac{r^2(r-1)n^{\frac{1}{2}}}{2(r-2)^{\frac{3}{2}}\sqrt{2\lfloor \log_{r-1}(\frac{(r-2)n+2}{r})\rfloor}}.$$

Proof. Let $u \in V(G)$ and n_i be the number of vertices at distance i from u. Thus,

$$w(u) = \sum_i i \cdot n_i, \quad \sum_i n_i = n.$$

Since the graph is r-regular, we have $n_i \leq r(r-1)^{i-1}$. Let s and c satisfy that

$$n = 1 + r + r(r-1) + \ldots + r(r-1)^{s-1} + c, \quad 0 \leq c < r(r-1)^s.$$

Thus we can bound $w(u)$ in the following way:

$$w(u) = \sum_{i=0}^{s+1} i \cdot n_i \geq 1r + 2r(r-1) + \ldots + sr(r-1)^{s-1} + (s+1)c.$$

In other words, a lower bound on $w(u)$ is attained if the breadth-search tree, rooted at u, is an almost complete tree with all leaves at distance s and maybe $s+1$ from u, and every non-leaf vertex is of degree r. So, we have

$$1 + (r-1) + \ldots + (r-1)^{s-1} = \frac{n-1-c}{r},$$

and hence

$$\frac{(r-1)^s - 1}{r-2} = \frac{n-1-c}{r},$$

which gives

$$s=\log_{r-1}\left(\frac{(r-2)n+2-c(r-2)}{r}\right). \tag{1}$$

From (1) and from $c<r(r-1)^s$ we get

$$\frac{(r-2)n+2}{r}=(r-1)^s+\frac{c(r-2)}{r}<(r-1)^s+(r-1)^s(r-2)=(r-1)^{s+1},$$

which means that $\log_{r-1}(\frac{(r-2)n+2}{r})<s+1$. Since $\log_{r-1}(\frac{(r-2)n+2}{r})\geq s$ by (1), we have $s=\lfloor\log_{r-1}(\frac{(r-2)n+2}{r})\rfloor$. Consequently,

$$\begin{aligned}
w(u)\geq sr(r-1)^{s-1} &= \lfloor\log_{r-1}(\frac{(r-2)n+2}{r})\rfloor\cdot r\cdot(r-1)^{\lfloor\log_{r-1}(\frac{(r-2)n+2}{r})\rfloor-1}\\
&\geq \lfloor\log_{r-1}(\frac{(r-2)n+2}{r})\rfloor r\frac{(r-2)n+2}{r}\frac{1}{(r-1)^2}\\
&= \lfloor\log_{r-1}(\frac{(r-2)n+2}{r})\rfloor\frac{(r-2)n+2}{(r-1)^2}.
\end{aligned}$$

Thus,

$$\begin{aligned}
SJ(G) &\leq \frac{m}{m-n+2}m\frac{1}{\sqrt{2w(u)}}\\
&\leq \frac{\frac{rn}{2}}{\frac{rn}{2}-n+2}\frac{rn}{2}\frac{1}{2\sqrt{\lfloor\log_{r-1}(\frac{(r-2)n+2}{r})\rfloor\frac{(r-2)n+2}{(r-1)^2}}}\\
&< \frac{r^2(r-1)n^{\frac{1}{2}}}{2(r-2)^{\frac{3}{2}}\sqrt{2\lfloor\log_{r-1}(\frac{(r-2)n+2}{r})\rfloor}}.
\end{aligned}$$

∎

Next, we consider the Szeged index of r-regular graphs.

Theorem 4. *Let G be an r-regular connected graph on n vertices, where n is even and $r\leq\frac{n}{2}$. Then*

$$S_z(G)\leq\frac{rn^3}{8}.$$

And this bound is tight.

Proof. By the definition, we know that $n_u(e)+n_v(e) \leq n$ and $n_0(e) \geq 0$. So the smaller the $n_0(e)$ is and the closer $n_u(e)$ and $n_v(e)$ are, and then the larger the Szeged index is. Hence,

$$S_z(G) = \sum_{e=uv\in E} n_u(e)n_v(e) \leq m\frac{n}{2}\frac{n}{2} \leq \frac{rn^3}{8}.$$

We say this bound is tight, namely, for given n and r, there exist a graph G satisfying that $S_z(G) = \frac{rn^3}{8}$. We construct such a graph as follows. Constitute a bipartite graph $B_{\frac{n}{2},r}$ with vertex classes $X = \{u_i : 1 \leq i \leq \frac{n}{2}\}$ and $Y = \{u'_i : 1 \leq i \leq \frac{n}{2}\}$ in which u_i join to the corresponding vertices u'_i , $u'_{i+1}, \dots, u'_{i+r-1}$, where the subscripts are taken modulo $\frac{n}{2}$. See Figure 1 for $B_{6,3}$.

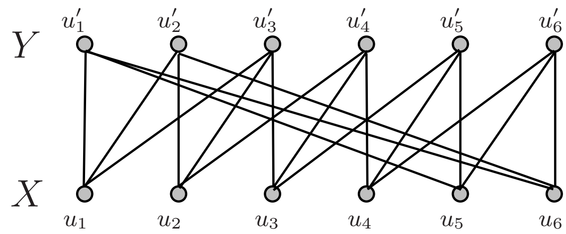

Figure 1: The graph $B_{6,3}$.

By some elementary calculations, we get $n_u(e) = n_u(e) = \frac{n}{2}$ for an arbitrary edge $e = uv$. Therefore,

$$S_z(B_{\frac{n}{2},r}) = \frac{rn^3}{8}.$$

The result is proved. ∎

Theorem 5. *Let G be an r-regular connected graph on n vertices. Then*

$$S_z^*(G) \leq \frac{rn^3}{8}.$$

And this bound is tight.

Proof. We know the sum of $n_u(e) + \frac{n_0(e)}{2}$ and $n_v(e) + \frac{n_0(e)}{2}$ is n. Therefore, the closer the above two values are, the larger the product is. So, if $n_u(e) + \frac{n_0(e)}{2} = n_v(e) + \frac{n_0(e)}{2} = \frac{n}{2}$, then the product is largest obviously. At this time,

$$S_z^*(G) \leq \frac{rn^3}{8}.$$

If for arbitrary n and r satisfying that nr is even, we can find a graph with the required conditions and the revised Szeged index is $\frac{rn^3}{8}$, then the theorem is proved obviously.

In the following, we will characterize such an r-regular graph $C_{n,r}$ with n vertices. First, we start from a cycle with n vertices, i.e., C_n. Since at least one of r and n is even, we consider two situations.

Case 1. One of r and n is odd.

For each vertex u in C_n, u is adjacent to every vertex of a path P_{r-2} which lies on C_n, satisfying that the distances in C_n between u and two endpoints of P_{r-2} are equal. Then we get an r-regular graph. As examples, see Figure 2 for $C_{8,5}$ and $C_{9,4}$.

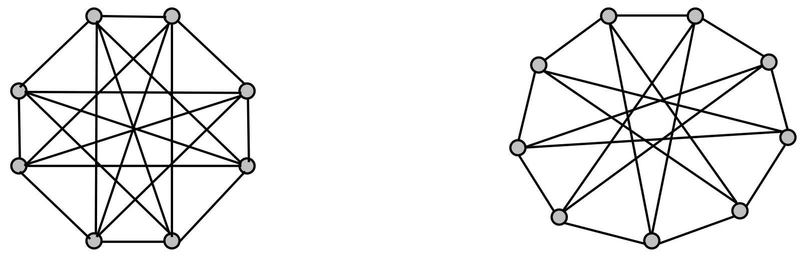

Figure 2: The graph $C_{8,5}$ (left) and $C_{9,4}$ (right).

Case 2. Both of r and n are even.

For each vertex u in C_n, find the symmetrical vertex v of u on C_n and join u to $\frac{r-2}{2}$ consecutive vertices on the left and right sides of v on C_n, respectively. Then we get an r-regular graph. See Figure 3 for $C_{6,4}$.

It is easy to calculate the values of $n_u(e)+\frac{n_0(e)}{2}$ and $n_v(e)+\frac{n_0(e)}{2}$ for each edge of $C_{n,r}$. ∎

Next, we will give a lower bound of the revised Szeged index.

Theorem 6. *Let G be an r-regular graph on n vertices with $r \geq 3$. Then*

$$S_z^*(G) \geq \frac{n(r^2+2r)(2n-r-2)}{8}.$$

Proof. From the above proof, we know the larger the difference value of $n_u(e)+\frac{n_0(e)}{2}$ and $n_v(e)+\frac{n_0(e)}{2}$ is, the lower the product is. Therefore, we need to find the

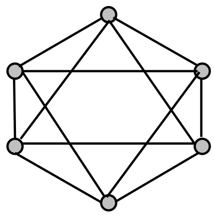

Figure 3: The graph $C_{6,4}$.

largest difference. For some edge $e(=uv)$ of G, we know that $r-1$ neighbors of u are either in $N_u(e)$ or $N_0(e)$. Obviously, the difference between $n_u(e)+\frac{n_0(e)}{2}$ and $n_v(e)+\frac{n_0(e)}{2}$ is largest when the graph satisfies the following conditions: u and v have $r-2$ common neighbors which form a complete subgraph K_{r-2}; the other neighbor x of u is adjacent to all neighbors of v. See Figure 4. In this case, $n_u(e)=2$, $n_v(e)=n-r$ and $n_0(e)=r-2$. So we get the conclusion

$$S_z^*(G)\geq\frac{rn}{2}(2+\frac{r-2}{2})(n-r+\frac{r-2}{2})\geq\frac{n(r^2+2r)(2n-r-2)}{8}.$$

∎

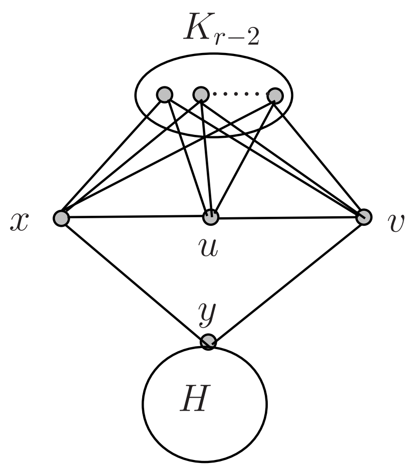

Figure 4: The graph G.

3. Fullerene graphs

Here we consider the chemical structure–fullerene.

Theorem 7. *Let G be a fullerene graph on $n \geq 60$ vertices. Then*

$$SJ(G) \leq \frac{9n}{\sqrt{n\sqrt{n}}}.$$

Proof. Let $u \in V(G)$ and n_i be the number of vertices at distance i from u. Then $n_0 = 1$ and $n_1 = 3$. Moreover, it is shown that $n_{i+1} \leq n_i + 3$ for $i \geq 1$. This immediately gives the bound $n_i \leq 3i$ for $i \geq 1$. We obtain a lower bound of $w(u)$ by assuming each $n_i = 3i$ for $i \geq 1$, as in this way we have fewer vertices at higher distance. So

$$w(u) = \sum_i i \cdot n_i \geq 1 * 3 + 2 * 6 + \ldots + s * 3s + (s+1)c,$$

for some s and c, where $0 \leq c < 3s+3$ and $1 + 3 + \cdots + 3s + c = n$. Hence,

$$3(1 + 2 + \cdots + s + (s+1)) \geq n,$$

and so

$$s^2 + 3s + 2 \geq \frac{2n}{3}.$$

Since $n \geq 60$, we have $s \geq 5$, and hence $s^2 \geq 3s + 2$, which gives $s \geq \sqrt{\frac{n}{3}}$. Since s is integer, we obtain

$$s \geq \left\lceil \sqrt{\frac{n}{3}} \right\rceil.$$

Consequently,

$$w(u) \geq 1 * 3 + 2 * 6 + \cdots + 3\lceil\sqrt{\frac{n}{3}}\rceil^2 + c(\lceil\sqrt{\frac{n}{3}}\rceil + 1) \geq 3 \sum_{j=1}^{\lceil\sqrt{\frac{n}{3}}\rceil} j^2 > \frac{n}{3}\sqrt{\frac{n}{3}}.$$

Thus,

$$SJ(G) \leq \frac{m}{m-n+2} m \frac{1}{\sqrt{2w(u)}} \leq \frac{\frac{rn}{2}}{\frac{rn}{2} - n + 2} \frac{rn}{2} \frac{1}{\sqrt{2\frac{n}{3}\sqrt{\frac{n}{3}}}} \leq \frac{9\sqrt{3\sqrt{3}}n}{2\sqrt{2n\sqrt{n}}} < \frac{9n}{\sqrt{n\sqrt{n}}}.$$

∎

We know that the smallest fullerene graph is the dodecahedral C_{20}. Other fullerenes are denoted by $C_{2n}, n = 12, 13, \ldots$. For each edge $e(= uv)$ of one fullerene, there are at least 2 vertices at the same distance to u and v. Particularly, for the five edges of the outer pentagonal or hexagonal faces, there are at least 4 such vertices. Then we can get Theorem 8 directly.

Theorem 8. *Let G be a fullerene graph on n vertices. Then*

$$S_z(G) < \frac{3n(n-2)^2}{8} - 5(n-3).$$

The following result can be obtained directly from Theorems 2.2 and 2.3.

Theorem 9. *Let G be a fullerene graph on* $n \geq 60$ *vertices. Then*

$$\frac{15n(2n-5)}{8} < S_z^*(G) \leq \frac{3n^3}{8}.$$

4. Cubic graphs

In [42], Knor et al. consider a special cubic graph H_n. In this section, we consider the Sum-Balaban and the (revised) Szeged index value of H_n.

Let $4|n$, and H_n be such a graph which has the cycle of length $3\frac{n}{4}$, in which every third vertex is doubled, see Figure 5 for H_{12}. In other words, H_n is obtained from $n/4$ copies of $K_4 - e$ joined by $n/4$ extra edges. Obviously, H_n is a cubic connected graph. And we can get the following conclusion.

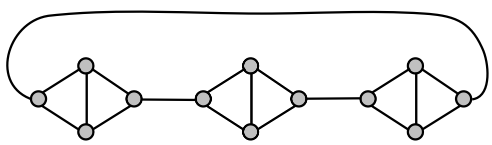

Figure 5: The graph H_{12}.

Theorem 10. *For positive n is divisible by 4, it holds*

$$SJ(H_n) \leq 6\sqrt{2}.$$

Proof. Let $\ell = \frac{3n}{4}$. First we give a lower bound for $w(u), u \in V(H_n)$. In order to do so, we find the total distance $cw(u)$ from u to the vertices of the original cycle. If l is even, then

$$cw(u) = 1+2+\cdots+\frac{\ell}{2}+1+2+\cdots+(\frac{\ell}{2}-1) = \frac{\ell^2}{4}.$$

Similarly, if ℓ is odd, then

$$cw(u) = 2(1+2+\cdots+\frac{\ell-1}{2}) = \frac{\ell^2-1}{4}.$$

As there is at least one vertex in H_n not on the original cycle and different from u, and as the distance of this vertex to u is at least one, for both the above cases we get

$$w(u) \geq cw(u)+1 > \frac{\ell^2}{4} = \frac{9n^2}{64}.$$

Hence,

$$SJ(H_n) \leq \frac{\frac{3n}{2}}{\frac{3n}{2}-n+2}\frac{3n}{2}\frac{1}{\sqrt{2\frac{9n^2}{64}}} = \frac{12n}{\sqrt{2}(n+4)} < 6\sqrt{2}.$$

∎

From the properties of this graph, we can get the following results easily.

Theorem 11. *For positive n divisible by 4, it holds*

$$S_z(H_n) = \begin{cases} \frac{5n(n-2)^2+4n}{16} & \text{if } \frac{n}{4} \text{ is odd,} \\ \frac{5n^3-8n^2+4n}{16} & \text{if } \frac{n}{4} \text{ is even.} \end{cases}$$

Theorem 12. *For positive n divisible by 4, it holds*

$$S_z^*(H_n) = \begin{cases} \frac{3n^3}{8} & \text{if } \frac{n}{4} \text{ is odd,} \\ \frac{3n^3-2n}{8} & \text{if } \frac{n}{4} \text{ is even.} \end{cases}$$

5. Summary and Conclusion

Knor et al. gave an upper bound for the Balaban index of r-regular graphs on n vertices and a better upper bound for fullerene graphs. They also suggested exploring similar bounds for other indices. In this paper, we consider the Sum-Balaban index and the (revised) Szeged index, and give bounds for these three indices of r-regular graphs, and also the cubic graphs and fullerene graphs, respectively. As a future work, it would be interesting to consider other topological indices for regular graphs.

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