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Extremal cacti of given matching number with respect to the distance spectral radius

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ABSTRACT

A cactus is a connected graph in which any two cycles have at most one common vertex. The distance spectral radius $\rho(G)$ of a graph G is the largest eigenvalue of the distance matrix $D(G)$. Recently, many researchers proposed the use of $\rho(G)$ as a molecular structure descriptor of alkanes. In this paper, we characterize n-vertex cyclic cactus with given matching number m which minimizes the distance spectral radius. The resulting cactus also minimizes the Hosoya index, the Wiener index and the Randić index in the same class of graphs.

1. Introduction

We only consider connected, simple and undirected graphs. Let $G = (V_G, E_G)$ be a simple graph on n vertices. We follow the notation and terminologies in [5,9] except otherwise stated.

Let $d_G(v)$ denote the degree of a vertex v in G and $N_G(v)$ be the set of vertices adjacent to v in G. A vertex v is called a pendant vertex of G if $d_G(v) = 1$ and the edge associated with a pendant vertex is called a pendant edge. Denote by $|U|$ the cardinality of the set U. For a vertex subset S of V_G, write $G[S]$, the subgraph induced by S. Let $G - v$, $G - uv$ denote the graph obtained from G by deleting the vertex $v \in V_G$, or the edge $uv \in E_G$, respectively (this notation is naturally extended if more than one vertex or edge is deleted). Similarly, $G + uv$ is obtained from G by adding an edge $uv \notin E_G$. For a connected graph G, an edge uv in E_G is called a *cut edge* if $G - uv$ is disconnected. Denote by P_n, S_n and K_n the path, the star and the complete graph with n vertices, respectively.

Two distinct edges in a graph G are *independent* if they do not have a common end vertex in G. A set of pairwise independent edges of G is called a *matching* of G, while a matching of maximum cardinality is a *maximum matching* of G. The *matching number* m of G is the cardinality of a maximum matching of G. Let M be a matching of G. The vertex v in G is *M-saturated* if v is incident with an edge in M, we also say that M saturates v; otherwise, v is *M-unsaturated*. A *perfect matching* M of G means that each vertex of G is M-saturated. Clearly, every perfect matching is maximum.

The *distance* between two vertices $u, v \in V_G$ is denoted by d_{uv} and is defined as the length of a shortest path between u and v in G. The *distance matrix* of G is denoted by $D(G)$ and is defined by $D(G) = (d_{uv})_{u,v \in V_G}$. It is easy to see that the matrix $D(G)$ is real symmetric, so all its eigenvalues are real [9]. The *distance spectral radius* $\rho(G)$ of G is the largest eigenvalue of the distance matrix $D(G)$. If in addition G is connected, $D(G)$ is non-negative and irreducible. By the Perron–Frobenius theory of

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non-negative matrices, $\rho(G)$ has multiplicity one and there exists a unique positive unit eigenvector, say $\mathbf{x} = (x_1, x_2, \dots, x_n)^T$, corresponding to $\rho(G)$. We refer to $\mathbf{x} = (x_1, x_2, \dots, x_n)^T$ as the distance Perron vector of G. Obviously, $0 < x_i < 1$ for $1 \le i \le n$. It will be convenient to associate a labeling of vertices of G (with respect to $\mathbf{x}$) in which x_v is the label of v. The *distance characteristic polynomial* of G, equal to $\det(xI - D)$, is denoted by $P(G, x)$ (or, for short, by $P(G)$). Also, the quadratic form $\mathbf{x}^T D(G)\mathbf{x}$ can be written as

$$\rho(G) = \mathbf{x}^T D(G)\mathbf{x} = 2 \sum_{\{u,v\} \subseteq V_G} d_{uv} x_u x_v.$$

The eigenvector equation $D(G)\mathbf{x} = \rho(G)\mathbf{x}$ can be interpreted as

$$\rho(G) x_v = \sum_{u \in V_G} d_{uv} x_u \tag{1.1}$$

Balaban et al. [2] proposed the use of $\rho(G)$ as a molecular descriptor, while in [13] it was successfully used to infer the extent of branching and model boiling points of alkanes. In recent years, the distance spectral radius has received much attention; see [1,3,4,7,15,18,19,21,24,26,30,31,33–36]. In particular, Ilić [15] characterized n-vertex trees with given matching number, which minimizes the distance spectral radius. Liu [19] characterized graphs with minimal distance spectral radius in three classes of simple connected graphs on n vertices: with fixed vertex connectivity, matching number and chromatic number, respectively. Zhang [35] and Lu and Luo [21] characterized unicyclic graphs with perfect matching and given matching number, respectively, which minimize the distance spectral radius. It is natural and interesting to consider the same problem in the class of cactus graphs, each of which is a connected graph in which any two cycles have at most one common vertex. Cacti have been an interesting topic in chemical and mathematical literature; see [6,8,12,14,16,17,22,23,27].

For a cactus G, we call it a *bundle* if all cycles of G have exactly one common vertex. A cactus G is called a cyclic cactus if G contains at least one cycle. Since Ilić in [15] characterized n-vertex trees with given matching number, we only consider cyclic cacti in this paper. Denote by $\mathscr{C}_n^m$ the set of all cyclic cacti on n vertices with matching number m. In this paper, we determine the distance spectral radius of graphs among $\mathscr{C}_n^m$. The corresponding extremal graphs are identified.

2. Preliminaries

Recall that the spectral radius of a non-negative irreducible matrix increases when an entry increases [25, p. 38]. Thus, we have the following lemma.

Lemma 2.1 [28]**.** *Let G be a connected graph with two nonadjacent vertices $u, v \in V_G$. Then $\rho(G + uv) < \rho(G)$.*

A *chain* in a graph G is a cycle C in G, such that $G - E_C$ has exactly $|V_C|$ components. A *generalized closed necklace* is a graph with a chain. The length of the chain is just the length of the cycle C.

Let G be consisted of a connected subgraph H and pendant graphs $G^i (1 \le i \le k)$ of order t_i , where $V_{G^i} \cap V_H = \{v_i\}$. Vertex v_i is called the *root* of the graph G^i on H. If $t_i \ge 2$, then G^i is called a nontrivial attaching graph to H with root v_i. If $V_{G^i} = \{v_i\}$, then G^i is called a trivial attaching graph to H. If in addition G^i is a subtree of G, then G^i is called a pendant tree to H of G.

From [8], we get the following useful lemmas.

Lemma 2.2 [8]**.** *Let G be a generalized closed necklace with a chain of odd length l where $l \ge 5$. If G' is the graph obtained from G by identifying three consecutive vertices on that chain, one of which has degree at least three, and creating two new pendant vertices at the identified vertex, then $\rho(G') < \rho(G)$.*

Lemma 2.3 [8]**.** *Let G be a generalized closed necklace with a chain of even length. If G' is the graph obtained from G by identifying two adjacent vertices on that chain, one of which has degree at least three, and creating a new pendant vertex at the identified vertex, then $\rho(G') < \rho(G)$.*

Lemma 2.4 [8]**.** *Let G be a graph with a clique K_s satisfying that $G - E_{K_s}$ has exactly s components. Let G^1 and G^2 be two nontrivial components of $G - E_{K_s}$ such that $u \in V_{K_s} \cap V_{G^1}$ and $v \in V_{K_s} \cap V_{G^2}$. If $G' = G - \sum_{w \in N_{G^2}(v)} vw + \sum_{w \in N_{G^2}(v)} uw$, then $\rho(G') < \rho(G)$.*

Further on we need the following lemmas.

Lemma 2.5 [10]**.** *Let B be a real symmetric $n \times n$ matrix and λ an eigenvalue of B with an eigenvector $\mathbf{x}$ all of whose entries are nonnegative. If $S_i(B) (1 \le i \le n)$ is the ith row sum of B, then*

$$\min_{1 \le i \le n} S_i(B) \leqslant \lambda \leqslant \max_{1 \le i \le n} S_i(B).$$

Moreover, if the row sums of B are not all equal and if all entries of x are positive, then both inequalities above are strict.

Lemma 2.6 [32]**.** *Let G be a connected graph and σ an automorphism of G. If $\mathbf{x}$ is the distance Perron vector of G, then $\sigma(u) = v$ leads to $x_u = x_v$.*

Lemma 2.7 [11]**.** *$\rho(C_n) = \frac{n^2}{4}$ if n is even; $\rho(C_n) = \frac{n^2-1}{4}$ if n is odd.*