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On multiplicative harmonic index of trees

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Abstract

The harmonic index is one of the best-known vertex-degree-based topological indices proposed by Fajtlowics in 1987 within some conjectures generated by the computer program Graffiti. It is formulated for a graph $\mathcal{G}$ as

$$H(\mathcal{G}) = \sum_{aa' \in E(\mathcal{G})} \frac{2}{d_{\mathcal{G}}(a) + d_{\mathcal{G}}(a')}.$$

The harmonic index has been shown to correlate well with the π-electronic energy of benzenoid hydrocarbons. The multiplicative version of this graph invariant was proposed by Kulli in 2016. In this paper, we obtain the maximum value of the multiplicative harmonic index over the set of trees with given order and maximum vertex degree and introduce the extremal trees.

Keywords: Vertex-degree-based topological indices, Maximum degree, Tree, Extremal problem.

AMS Mathematical Subject Classification [2010]: 05C05, 05C07, 05C35

1 Introduction

Throughout this paper, our graphs are considered to be simple, connected, and finite. Let $\mathcal{G}$ be a graph with vertex set $V(\mathcal{G})$ and edge set $E(\mathcal{G})$. The *open neighborhood* $N_{\mathcal{G}}(a)$ of $a \in V(\mathcal{G})$ is the set of vertices of $\mathcal{G}$ adjacent to a. The *degree* $d_{\mathcal{G}}(a)$ is the order of $N_{\mathcal{G}}(a)$. The *distance* $d_{\mathcal{G}}(a, a')$ between $a, a' \in V(\mathcal{G})$ is the length of any shortest path in $\mathcal{G}$ connecting the vertices a and a'.

Chemical compounds are usually modeled by molecular graphs. A *molecular graph* is a graph associated with the structural graph of a molecular structure in which the vertices represent atoms of the structure and edges represent chemical bonds. In mathematical chemistry, the physico-chemical properties of chemical structures are modeled via molecular structure descriptors which are refereed to as topological indices. A *topological index* is a real value associated with molecular graphs of chemical compounds that describes their topology and are invariant under graph isomorphism. Topological indices are used for correlation analysis

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in theoretical and environmental chemistry, pharmacology, biology and toxicology (see, for example, [4, 10]). Topological indices are classified into different categories among which *vertex-degree-based* indices are more well-known. These indices are helpful measures in analyzing various properties of chemical compounds like viscosity, entropy, enthalpy of vaporization, gyrational radius and boiling point.

The harmonic index is among the best-known and well-investigated vertex-degree-based indices in mathematical chemistry. This index was proposed by Fajtlowics [5] in 1987 within some conjectures generated by the computer program Graffiti. It is formulated for a graph $\mathcal{G}$ as

$$H(\mathcal{G}) = \sum_{aa' \in E(\mathcal{G})} \frac{2}{d_{\mathcal{G}}(a) + d_{\mathcal{G}}(a')}.$$

The harmonic index correlates well with the π-electronic energy of benzenoid hydrocarbons. Further results on mathematical properties and applications of the harmonic index can be found in [1, 2, 9] and the references quoted therein.

In 2016, Kulli [7] put forward the multiplicative version of the harmonic index. This invariant is defined for a graph $\mathcal{G}$ as

$$H^*(\mathcal{G}) = \prod_{aa' \in E(\mathcal{G})} \frac{2}{d_{\mathcal{G}}(a) + d_{\mathcal{G}}(a')}.$$

The mathematical and chemical properties of this invariant have been the subject of some recent publications (see, for example, [3, 6, 8]).

A basic problem in chemical graph theory is to determine the minimum and maximum values of graph invariants within the set of graphs with fixed graph parameters. Among various collection of graphs, trees are more investigated due to the fact that many classes of chemical graphs are tree. In this paper, we study the maximum value of the multiplicative harmonic index over all trees with given order and maximum vertex degree and identify the extremal trees.

2 Main results

A *rooted tree* is a tree with a special vertex as the *root*. A *leaf* of a tree is a vertex of degree one. A tree with exactly one vertex of degree greater than two is said to be a *spider*. The vertex of a spider with largest vertex degree is called the *center* of the spider. A *leg* of a spider is a path connecting its center to a leaf. A star is a spider in which all legs have length one. Also a path can be assumed as a spider with one leg or two legs.

For positive integers n and Δ, we denote by $\mathcal{T}_{n,\Delta}$ the set of all trees with n vertices and maximum degree Δ.

We need the following propositions in the proof of our main theorem.

Proposition 2.1. *Let $T \in T(n, \Delta)$ be a rooted tree whose root is on a vertex ρ of degree Δ. Let T have a vertex $\omega \neq \rho$ with $d_T(\omega) \geq 3$ and maximum distance from ρ such that at least two neighbors ω_1 and ω_2 of ω in T be leaf. If $T' \in T(n, \Delta)$ is the tree obtained from T by removing the edge $\omega\omega_1$ and adding the edge $\omega_1\omega_2$, then $H^*(T') > H^*(T)$.*

Proposition 2.2. *Let $T \in T(n, \Delta)$ be a rooted tree whose root is on a vertex ρ of degree Δ. Let T have a vertex $\omega \neq \rho$ with $d_T(\omega) \geq 3$ and maximum distance from ρ such that exactly one neighbor ω_1 of ω in T be* *a leaf and let $\omega\alpha_1\alpha_2...\alpha_p$, $p \geq 2$ be a path in T. If $T' \in T(n,\Delta)$ is the tree obtained from T by removing the edge $\omega\omega_1$ and adding the edge $\alpha_p\omega_1$, then $H^*(T') > H^*(T)$.*

Proposition 2.3. *Let $T \in T(n,\Delta)$ be a rooted tree whose root is on a vertex ρ of degree Δ. Let T have a vertex $\omega \neq \rho$ with $d_T(\omega) \geq 3$ and maximum distance from ρ such that none of the neighbors of ω in T be a leaf and let $\omega\alpha_1\alpha_2\dots\alpha_p$ and $\omega\beta_1\beta_2\dots\beta_q$, $p,q \geq 2$, be two paths in T. If $T' \in T(n,\Delta)$ is the tree obtained from T by removing the vertices $\alpha_1,\alpha_2,\dots,\alpha_p$ and adding the path $\beta_q\alpha_1\alpha_2\dots\alpha_p$, then $H^*(T') > H^*(T)$.*

From the above propositions, we reach the following lemma.

Lemma 2.4. *Let $T \in T_{n,\Delta}$ be rooted at ω, where ω is a vertex with $d_T(\omega) = \Delta$. Let T contain a vertex except ω of degree more than two. Then there exists a tree $T' \in T_{n,\Delta}$ such that $H^*(T') > H^*(T)$.*

Lemma 2.5. *Let $S \in T_{n,\Delta}$ be a spider with center ω where $d_S(\omega) = \Delta \geq 3$ and let S have at least a leaf α_1 and a leg $\omega\beta_1\beta_2\dots\beta_q$, $q \geq 2$. If $S' \in T_{n,\Delta}$ is the spider obtained from S by removing the edge $\beta_q\beta_{q-1}$ and adding the edge $\beta_q\alpha_1$, then $H^*(S') > H^*(S)$.*

From Lemmas 2.4 and 2.5, we get the main theorem of the paper.

Theorem 2.6. *For $T \in T_{n,\Delta}$,*

$$H^*(T) \leq \begin{cases} (\frac{2}{\Delta+1})^{2\Delta-n+1} \times (\frac{2}{\Delta+2})^{n-\Delta-1} \times (\frac{2}{3})^{n-\Delta-1} & \text{if } \Delta > \frac{n-1}{2}, \\ (\frac{2}{\Delta+2})^{\Delta} \times (\frac{2}{3})^{\Delta} \times (\frac{1}{2})^{n-2\Delta-1} & \text{if } \Delta \leq \frac{n-1}{2}. \end{cases}$$

The equality holds if and only if T is a spider whose all legs have length at most two or all legs have length at least two.

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