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Note

On the general sum-connectivity index of trees with given number of pendent vertices

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ABSTRACT

The general sum-connectivity index of a graph G is defined as $\chi_\alpha(G) = \sum_{uv\in E(G)}(d(u)+d(v))^\alpha$, where $d(u)$ denotes the degree of a vertex u in G and α is a real number. In this paper, we present the maximum general sum-connectivity indices of trees and chemical trees with given number of pendent vertices for $-1 \le \alpha < 0$. The corresponding extremal graphs are also characterized.

1. Introduction

Topological indices are numbers associated with chemical structures derived from their hydrogen-depleted graphs as a tool for compact and effective description of structural formulas which are used to study and predict the structure–property correlations of organic compounds. Let G be a simple graph with vertex set $V(G)$ and edge set $E(G)$. The Randić index $R(G)$, proposed by Randić [14] in 1975, is defined as

$$R(G) = \sum_{uv\in E(G)} \frac{1}{\sqrt{d(u)d(v)}},$$

where $d(u)$ (or $d_G(u)$) denotes the degree of a vertex u of G. The Randić index is one of the most successful molecular descriptors in structure–property and structure–activity relationship studies [3,8,18]. Mathematical properties of this descriptor have been studied extensively (see [7,10–12] and the references cited therein).

With motivation from the Randić index, the sum-connectivity index $\chi(G)$ and the general sum-connectivity index $\chi_\alpha(G)$ of a graph G were recently proposed by Zhou and Trinajstić [27,28] and defined as

$$\chi(G) = \sum_{uv\in E(G)} \frac{1}{\sqrt{d(u)+d(v)}}$$

and

$$\chi_\alpha(G) = \sum_{uv\in E(G)} (d(u)+d(v))^\alpha,$$

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where α is a real number. It has been found that the sum-connectivity index and the Randić index correlate well between themselves and with the π-electronic energy of benzenoid hydrocarbons [13]. The harmonic index $H(G)$ of a graph G is another variant of the Randić index. This index first appeared in [6] and is defined as

$$H(G) = \sum_{uv \in E(G)} \frac{2}{d(u) + d(v)}.$$

Note that both the sum-connectivity index and the harmonic index can be viewed as particular cases of the general sum-connectivity index since $\chi(G) = \chi_{-\frac{1}{2}}(G)$ and $H(G) = 2\chi_{-1}(G)$.

In the study of topological indices in general, it is often of interest to consider the extremal values of a certain index among graphs under some constraints. Along this line, the extremal values of the general sum-connectivity index have been extensively explored. Zhou and Trinajstić [28] determined the minimum general sum-connectivity index of trees for all $\alpha \neq 0$ and the maximum general sum-connectivity index of trees for $\alpha > \alpha_0 \approx -1.4094$ and $\alpha \neq 0$. Du, Zhou and Trinajstić [5] found the maximum general sum-connectivity index of trees for $\alpha < \alpha_1 \approx -4.3586$ and characterized the corresponding extremal trees. Tomescu and Kanwal [23] considered the minimum general sum-connectivity indices of trees with given number of pendent vertices and diameter for $-1 \leq \alpha < 0$, respectively. Tomescu and Arshad [20] determined the minimum general sum-connectivity index of unicyclic graphs with given number of pendent vertices for $-1 \leq \alpha < 0$ and characterized the corresponding extremal graphs. Tache [15] and Zhu and Lu [29] gave the maximum general sum-connectivity indices of bicyclic graphs and tricyclic graphs for $\alpha \geq 1$, respectively. Tomescu [19] considered the minimum general sum-connectivity index of graphs (triangle-free graphs, respectively) with minimum degree at least 2 for $-1 \leq \alpha < \alpha_2 \approx -0.8670$ ($-1 \leq \alpha < \alpha_3 \approx -0.8171$, respectively). See [1,4,9,16,17,21,22,24] for more mathematical properties of this index.

In this work, we study the general sum-connectivity indices of trees and chemical trees with given number of pendent vertices. We determine the maximum general sum-connectivity indices of trees and chemical trees with n vertices and k pendent vertices for $-1 \leq \alpha < 0$. The corresponding extremal graphs are also characterized.

2. Preliminaries

Let G be a graph. For any vertex $v \in V(G)$, we use $N_G(v)$ (or $N(v)$ if there is no ambiguity) to denote the set of neighbors of v in G. Let n_i be the number of vertices of degree i in G. We use $E_2(G)$ to denote the set of edges in G such that for any edge $uv \in E_2(G)$, we have $d(u) = d(v) = 2$. The maximum degree of G is denoted by $\Delta(G)$. A pendent vertex is a vertex of degree 1 and a non-pendent vertex is a vertex of degree at least 2. An edge incident with a pendent vertex is called a pendent edge. We say a path $P = v_0v_1 \dots v_s$ of G is a pendent path if v_0 is a pendent vertex, $d(v_s) \geq 3$ and $d(v_1) = \cdots = d(v_{s-1}) = 2$ (unless $s = 1$). We use $\mathcal{P}(G)$ to denote the set of all pendent paths in G. Let $G - uv$ be the graph obtained from G by deleting the edge $uv \in E(G)$. We use P_n and S_n to denote the path and the star on n vertices, respectively. We write $A := B$ to rename B as A.

A chemical tree is a tree with maximum degree at most 4. Let $\mathcal{T}_{n,k}$ and $\mathcal{CT}_{n,k}$ be the set of trees and chemical trees with n vertices and k pendent vertices, respectively, where $2 \leq k \leq n-1$. A tree T is called a $(k, 3)$-regular tree if T contains k pendent vertices and every non-pendent vertex has degree 3 in T. It is easy to calculate that every $(k, 3)$-regular tree has $2k - 2$ vertices. We use $\mathcal{T}^*_{n,k}$ to denote the set of trees on n vertices obtained from a $(k, 3)$-regular tree by adding at least one new vertex on each pendent edge. Note that each tree $T \in \mathcal{T}^*_{n,k}$ can also be stated as follows: T is a tree on n vertices, there are $k-2$ vertices of maximum degree 3 in T which induce a tree and any of these vertices is adjacent to either another vertex of degree 3 or a vertex of degree 2. Clearly, every tree in $\mathcal{T}^*_{n,k}$ contains k pendent vertices, $n-2k+2$ vertices of degree 2 and $k-2$ vertices of degree 3. Since $\mathcal{T}_{n,2} = \mathcal{CT}_{n,2} = \{P_n\}$, $\mathcal{T}_{n,n-1} = \{S_n\}$ and $\mathcal{CT}_{n,n-1} = \{S_n | 3 \leq n \leq 5\}$, we only consider $3 \leq k \leq n-2$ in the following arguments.

In order to prove our main results, we need the following three transformations on a tree T which were introduced by Zhang, Lu and Tian [26].

(i) Let uv be an edge in T. If T_{uv} is the graph obtained from T by contracting the edge uv, i.e., identifying the two vertices u and v in $T - uv$, we say that T_{uv} is obtained from T by Transformation I. Hence $|V(T_{uv})| = |V(T)| - 1$.

(ii) Let v be a vertex in T with $N(v) = V' \cup V''$ such that $V' \cap V'' = \emptyset$, $|V'| = s_1 \geq 1$ and $|V''| = s_2 \geq 1$. If $T_{v\to(s_1,s_2)}$ is the graph obtained from T by splitting the vertex v into two new vertices v' and v'', connecting v' and v'', and connecting v' to all vertices in V' and v'' to all vertices in V'', we say that $T_{v\to(s_1,s_2)}$ is obtained from T by Transformation II. Clearly, $|V(T_{v\to(s_1,s_2)})| = |V(T)| + 1$.

(iii) Let v be a vertex in T with $d(v) = s \geq 4$. If $T_{v\to(3-\text{reg})}$ is the graph obtained from T by replacing the vertex v with an $(s, 3)$-regular tree T' such that each vertex in $N(v)$ and each pendent vertex of T' are identified one by one, we say that $T_{v\to(3-\text{reg})}$ is obtained from T by Transformation III (see Fig. 1 for an illustration). By the construction of $T_{v\to(3-\text{reg})}$, it is easy to see that $|T_{v\to(3-\text{reg})}| = |V(T)| + s - 3$.

We now give several auxiliary lemmas by applying the above transformations. These lemmas will then be used to prove our main results in Section 3.