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# Bounds on the Balaban index of trees *†

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**Abstract**

The Balaban index of a connected (molecular) graph $G$ is defined as $J(G) = \frac{m}{\mu+1} \sum\limits_{uv \in E(G)} (D_u D_v)^{-1/2}$. In this paper, sharp upper and lower bounds on the Balaban index of trees are reported.

## 1 Introduction

The graphs considered in this paper are finite, undirected, connected and simple (no loops or multiple edges). The sets of vertices and edges of a graph $G$ are denoted by $V(G)$ and $E(G)$, respectively. A vertex with degree 1 is called a *leaf*.

If vertices $u$ and $v$ are connected in $G$, the *distance* between $u$ and $v$ in $G$, denoted by $D_{uv}$, is the length of a shortest $(u, v)$-path in $G$. The *diameter* of $G$ is the maximum distance between two vertices of $G$, denoted by $d(G)$. The *distance matrix* of $G$ is the matrix $D(G) = [d_{ij}]_{n\times n}$, where $d_{ij}$ is the distance between $v_i$ and $v_j$.

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Let $D_u = \sum_{v \in V(G)} D_{uv}$ be the distance sum of vertex $u$ in $G$. The Balaban index (also called the average distance-sum connectivity) of graph $G$ is defined as

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

where $m$ is the number of edges and $\mu$ is the cyclomatic number of $G$. Note that the cyclomatic number of $G$ 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.

In [5], Zhou and Trinajstić obtained the upper and lower bounds on the Balaban index of connected graphs using algebraic methods. In this paper, we study the bounds on the Balaban index of trees.

## 2 Main Results

**Theorem 2.1** *If $T$ is a tree with $n$ vertices, then $J(T) \leq (2n-3)^{-1/2}(n-1)^{3/2}$, with equality if and only if $T$ is a star.*

**Proof.** Since $T$ is a tree with $n$ vertices, we have $m = n - 1$ and $\mu = 0$. Thus

$$J(T) = (n-1) \sum_{uv \in E(T)} (D_u D_v)^{-1/2}.$$

If $d(T) = 1$, then $T$ is an edge and $J(T) = 1$. The theorem obviously holds.

Otherwise $d(T) \geq 2$.

Consider the distance matrix $[d_{ij}]_{n \times n}$ of $T$. We have the following properties:

(1) the diagonal entries are 0 and the other entries are positive integers;

(2) the entries in column $u$ corresponding to the vertices except $u$, which are not neighbors of $u$, are at least 2;

(3) the $u$ column sum is $D_u$;

(4) $D_u \geq n-1$ and $D_u = n-1$ happens for at most one time.

If $d(T) = 2$, then $T$ is a star and $D_u = n-1$ or $2n-3$ for each $u \in V(T)$. Thus we have $J(T) = (2n-3)^{-1/2}(n-1)^{3/2}$.

Otherwise $d(T) \geq 3$.

Let $x \in V(T)$ with $d(x) = \Delta(T)$ and $x$ be the root of $T$. Then the other vertices of $T$ can be divided into levels by the distance on $x$ (see Figure 1). Note that the vertices in the same level are independent.

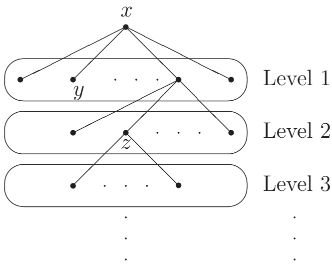


Figure 1. The root $x$ and the levels of $T$

Let $Y$ be the set of the vertices in level 1 and $y \in Y$. To simplify the notations, let $|Y| = \Delta(T) = t$ and $d(y) = s$ $(1 \leq s \leq t)$. By the properties (1)-(3) of distance matrix of $T$, we have $D_x \geq n-1+(n-1-t) = 2n-2-t$ and $D_y \geq n-1+(n-1-s) = 2n-2-s \geq 2n-2-t$. Similarly for any vertex $v$ in level $i$ $(i \geq 2)$, $D_v \geq 2n-2-t$. Since $d(T) \geq 3$, we have $2 \leq t \leq n-2$.

If $t < \frac{n}{2}$, then we have

$$\begin{aligned} J(T) &= (n-1) \sum_{uv \in E(T)} (D_u D_v)^{-1/2} \\ &\leq (n-1)^2[(2n-2-t)^2]^{-1/2} \\ &< (n-1)^2[(2n-2-\frac{n}{2})^2]^{-1/2} \\ &= (n-1)^2[(\frac{3}{2}n-2)^2]^{-1/2} \end{aligned}$$

Since

$$(\frac{3}{2}n-2)^2 = \frac{9}{4}n^2 - 6n + 4 > 2n^2 - 5n + 3 = (n-1)(2n-3), \; n \geq 4,$$

we have

$$J(T) < (n-1)^2[(n-1)(2n-3)]^{-1/2} = (2n-3)^{-1/2}(n-1)^{3/2}.$$

Otherwise $t \geq \frac{n}{2}$.

From the proof above, we have $D_x \geq 2n-2-t$. Additionally, we have $D_y \geq n-1+(t-1) = n+t-2$.

Let $Z$ be the set of the vertices in level 2 and $z \in Z$. Then we have $D_z \geq n-1+1+2(t-1) = n+2t-2 \geq 2n-2$. Similarly for any vertex $w$ in level $i$ ($i \geq 3$), $D_w \geq n+3t-2 > 2n-3 > n-1$. Thus we have

$$\begin{aligned} J(T) &= (n-1) \sum_{uv \in E(T)} (D_u D_v)^{-1/2} \\ &= (n-1)[\sum_{y \in Y} (D_x D_y)^{-1/2} + \sum_{\substack{y \in Y, z \in Z \\ yz \in E(T)}} (D_y D_z)^{-1/2} + \sum_{\substack{u \notin Y \\ uv \in E(T)}} (D_u D_v)^{-1/2}] \\ &< (n-1)\{t[(2n-2-t)(n+t-2)]^{-1/2} + (n-1-t)[(n-1)(2n-3)]^{-1/2}\} \end{aligned}$$

Since

$$\begin{aligned} & (2n-2-t)(n+t-2) \\ =\ & (2n-3+1-t)(n-1+t-1) \\ =\ & (2n-3)(n-1) + (1-t)(n-1) + (t-1)(2n-3) - (t-1)^2 \\ =\ & (2n-3)(n-1) + (t-1)(n-2) - (t-1)^2 \\ =\ & (2n-3)(n-1) + (t-1)[(n-2)-(t-1)] \\ >\ & (2n-3)(n-1), \end{aligned}$$

we have

$$J(T) < (n-1)^2[(n-1)(2n-3)]^{-1/2} = (2n-3)^{-1/2}(n-1)^{3/2}.$$

Therefore, $J(T) \leq (2n-3)^{-1/2}(n-1)^{3/2}$, with equality if and only if $T$ is a star. This completes the proof of Theorem 2.1. $\square$

**Theorem 2.2** *If $T$ is a tree, then $J(T) \geq (n-1)\sum_{i=1}^{n-1}(D_i D_{i+1})^{-1/2}$, where $D_i = \frac{(n-i+1)(n-i)}{2} + \frac{(i-1)i}{2}$, with equality if and only if $T$ is a path.*

**Proof.** Since $T$ is a tree with $n$ vertices, we have $m = n-1$ and $\mu = 0$. Thus

$$J(T) = (n-1) \sum_{uv \in E(T)} (D_u D_v)^{-1/2}.$$

If $d(T) = n-1$, then $T$ is a path and $J(T) = (n-1)\sum_{i=1}^{n-1}(D_i D_{i+1})^{-1/2}$, where $D_i = \frac{(n-i+1)(n-i)}{2} + \frac{(i-1)i}{2}$.

$$D(P_n) = \begin{array}{c} \left(\begin{array}{cccccc} 0 & 1 & 2 & 3 & \cdots & n-1 \\ 1 & 0 & 1 & 2 & \cdots & n-2 \\ 2 & 1 & 0 & 1 & \cdots & n-3 \\ \vdots & \vdots & \ddots & \ddots & \ddots & \vdots \\ n-1 & n-2 & n-3 & n-4 & \cdots & 0 \end{array}\right) \end{array} \begin{array}{c} D_1 \\ D_2 \\ D_3 \\ \vdots \\ D_n \end{array}$$

Note that $\{D_i\}$ has the following properties:

(i) $\{D_i\}$ is a symmetric sequence with $D_i = D_{n-i+1}$, $i = 1, 2, \ldots \frac{n}{2}$ for $n$ is even ($\frac{n-1}{2}$ for $n$ is odd, respectively);

(ii) $D_i > D_{i+1}$ $(1 \leq i \leq \frac{n}{2} - 1$ or $\frac{n-1}{2})$.

Otherwise $d(T) \leq n-2$.

Consider the distance matrix $[d_{ij}]_{n\times n}$ of $T$. We have the following properties:

(1) the diagonal entries are 0 and the other entries are positive integers less than $n-2$;

(2) the $u$ column sum is $D_u$.

Let $P = v_1 v_2 \cdots v_k$ $(k = d(T) \leq n-2)$ be a longest path in $T$. Since $P$ is longest, we have that $v_1$ and $v_k$ are leaves. Let $v_1$ be the root of $T$. Then the other vertices of $T$ can be divided into levels by the distance on $v_1$ (see Figure 2). Note that the vertices in the same level are independent.

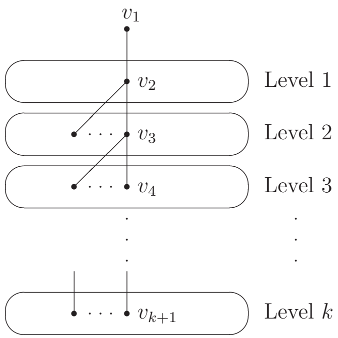


Figure 2. The root $v_1$ and the levels of $T$

Let $L_i$ be the set of vertices in level $i$ $(1 \leq i \leq k)$. For any vertex $x_i \in L_i$, comparing the distance matrix of $T$ with that of a path, we are easy to have $D_{x_i} < D_{i+1}$ $(1 \leq i \leq k \leq n-2)$. Furthermore, $D_{v_1} < D_1$.

Let $r_i$ be the number of edges between level $i$ and level $i+1$ $(1 \leq i \leq k-1)$. Note that $\sum\limits_{i=1}^{k-1} r_i = n-2$. Then we have

$$\begin{aligned} J(T) &= (n-1) \sum_{uv \in E(T)} (D_u D_v)^{-1/2} \\ &= (n-1)[(D_{v_1} D_{v_2})^{-1/2} + \sum_{\substack{x_i x_{i+1} \in E(T) \\ 1 \leq i \leq k-1}} (D_{x_i} D_{x_{i+1}})^{-1/2}] \\ &> (n-1)[(D_1 D_2)^{-1/2} + (D_2 D_3)^{-1/2} + \cdots + (D_k D_{k+1})^{-1/2} + \\ &\quad (r_1 - 1)(D_2 D_3)^{-1/2} + (r_2 - 1)(D_3 D_4)^{-1/2} + \ldots + (r_{k-1} - 1)(D_k D_{k+1})^{-1/2}] \end{aligned}$$

Since $D_1 (= D_n) > D_2 (= D_{n-1}) > \cdots > D_{\frac{n}{2}} (= D_{\frac{n}{2}+1})$ or $D_{\frac{n+1}{2}}$ for $n$ is odd, we have

$$\frac{1}{\sqrt{D_1 D_2}} (= \frac{1}{\sqrt{D_{n-1} D_n}}) < \frac{1}{\sqrt{D_2 D_3}} (= \frac{1}{\sqrt{D_{n-2} D_{n-1}}}) < \cdots < \frac{1}{\sqrt{D_{\frac{n}{2}} D_{\frac{n}{2}+1}}} \text{ or }$$

$$\frac{1}{\sqrt{D_{\frac{n-1}{2}} D_{\frac{n+1}{2}}}} (= \frac{1}{\sqrt{D_{\frac{n+1}{2}} D_{\frac{n+3}{2}}}}) \text{ for } n \text{ is odd.}$$

Thus we have

$$J(T) > (n-1) \sum_{i=1}^{n-1} (D_i D_{i+1})^{-1/2}.$$

Therefore, we have $J(T) \geq (n-1) \sum\limits_{i=1}^{n-1} (D_i D_{i+1})^{-1/2}$, where $D_i = \frac{(n-i+1)(n-i)}{2} + \frac{(i-1)i}{2}$, with equality if and only if $T$ is a path. This completes the proof of Theorem 2.2. $\square$

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