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Bounds on the Balaban Index

Bo Zhou[a,*] and Nenad Trinajstić[b]

[a]*Department of Mathematics, South China Normal University, Guangzhou 510631, P. R. China*

[b]*The Ruđer Bošković Institute, P. O. Box 180, HR-10002 Zagreb, Croatia*

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The Balaban index of a connected (molecular) graph G is defined as $J = J(\mathrm{G}) = \frac{m}{\mu+1} \sum_{uv\in \mathrm{E(G)}} (D_u D_v)^{-1/2}$ where m is the number of edges, μ is the cyclomatic number, D_u is the sum of distances between vertex u and all other vertices of G, and the summation goes over all edges from the edge set E(G). The Balaban index is one of the widely used topological indices for QSAR and QSPR studies. In this paper, tight lower and upper bounds are reported for the Balaban index.

INTRODUCTION

Let G be a simple connected graph with vertex set V(G) and edge set E(G).[1] The distance between vertices u and v in G is denoted by D_{uv}. Let $D_u = \sum_{v\in \mathrm{V(G)}} D_{uv}$ be the distance sum of vertex u in G.[2,3] The Balaban index (also called the average distance-sum connectivity) of graph G is defined as:[4,5]

$$J = J(\mathrm{G}) = \frac{m}{\mu+1} \sum_{uv\in \mathrm{E(G)}} (D_u D_v)^{-1/2}$$

where m is the number of edges and μ is the cyclomatic number of G. Note that the cyclomatic number is the minimum number of edges that must be removed from G in order to transform it to an acyclic graph; it can be calculated using $\mu = m - n + 1$ where n is the number of vertices.[1]

The Balaban index appears to be a very useful molecular descriptor with attractive properties.[6,7] It has also been extended to weighted graphs[8–12] and used successfully in QSAR/QSPR modeling, see Refs. 13 and 14. Several of its recent uses can be found in Refs. 15–17. In this article, we report some lower and upper bounds for the Balaban index.

RESULTS

Recall the Hosoya definition of the Wiener index of the connected graph G:[18]

$$W = W(\mathrm{G}) = \frac{1}{2} \sum_{u\in \mathrm{V(G)}} D_u .$$

Let G be a graph with vertex set $\mathrm{V(G)} = \{v_1, v_2, ..., v_n\}$. For $u \in \mathrm{V(G)}$, $\Gamma(u)$ denotes the set of its (first) neighbors in G and the degree of u is $d_u = |\Gamma(u)|$. The adjacency matrix $\boldsymbol{A}$ of G is an $n \times n$ matrix ($\boldsymbol{A}_{ij}$), such that $\boldsymbol{A}_{ij} = 1$ if the vertices v_i and v_j are adjacent and 0 otherwise.[19] Since $\boldsymbol{A}$ is symmetric, its eigenvalues are real. Let $\rho = \rho(\mathrm{G})$ be the maximum eigenvalue of the adjacency matrix of G, which has been proposed by Cvetković and Gutman[20] as a measure of molecular

* Author to whom correspondence should be addressed. (E-mail: zhoubo@scnu.edu.cn)

branching. See Ref. 21 for more details on the properties of ρ.

For a vector $\boldsymbol{x}$, $\boldsymbol{x}^T$ denotes its transpose. For a graph G, $(x_1, x_2,..., x_n)^T$ is an eigenvector of $\boldsymbol{A}$ belonging to the eigenvalue ρ if and only if $\sum_{v\in\Gamma(u)} x_v = \rho x_u$ for any $u \in$ V(G). A graph is a semiregular bipartite graph of degrees r_1 and r_2 if it is bipartite and each vertex in one part of the bipartition has degree r_1 and each vertex in the other part of the bipartition has degree r_2.

Theorem 1. – Let G be a connected graph with $n \geq 2$ vertices and m edges. Then:

$$J \geq \frac{m^3}{(m-n+2)\rho W} \tag{1}$$

with equality if and only if either G is a regular graph with equal distance sums for all vertices, or else G is a semiregular bipartite graph of degrees r_1 and r_2, such that $\frac{r_1}{r_2} = \frac{D_u}{D_v}$ for any vertex u in the part with degree r_1 and any vertex v in the other part with degree r_2.

Proof: Note that for any n-dimensional column vector $\boldsymbol{x}$ with positive entries, $\rho \geq \frac{\boldsymbol{x}^T \boldsymbol{A}\boldsymbol{x}}{\boldsymbol{x}^T \boldsymbol{x}}$ with equality if and only if $\boldsymbol{x}$ is an eigenvector belonging to ρ; see, *e.g.* Ref 22. Setting $\boldsymbol{x} = (\sqrt{D_{v_1}}, \sqrt{D_{v_2}}, \dots, \sqrt{D_{v_n}})^T$ we have:

$$\rho \geq \frac{1}{W} \sum_{uv\in \mathrm{E(G)}} (D_u D_v)^{1/2}$$

with equality if and only if $\sum_{v\in\Gamma(u)} \sqrt{D_v} = \rho\sqrt{D_u}$ for any $u \in$ V(G). By the Cauchy-Schwarz inequality:

$$\sum_{uv\in \mathrm{E(G)}} (D_u D_v)^{-1/2} \geq \frac{m^2}{\sum_{uv\in \mathrm{E(G)}} (D_u D_v)^{1/2}}$$

with equality if and only if $D_u D_v$ is a constant for any $uv \in$ E(G). It follows that:

$$\sum_{uv\in \mathrm{E(G)}} (D_u D_v)^{-1/2} \geq \frac{m^2}{\rho W}$$

from which (1) follows.

Suppose that equality holds in (1). Then equality must apply in the first and second of the displayed equations of the previous paragraph, so that $\sum_{v\in\Gamma(u)} \sqrt{D_v} = \rho\sqrt{D_u}$ for any $u \in$ V(G) and $D_u D_v$ is a constant for any $uv \in$ E(G). Thus $d_u\sqrt{D_v} = \rho\sqrt{D_u}$ and $d_v\sqrt{D_u} = \rho\sqrt{D_v}$ for any $uv \in$ E(G). It is easily seen that $d_u d_v$ is a constant for any $uv \in$ E(G). Therefore, either G is a regular graph such that D_u is a constant for every $u \in$ V(G) or else G is a semiregular bipartite graph of degrees, say r_1 and r_2, such that $\frac{r_1}{r_2} = \frac{D_u}{D_v}$ for any vertex u in the part with degree r_1 and any vertex v in the other part with degree r_2. Conversely, it is easily seen that if G satisfies the conditions in the second part of the theorem, then equality holds in (1). □

We note that graphs with equal distance sums for all vertices may be regular, *e.g.*, vertex-transitive graphs, strongly regular graphs and distance-regular graphs, but may also be non-regular, *e.g.*, the graph whose vertex set can be partitioned into $4p + 2$ subsets V_i for an integer $p \geq 1$ and $i \in \{1,2,..., 4p + 2\}$ such that $|V_i| = 1$ for odd i, $|V_i| = r \geq 2$ for even i, each vertex in an odd-i V_i is adjacent (exactly) to those $2r$ vertices in $V_{i-1} \cup V_{i+1}$ (where the subscripts are modulo $4p + 2$), and the vertices in each individual even-i V_i are all further adjacent to one another (so that their degree is $r + 1$), for which distance sums are all equal to $(2p^2 + 2p + 1)r + 2p^2 + 2p$. If $p = 1$ and $r = 2$ this graph was noted in Ref. 23.

The clique number of a graph is the number of vertices in the largest complete subgraph of the graph.[24] Let G be a connected graph with $n \geq 2$ vertices and m edges. Then $\rho \leq \sqrt{2m-n+1}$ with equality if and only if G is the star or complete graph;[25] moreover, if the clique number of G is $k \geq 2$, then $\rho \leq \sqrt{\frac{2(k-1)m}{k}}$ with equality if and only if G is a complete bipartite graph for $k = 2$ or a regular complete k-partite graph for $k \geq 3$.[26] Thus, as a consequence of Theorem 1, we have the following corollaries.

Corollary 2. **–** Let G be a connected graph with $n \geq 2$ vertices and m edges. Then:

$$J \geq \frac{m^3}{W(m-n+2)\sqrt{2m-n+1}} \tag{2}$$

with equality if and only if G is a complete graph.

Note that $\frac{m^3}{(m-n+2)\sqrt{2m-n+1}}$ achieves its minimum value when $m = s_n = \frac{7n-12+\sqrt{13n^2-60n+72}}{6}$ for $2 \leq n - 1 \leq m \leq \frac{n(n-1)}{2}$ and that $s_n < \frac{n(n-1)}{2}$ for $n \geq 3$. Thus, J for a connected graph G with $n \geq 3$ vertices is given by:

$$J > \frac{(7n-12+\sqrt{s_n})^3}{12\sqrt{3}\,W(n+\sqrt{s_n})\sqrt{4n-9+\sqrt{s_n}}}.$$

Corollary 3. – Let G be a connected graph with $n \geq 2$ vertices, m edges and clique number $k \geq 2$ Then:

$$J \geq \frac{m^2\sqrt{km}}{W(m-n+2)\sqrt{2(k-1)}} \tag{3}$$

with equality if and only if G is a regular complete k-partite graph.

Remark. – We note that (3) is obtained by an upper bound for ρ which has been proven elsewhere[25] by using a result of Motzkin and Straus:[27] for a graph G with the clique number k and for $x_u \ge 0$, $u \in V(G)$ with $\sum_{u\in V(G)} x_u = 1$:

$$\sum_{uv\in E(G)} x_u x_v \le \frac{k-1}{2k}$$

with equality if and only if the subgraph induced by vertices $u \in V(G)$ with $x_u > 0$ is a complete k-partite graph, such that the sum of the x_u's in each part is the same. Assume $x_u = \frac{D_u}{2W}$ for $u \in V(G)$. Then $x_u > 0$ for $u \in V(G)$ with $\sum_{u\in V(G)} x_u = 1$ and thus:

$$\sum_{uv\in E(G)} \frac{D_u}{2W}\cdot\frac{D_v}{2W} \le \frac{k-1}{2k}$$

with equality if and only if G is a complete k-partite graph, say $G = K_{n_1,\ldots,n_k}$ with $n_i(n + n_i - 2) = \frac{2W}{k} = n_j(n + n_j - 2)$ for any $1 \le i < j \le k$ or equivalently, G is a regular complete k-partite graph. By the Cauchy-Schwarz inequality:

$$\sum_{uv\in E(G)} (D_uD_v)^{-1/2} \ge \frac{m^2}{\sum_{uv\in E(G)} (D_uD_v)^{1/2}} \ge$$

$$\frac{m^2}{\left(m\sum_{uv\in E(G)} D_uD_v\right)^{1/2}} \ge$$

$$\frac{m^2}{\left(m\frac{2(k-1)}{k}W^2\right)^{1/2}} = \sqrt{\frac{km}{2(k-1)}}\,\frac{m}{W},$$

from which (3) follows. Equality holds in (3) if and only if all inequalities above are equalities, *i.e.,* G is a regular complete k-partite graph.

Theorem 4. – Let G be a connected graph with $n \ge 2$ vertices, m edges and maximum degree Δ. Assume $\overline{D} = \max_{u\in V(G)} D_u$ and $\underline{D} = \max_{u\in V(G)} D_u$. Then:

$$J \le \frac{m}{2(m-n+2)}\left[\frac{n\Delta}{2n-2-\Delta} - \frac{(\sqrt{\overline{D}}-\sqrt{\underline{D}})^2}{m\overline{D}\underline{D}}\right] \quad (4)$$

with equality if and only if G is a regular graph with diameter at most two.

Proof: It can be seen that:

$$2\sum_{uv\in E(G)} (D_uD_v)^{-1/2} = \sum_{u\in V(G)} \frac{d_u}{D_u} - \sum_{uv\in E(G)}\left(\frac{1}{\sqrt{D_u}} - \frac{1}{\sqrt{D_v}}\right)^2.$$

Note that for any $u \in V(G)$, $D_u \ge 2(n-1) - d_u$ with equality if and only if the distance between u and any other vertex is at most two. Then since $f(x) = \frac{x}{2(n-1)-x}$ is increasing for $x \le \Delta \le n-1$, we have:

$$\sum_{u\in V(G)} \frac{d_u}{D_u} \le \sum_{u\in V(G)} \frac{d_u}{2(n-1)-d_u} \le \frac{n\Delta}{2(n-1)-\Delta}$$

with equalities if and only if G is a regular graph with diameter at most two. By the Cauchy-Schwarz inequality:

$$\sum_{uv\in E(G)}\left(\frac{1}{\sqrt{D_u}} - \frac{1}{\sqrt{D_v}}\right)^2 \ge$$

$$\frac{1}{m}\left(\sum_{uv\in E(G)}\left|\frac{1}{\sqrt{D_u}} - \frac{1}{\sqrt{D_v}}\right|\right)^2 \ge \frac{1}{m}\left(\frac{1}{\sqrt{\underline{D}}} - \frac{1}{\sqrt{\overline{D}}}\right)^2$$

with equalities if and only if $D_u = D_v$ for any $uv \in E(G)$. It is now easily seen that from this expression, (4) follows. From the arguments above, equality holds in (4) if and only if all inequalities above are equalities. Note that if G is a regular graph with diameter at most two, then $D_u = D_v$ for any $uv \in E(G)$. Thus, the result follows. □

Let G be a connected graph with $n \ge 2$ vertices, m edges and maximum degree Δ. According to Theorem 4:

$$J \le \frac{nm\Delta}{2(m-n+2)(2n-2-\Delta)} \quad (5)$$

with equality if and only if G is a regular graph with diameter at most two. Thus:

$$J \le \frac{nm}{2(m-n+2)}$$

with equality if and only if G is a complete graph.

Theorem 5. – Let G be a connected graph with $n \ge 2$ vertices and m edges. Then:

$$J \le \frac{m}{2(m-n+2)}\,\rho\sum_{u\in V(G)} \frac{1}{D_u} \quad (6)$$

with equality if and only if $\sum_{v\in\Gamma(u)} D_v^{-1/2} = \rho D_u^{-1/2}$ for any $u \in V(G)$.

Proof: Setting $\boldsymbol{x} = (D_{v_1}^{-1/2}, D_{v_2}^{-1/2}, \ldots, D_{v_n}^{-1/2})^T$ in $\rho \ge \frac{\boldsymbol{x}^T\boldsymbol{A}\boldsymbol{x}}{\boldsymbol{x}^T\boldsymbol{x}}$ we have:

$$\rho \geq \frac{2 \sum_{uv \in E(G)} (D_u D_v)^{-1/2}}{\sum_{u \in V(G)} \frac{1}{D_u}}$$

with equality if and only if $\sum_{v \in \Gamma(u)} D_v^{-1/2} = \rho D_u^{-1/2}$ for any $u \in V(G)$. □

Let G be a connected graph with $n \geq 2$ vertices, m edges and minimum degree δ. Note that:

$$\sum_{u \in V(G)} \frac{1}{D_u} \leq \sum_{u \in V(G)} \frac{1}{2(n-1)-d_u} \leq \frac{n}{2(n-1)-\delta}.$$

According to Theorem 5, we have the following corollaries.

Corollary 6. – Let G be a connected graph with $n \geq 2$ vertices, m edges and minimum degree δ. Then:

$$J \leq \frac{mn}{2(m-n+2)(2n-2-\delta)} \rho \tag{7}$$

with equality if and only if G is a regular graph with diameter at most two.

Corollary 7. – Let G be a connected graph with n vertices, m edges and minimum degree δ and clique number $k \geq 2$. Then:

$$J \leq \frac{mn}{2(m-n+2)(2n-2-\delta)} \sqrt{\frac{2(k-1)m}{k}}$$

with equality if and only if G is a regular complete k-partite graph.

Since $\delta \leq \rho$ (see Ref. 21), the upper bound in (7) is better than the one in (5).

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SAŽETAK

Granice Balabanova indeksa

Bo Zhou i Nenad Trinajstić

Balabanov indeks definira se sljedećim izrazom $J = J(\mathrm{G}) = \frac{m}{\mu+1}\sum_{uv\in \mathrm{E(G)}}(D_u D_v)^{-1/2}$ gdje je m broj bridova u (molekularnome) grafu G, μ ciklomatski broj, D_u zbroj udaljenosti između čvora u i svih drugih čvorova u G, a zbroj u gornjem izrazu ide preko svih bridova u G. Balabanov indeks jedan je od najviše rabljenih molekularnih deskriptora u QSPR i QSAR modeliranju. Ovaj članak sadrži razmatranje o donjoj i gornjoj granici Balabanova indeksa.