Trees with the First Three Smallest and Largest Generalized Topological Indices *

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Abstract

Let T be a tree and d_v the degree of its vertex v. In this paper, we investigate the following topological indices for a tree T: $\sum\limits_{u\in V(T)} d_v^m$, $\sum\limits_{u\in V(T)} d_v^{-m}$, $\sum\limits_{u\in V(T)} d_v^{1/m}$, $\sum\limits_{u\in V(T)} d_v^{-1/m}$, where $m \geq 2$ is an integer. All trees with the smallest, the second and third smallest values of the four topological indices are characterized. The same is done for all trees with the largest, the second and third largest values of these indices.

Keywords: tree; chemical tree; topological index

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1 Introduction

It is well known that a topological index of molecules determines a large number of molecular properties such as boiling points, molecular volumes, energy levels, electronic populations, etc., see [8,10] for details. A topological index of molecules is a numeric quantity that is mathematically derived in a direct and unambiguous manner from the structural graph of a molecule. Since isomorphic graphs possess identical values for any given topological index, these indices are referred to as graph invariants. Many topological indices have been developed through the years and correlated with many physicochemical properties [1,3-7,9,12].

Let $G = (V(G), E(G))$ denote a graph with $V(G)$ as the set of vertices and $E(G)$ as the set of edges. The Randić index of G defined in [10] is

$$\chi(G) = \sum_{uv\in E(G)} \frac{1}{\sqrt{d_u d_v}},$$

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where d_v denotes the degree of the vertex v in G. Randić demonstrated that his index is well correlated with a variety of physico-chemical properties of alcanes. The index χ became one of the most popular molecular descriptors, see [1,4-5,10-12]. The zeroth-order Randić index $\chi^0(G)$ of G defined by Kier and Hall [8] is

$$\chi^0(G) = \sum_{v \in V(G)} \frac{1}{\sqrt{d_v}}.$$

Pavlović [12] gave the unique graph with the largest value of $\chi^0(G)$. In [6], Li el al. investigated the same problem for the topological index $M_1(G)$, a Zagreb index [13], which is defined as

$$M_1(G) = \sum_{v \in V(G)} d_v^2.$$

By observing the common appearance of the Randić index and the Zagreb index, we can formulate four generalized topological indices for a (molecular) graph G as follows:

(i) $\alpha_m(G) = \sum\limits_{u \in V(G)} d_v^m$,

(ii) $\alpha_{-m}(G) = \sum\limits_{u \in V(G)} d_v^{-m}$,

(iii) $\alpha_{1/m}(G) = \sum\limits_{u \in V(G)} d_v^{1/m}$,

(iv) $\alpha_{-1/m}(G) = \sum\limits_{u \in V(G)} d_v^{-1/m}$,

where m is a positive integer, usually, at least 2. One can see that if we take $m = 2$, the above index (i) is the Zagreb index M_1, and the above index (iv) is the zeroth-order Randić index $\chi^0(G)$. It is easy to see that there is a unified formulation for the four indices, that is, $\alpha_m(G) = \sum\limits_{u \in V(G)} d_v^m$, in which m can be any integers (including negative integers) or any of the fractions $\frac{1}{k}$ for any nonzero integers k. However, because sometimes they present different properties, we have to distinguish them in discussions. So, we prefer to use different notations for the four indices. In this paper, we shall investigate the above four topological indices for special graphs of chemical interest–trees. We characterize all trees with the smallest, the second and third smallest values of the four topological indices. The same is done for all trees with the largest, the second and third largest values of these indices.

Throughout this paper, we consider finite and simple graphs only. We denote, respectively, by S_n and P_n the star and path with n vertices. By $S_{n,m}$ we denote the graph obtained from S_{n+2} and S_{m+1} by identifying an end-vertex of S_{n+2} with the center of S_{m+1}. For a graph G, we denote by $D(G)$ the degree sequence of G, that is, if the degree sequence of G is $d_1, d_2, \cdots, d_n$, then $D(G) = [d_1, d_2, \cdots, d_n]$. Furthermore, $D(G) = [x_1^{a_1}, x_2^{a_2}, \cdots, x_t^{a_t}]$ means that G has a_i vertices of degree x_i, where $i = 1, 2, \cdots, t$. Denote by $\mathcal{T}^1$ the set of trees T with n vertices and $D(T) = [3, 2^{n-4}, 1^3]$ and by $\mathcal{T}^2$ the set of trees T with n vertices and $D(T) = [3^2, 2^{n-6}, 1^4]$. Undefined notations and terminology will conform to those in [2].

2 The Extremal Values for the Four Indices of Trees

For convenience, in the sequel we always assume that G is a graph with $D(G) = [d_1, d_2, \cdots, d_n]$ such that $d_i \geq d_j + 2$, and G' is a graph obtained from G by replacing the pair (d_i, d_j) by the pair $(d_i - 1,\ d_j + 1)$, that is, $D(G') = [d_1, d_2, \cdots, d_{i-1}, d_i - 1, d_{i+1}, \cdots, d_{j-1}, d_j + 1, d_{j+2}, \cdots, d_n]$.

Lemma 1. For two graphs G and G', we have
(i) $\alpha_m(G) > \alpha_m(G')$;
(ii) $\alpha_{-m}(G) > \alpha_{-m}(G')$;
(iii)$\alpha_{1/m}(G) < \alpha_{1/m}(G')$;
(iv) $\alpha_{-1/m}(G) > \alpha_{-1/m}(G')$.

Proof. (i) Note that

$$\begin{aligned}&d_i^m + d_j^m - (d_i-1)^m - (d_j+1)^m\\ &= (d_i - 1 + 1)^m + (d_j + 1 - 1)^m - (d_i-1)^m - (d_j+1)^m\\ &= \sum_{k=1}^m \begin{pmatrix} m \\ k \end{pmatrix} \left((d_i-1)^{m-k} + (-1)^k (d_j+1)^{m-k}\right).\end{aligned}$$

So, by $d_i \geq d_j + 2$, we have

$$\alpha_m(G) - \alpha_m(G') = \sum_{k=1}^{m} \begin{pmatrix} m \\ k \end{pmatrix} \left((d_i-1)^{m-k} + (-1)^k (d_j+1)^{m-k}\right) > 0.$$

(i) is thus proved.
(ii) By $d_i \geq d_j + 2$, we have

$$\begin{aligned}&\tfrac{1}{d_i^m} + \tfrac{1}{d_j^m} - \tfrac{1}{(d_i-1)^m} - \tfrac{1}{(d_j+1)^m}\\ &= \tfrac{(d_i-1)^m - d_i^m}{(d_i-1)^m d_i^m} + \tfrac{(d_j+1)^m - d_j^m}{(d_j+1)^m d_j^m}\\ &= \sum_{k=1}^{m} \begin{pmatrix} m \\ k \end{pmatrix} \left(\tfrac{1}{d_j^k (d_j+1)^m} + (-1)^k \tfrac{1}{d_i^k (d_i-1)^m}\right) > 0.\end{aligned}$$

This implies (ii).
(iii) By $d_i \geq d_j + 2$, it follows that

$$\begin{aligned}&\sqrt[m]{d_i} + \sqrt[m]{d_j} - \sqrt[m]{d_i - 1} - \sqrt[m]{d_j + 1}\\ &= \frac{1}{\sum_{k=1}^m \sqrt[m]{d_i^{m-k}(d_i-1)^{k-1}}} - \frac{1}{\sum_{k=1}^m \sqrt[m]{d_j^{m-k}(d_j+1)^{k-1}}} < 0.\end{aligned}$$

This implies (iii).
(iv) Similar to (iii), for $d_i \geq d_j + 2$ we have

$$\begin{aligned}&\tfrac{1}{\sqrt[m]{d_i}} + \tfrac{1}{\sqrt[m]{d_j}} - \tfrac{1}{\sqrt[m]{d_i-1}} - \tfrac{1}{\sqrt[m]{d_j+1}}\\ &= \frac{-1}{\sqrt[m]{d_i}\sqrt[m]{d_i-1}\sum_{k=1}^m \sqrt[m]{d_i^{m-k}(d_i-1)^{k-1}}} + \frac{1}{\sqrt[m]{d_j}\sqrt[m]{d_j+1}\sum_{k=1}^m \sqrt[m]{d_j^{m-k}(d_j+1)^{k-1}}} > 0.\end{aligned}$$

So, (iv) is implied. $\square$

From Lemma 1, one can see that there are many topological indices $f(G)$ such that $f(G) > f(G')$ or $f(G) < f(G')$. In the following, we shall investigate the extremal trees with respect to a topological index $f(G)$ such that $f(G) > f(G')$ or $f(G) < f(G')$.

Theorem 1. Let $f(G)$ be a topological index such that $f(G) > f(G')$. Then for a tree T with n vertices, we have

(i) $f(T)$ attains the largest value if and only if $T \cong S_n$, $f(T)$ attains the second largest value if and only if $T \cong S_{n-3,1}$ and $f(T)$ attains the third largest value if and only if $T \cong S_{n-4,2}$.

(ii) $f(T)$ attains the smallest value if and only if $T \cong P_n$, $f(T)$ attains the second smallest value if and only if $T \in \mathcal{T}^1$ and $f(T)$ attains the third smallest value if and only if $T \in \mathcal{T}^2$.

Proof. (i) Let T be a tree with n vertices and $D(T) = [x_1, x_2, \cdots, x_n]$. Note that if $T \ncong S_n$, then there must be a pair (x_i, x_j) such that $n-2 \geq x_i \geq x_j \geq 2$. We construct a graph T_1 by replacing the pair (x_i, x_j) by the pair (x_i+1, x_j-1). According to the condition of the theorem, we take $G = T_1$ and $G' = T$. Thus, it is not hard to see that $f(T_1) > f(T)$. Repeating the above operation until there is no pair (x_i, x_j) such that $n-2 \geq x_i \geq x_j \geq 2$, we can obtain a tree sequence $T, T_1, T_2, \cdots, T_{s-1}, T_s$ such that $T_s \cong S_n$, that is, $D(T_s) = [n-1, 1^{n-1}]$. Clearly, $f(T) < f(T_1) < f(T_2) < \cdots < f(T_{s-1}) < f(S_n)$. So, for any tree $T \ncong S_n$, $f(T) < f(S_n)$.

Since S_n is obtained from T_{s-1} by replacing the pair (x_i, x_j) by the pair (x_i+1, x_j-1) and $D(S_n) = [n-1, 1^{n-1}]$, where $n-2 \geq x_i \geq x_j \geq 2$, one can see that $D(T_{s-1}) = [n-2, 2, 1^{n-2}]$ and T_{s-1} must be $S_{n-3,1}$. Similarly, $D(T_{s-2})$ has the following two cases: $D(T^1_{s-2}) = [n-3, 2, 2, 1^{n-3}]$ and $D(T^2_{s-2}) = [n-3, 3, 1, 1^{n-3}]$. Note that $T^2_{s-2} \cong S_{n-4,2}$ and $D(T^2_{s-2})$ can be obtained by replacing the pair $(2,2)$ of $D(T^1_{s-2})$ by the pair $(3,1)$. From the condition of the theorem, we have that $f(S_{n-4,2}) > f(P_{n-4,4})$ and $f(S_n) > f(S_{n-3,1}) > f(S_{n-4,2}) > f(T_{s-i}) > f(T)$ for all $T \notin \{S_n, S_{n-3,1}, S_{n-4,2}\}$ and $i \geq 3$. The proof of (i) is thus complete.

(ii) Let T' be a tree with n vertices and let its degree sequence be $y_1, y_2, \cdots, y_n$. It is not difficult to see that if $T' \ncong P_n$, then there must be a pair (y_i, y_j) such that $y_i \geq y_j + 2$. We construct a graph T'_1 by replacing the pair (y_i, y_j) by the pair $(y_i - 1, y_j + 1)$. From the condition of the theorem, we have $G = T'$ and $G' = T'_1$. So, $f(T') > f(T'_1)$. Repeating the above operation until there is no pair (y_i, y_j) such that $y_i - y_j \geq 2$ for all i, j, we can obtain a tree sequence $T', T'_1, T'_2, \cdots, T'_{s-1}, T'_s$ such that $T'_s \cong P_n$. Clearly, $f(T') > f(T'_1) > f(T'_2) > \cdots > f(T'_{s-1}) > f(P_n)$. So, for any tree $T' \ncong P_n$, $f(T') > f(P_n)$.

Note that $D(P_n) = [2^{n-2}, 1^2]$ and P_n is obtained from T'_{s-1} by replacing the pair (y_i, y_j) by the pair $(y_i - 1, y_j + 1)$, where $y_i \geq y_j + 2$. It is easy to see that $D(T'_{s-1}) = [3, 2^{n-4}, 1^3]$. So, $T'_{s-1} \in \mathcal{T}^1$. Similarly, $D(T'_{s-2})$ has the following cases: $D(T'^1_{s-2}) = [3, 3, 2^{n-6}, 1^4]$, or $D(T'^2_{s-2}) = [4, 2, 2^{n-6}, 1^4]$. By using the pair $(3,3)$ to replace the pair $(4,2)$, we obtain $[3, 3, 2^{n-6}, 1^4]$ from $[4, 2, 2^{n-6}, 1^4]$. So, from the condition of the theorem we have $f(T'^2_{s-2}) > f(T'^1_{s-2})$. Since $T'^1_{s-2} \in \mathcal{T}^2$, we have $f(P_n) < f(T^1) < f(T^2\} < f(T'_{s-i}) < f(T')$ for all $T' \notin \{P_n\} \cup \mathcal{T}^1 \cup \mathcal{T}^2$ and $i \geq 3$, where $T^1 \in \mathcal{T}^1$ and $T^2 \in \mathcal{T}^2$. This completes the proof of (ii). $\square$

Similar to the proof of Theorem 1, we can show

Theorem 2. Let $f(G)$ be a topological index such that $f(G) < f(G')$. Then for a tree T with n vertices, we have

(i) $f(T)$ attains the smallest value if and only if $T \cong S_n$, $f(T)$ attains the second smallest value if and only if $T \cong S_{n-3,1}$ and $f(T)$ attains the third smallest value if and only if $T \cong S_{n-4,2}$.

(ii) $f(T)$ attains the largest value if and only if $T \cong P_n$, $f(T)$ attains the second largest value if and only if $T \in \mathcal{T}^1$ and $f(T)$ attains the third largest value if and only if $T \in \mathcal{T}^2$.

From Lemma 1, one can see that the topological indices $\alpha_m(G)$, $\alpha_{-m}(G)$ and $\alpha_{-1/m}(G)$ have the property that $f(G) > f(G')$; whereas $\alpha_{1/m}(G)$ has the property that $f(G) < f(G')$. So, from Theorems 1 and 2 it is not hard to get the smallest, the second and third smallest values of the above four topological indices, as well as the largest, the second and third largest values of these indices. In the following, we give the smallest and the largest values and omit other values.

Corollary 1. For a tree T with n vertices, we have

(i) $(n-2)2^m + 2 \leq \alpha_m(T) \leq (n-1)^m + n - 1$,

(ii) $(n-2)2^{-m} + 2 \leq \alpha_{-m}(T) \leq (n-1)^{-m} + n - 1$,

(iii)$(n-2)2^{1/m} + 2 \geq \alpha_{1/m}(T) \geq (n-1)^{1/m} + n - 1$,

(iv) $(n-2)2^{-1/m} + 2 \leq \alpha_{-1/m}(T) \leq (n-1)^{-1/m} + n - 1$

and for each of the inequalities, the equality on the left-hand side holds if and only if $T \cong P_n$; whereas the equality on the right-hand side holds if and only if $T \cong S_n$.

Theorem 3. Let $f(G)$ be a topological index such that $f(G) > f(G')$. Then for a chemical tree T with n vertices and $n-2 = 3a+i, i = 0,1,2$, we have

(i) $f(T)$ attains the largest value if and only if $D(T) = [4^a, i+1, 1^{n-a-1}]$,

(ii) $f(T)$ attains the second largest value if and only if $D(T) = [4^{a-1}, 3, 2, 1^{n-a-1}]$ for $i = 1$, $D(T) = [4^{a-1}, 3^2, 1^{n-a-1}]$ for $i = 2$ and $D(T) = [4^a, 2^2, 1^{n-a-2}]$ for $i = 3$, where a chemical tree is such a tree that has no vertex with degree greater than 4 .

Proof. (i) Let T be a chemical tree with n vertices and let its degree sequence be $z_1, z_2, \cdots, z_n$. Assume that $4 > z_i \geq z_j \geq 2$. We construct the graph T_1 by replacing the pair (z_i, z_j) by the pair (z_i+1, z_j-1). According to the condition of the theorem, we have $G = T_1$ and $G' = T$. Thus, it is not hard to see that $f(T_1) > f(T)$. Repeating the above operation until there is no pair (z_i, z_j) such that $3 \geq z_i \geq z_j \geq 2$, we can obtain a tree sequence $T, T_1, T_2, \cdots, T_{s-1}, T_s$. So, $f(T) < f(T_1) < f(T_2) < \cdots < f(T_{s-1}) < f(T_s)$ and T_s has some vertices of degree 4 or some vertices of degree 1 except for at most one vertex of degree 2 or degree 3. We denote, respectively, by a, b, c and d the number of the vertices of degrees 4,3,2 and 1. Then we have

$$\begin{cases} 4a+3b+2c+d &=& 2n-2. \\ a+b+c+d &=& n. \\ b+c &\leq& 1. \end{cases}$$

From the above equations, we have

(1) $a = \frac{n-2}{3}, b = c = 0$ and $d = n-a$ if $n-2 \equiv 0 (mod 3)$;

(2) $a = \frac{n-3}{3}, b = 0, c = 1$ and $d = n-a-1$ if $n-2 \equiv 1 (mod 3)$;

(3) $a = \frac{n-4}{3}, b = 1, c = 0$ and $d = n-a-1$ if $n-2 \equiv 2 (mod 3)$.

This completes the proof of (i).

(ii) For $i = 3$, from the proof of (i) we know that $D(T_s) = [4^a, 3, 1^{n-a-1}]$. Since $D(T_s)$ is obtained from T_{s-1} by replacing the pair (x_i, x_j) by the pair (x_i+1, x_j-1), where $3 \geq x_i \geq x_j \geq 2$, one can see that $D(T_{s-1})$ has the following two cases: $D(T^1_{s-1}) = [4^a, 2^2, 1^{n-a-2}]$ and $D(T^2_{s-1}) = [4^{a-1}, 3^2, 2, 1^{n-a-2}]$. Note that $D(T^1_{s-1})$ can be obtained by replacing the pair $(3,3)$ of $D(T^2_{s-1})$ by the pair $(4,2)$. From the condition of the theorem, we have that $f(T^1_{s-1}) > f(T^2_{s-1})$. For $i = 1,2$, by a similar argument to the case $i = 3$, the proof of (ii) can be complete. □

Similarly, we have

Theorem 4. Let $f(G)$ be a topological index such that $f(G) < f(G')$. Then for a chemical tree T with n vertices and $n-2 = 3a+i, i = 0,1,2$, we have

(i) $f(T)$ attains the smallest value if and only if $D(T) = [4^a, i+1, 1^{n-a-1}]$,

(ii) $f(T)$ attains the second smallest value if and only if $D(T) = [4^{a-1}, 3, 2, 1^{n-a-1}]$ for $i = 1$, $D(T) = [4^{a-1}, 3^2, 1^{n-a-1}]$ for $i = 2$ and $D(T) = [4^a, 2^2, 1^{n-a-2}]$ for $i = 3$.

From Lemma 1 and Theorems 3 and 4, we have

Corollary 2. For a chemical tree T with n vertices and $n-2 = 3a+i, i = 0,1,2$, we have

(i) $\alpha_m(T) \leq a \times 4^m + (i+1)^m + n - 1 - a$,

(ii) $\alpha_{-m}(T) \leq a \times 4^{-m} + (i+1)^{-m} + n - 1 - a$,

(iii)$\alpha_{1/m}(T) \geq a \times 4^{1/m} + (i+1)^{1/m} + n - 1 - a$,

(iv) $\alpha_{-1/m}(T) \leq a \times 4^{-1/m} + (i+1)^{-1/m} + n - 1 - a$,

and for each of the inequalities, the equality holds if and only if T has a vertices of degree 4, one vertex of degree $i+1$ and $n-a-1$ vertices of degree 1.

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