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journal homepage: www.elsevier.com/locate/damCacti with n -vertices and t cycles having extremal Wiener indexIvan Gutman^{a,b}, Shuchao Li^c, Wei Wei^{c,*}^a Faculty of Science, University of Kragujeva, 34000 Kragujevac, Serbia^b State University of Novi Pazar, Novi Pazar, Serbia^c Faculty of Mathematics and Statistics, Central China Normal University, Wuhan 430079, People's Republic of China

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ABSTRACT

The Wiener index $W(G)$ of a connected graph G is the sum of distances between all pairs of vertices of G . A connected graph G is said to be a cactus if each of its blocks is either a cycle or an edge. Let $\mathcal{G}_{n,t}$ be the set of all n -vertex cacti containing exactly t cycles. Liu and Lu (2007) determined the unique graph in $\mathcal{G}_{n,t}$ with the minimum Wiener index. We now establish a sharp upper bound on the Wiener index of graphs in $\mathcal{G}_{n,t}$ and identify the corresponding extremal graphs.

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1. Introduction

In this paper, we consider connected simple and finite graphs, and refer to Bondy and Murty [1] for notation and terminologies used but not defined here.

Let $G = (V_G, E_G)$ be a graph with vertex set V_G and edge set E_G . By $G - v$ and $G - uv$ we denote the graph obtained from G by deleting a vertex $v \in V_G$, or an edge $uv \in E_G$, respectively. (This notation is naturally extended if more than one vertex or edge are deleted.) Similarly, $G + uv$ is obtained from G by adding an edge $uv \notin E_G$.

As usual, let P_n and C_n , respectively, denote the path and cycle on n vertices.

The distance, $d_G(u, v)$, between two vertices u, v of G is the length of a shortest u - v path in G [3].

The Wiener index is defined as the sum of distances between all pairs of vertices, namely as

$$W(G) = \sum_{\{u,v\} \subseteq V_G} d_G(u, v) = \frac{1}{2} \sum_{v \in V_G} D_v(G)$$

where $D_v(G) = \sum_{u \in V_G} d_G(u, v)$. This distance-based graph invariant was introduced in 1947 [21], but was first considered in the mathematical literature only 30 years later [8]. Nowadays, the Wiener index is a well-known and much studied graph invariant; for reviews see [4,5,7,13,22]. It was also named “gross status” [11], “total status” [3], “graph distance” [8,9], and “transmission” [15,19]. In addition to its numerous applications in chemistry [5,10,18] the Wiener index has also found interesting applications in connection with computer networks [6].

A connected graph G is said to be a *cactus* if any two of its cycles have at most one common vertex. Let $\mathcal{G}_{n,t}$ be the set of all n -vertex cacti, each containing exactly t cycles. A graph is a *chain cactus* if each block has at most two cut vertices and each cut vertex is shared by exactly two blocks. Obviously, any chain cactus with at least two blocks contains exactly two blocks

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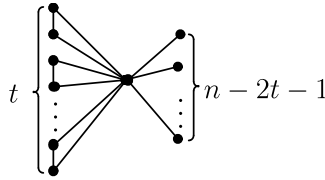


Fig. 1. The graph $G^*(n, t)$.

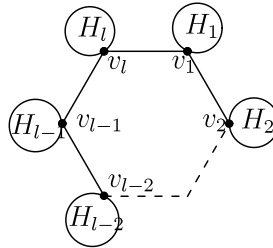


Fig. 2. The graph G .

that have only one cut-vertex. Such blocks are called *terminal blocks*. A *triangle-chain* of length k on $2k + 1$ vertices is a graph obtained from a path P_{k+1} by replacing each of its edges by a triangle. An *end* in a triangle-chain is a vertex of degree 2, with a neighbor of degree 2. The *saw graph*, denoted by $Sw(p, q; l)$, is the cactus obtained by joining an end of a triangle-chain of length p with the end of another triangle-chain of length q by a path of length l .

A motivation for the present study is that in 2007 Liu and Lu [14] determined the element of $\mathcal{G}_{n,t}$ with the minimum Wiener index. Since then, finding the maximal element(s) in $\mathcal{G}_{n,t}$ remained an open problem. Another motivation is the following conjecture, proposed by Bose, Nath and Paul in 2011 [2]:

Conjecture 1.1. $Sw(\lfloor t/2 \rfloor, \lceil t/2 \rceil; 2n - t - 1)$ uniquely maximizes the distance spectral radius among all cacti on n vertices with t cycles.

Motivated by Conjecture 1.1, we now propose:

Conjecture 1.2. $Sw(\lfloor t/2 \rfloor, \lceil t/2 \rceil; 2n - t - 1)$ uniquely maximizes the Wiener index among all cacti on n vertices with t cycles.

In this paper, we introduce several graph transformations to study $W(G)$ of cacti. Using their mathematical properties established, we determine a sharp upper bound on the Wiener index of cacti in $\mathcal{G}_{n,t}$, and provide a confirmative solution for Conjecture 1.2.

In what follows, we shall need the next two lemmas.

Lemma 1.3 ([16,17]). Let G_1 and G_2 be two connected graphs with disjoint vertex sets where $u_1 \in V_{G_1}$, $u_2 \in V_{G_2}$. Construct the graph G by identifying the vertices u_1 and u_2 , and denote the new vertex by u . Then

$$W(G) = W(G_1) + W(G_2) + (n_1 - 1)D_{u_2}(G_2) + (n_2 - 1)D_{u_1}(G_1)$$

where $|V_{G_i}| = n_i$ for $i = 1, 2$.

Let the cactus $G^*(n, t)$ be obtained from t triangles, all sharing a common vertex, and $n - 2t - 1$ pendant edges attached to the same vertex, as depicted in Fig. 1. Liu and Lu [14] demonstrated that this is the unique graph with minimum Wiener index in $\mathcal{G}_{n,t}$.

Lemma 1.4 ([14]). Let $G \in \mathcal{G}_{n,t}$, such that $n \geq 7$ and $t \geq 0$. Then $W(G) \geq W(G^*(n, t))$ with equality if and only if $G \cong G^*(n, t)$.

2. Some properties of the Wiener index

In this section, we examine the monotonicity of the Wiener index under some graph transformations.

Let H_i be a connected graph with $x_i \in V_{H_i}$ and suppose that $|V_{H_i}| = n_i$ for $i = 1, 2, \dots, \ell$ with $n_1 = \max\{n_1, n_2, \dots, n_\ell\}$. Let $C_\ell = v_1 v_2 \dots v_\ell v_1$ be a cycle of length $\ell \geq 4$. The graph G is obtained from C_ℓ and H_1, \dots, H_ℓ by identifying x_i with v_i for $i = 1, 2, \dots, \ell$ (see Fig. 2). The graph G' is obtained from G by deleting the edge $v_1 v_\ell$ and adding an edge $v_{\ell-2} v_\ell$, i.e., $G' = G - v_1 v_\ell + v_{\ell-2} v_\ell$.

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