Ordering n-vertex cacti with matching number q by their spectral radii

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ORDERING \( n \)-VERTEX CACTI WITH MATCHING NUMBER \( q \) BY THEIR SPECTRAL RADII

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Abstract. A connected graph \( G \) is a cactus if any two of its cycles have at most one common vertex. Denote by \( \mathcal{C}_{n,q} \) the set of \( n \)-vertex cacti with matching number \( q \). Huang, Deng and Simić [23] identified the unique graph with the maximum spectral radius among \( 2q \)-vertex cacti with perfect matchings. In this paper, as a continuance of it, the largest and second largest spectral radii together with the corresponding graphs among \( \mathcal{C}_{n,q} \) are determined. Consequently, the first two largest spectral radii together with cacti having perfect matchings are also determined.

Mathematics Subject Classification (2010): 05C50, 15A18.
Key words: Cactus, spectral radius, matching number.

1. Introduction. We consider only simple graphs (i.e. finite, undirected graphs without loops or multiple edges). Let \( G = (V_G, E_G) \) be a simple graph on \( n \) vertices and \( m \) edges (so \( n = |V_G| \) is its order, and \( m = |E_G| \) is its size), and let \( A_G \) be its adjacency matrix. Since \( A_G \) is symmetric, its eigenvalues are real. Without loss of generality, we can write them as \( \lambda_1(G) \geq \lambda_2(G) \geq \cdots \geq \lambda_n(G) \), and call them the eigenvalues of \( G \). The characteristic polynomial of \( G \) is just \( \det(xI - A_G) \), denoted by \( \phi(G;x) \) (or \( \phi(G) \) for short). The largest eigenvalue \( \lambda_1(G) \) is called the spectral radius of \( G \), denoted by \( \rho(G) \). If \( G \) is connected, then \( A_G \) is irreducible and by the Perron-Frobenius theory of non-negative matrices (see [10]), \( \rho(G) \) has multiplicity one and there exists a unique positive unit eigenvector corresponding to \( \rho(G) \). We shall refer to such an eigenvector as the Perron vector of \( G \). Its components can be considered as the vertex weights of \( G \). We call \( G \) a cactus if any two of its cycles have at most one common vertex.

Throughout we denote by \( P_n \), \( S_n \) and \( C_n \) the path, star and cycle on \( n \) vertices, respectively. \( G - v \), \( G - uv \) denote the graph obtained from \( G \) by deleting vertex

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\( v \in V_G \), or edge \( uv \in E_G \), respectively (this notation is naturally extended if more than one vertex or edge is deleted). Similarly, \( G + v \) and \( G + uv \) are obtained from \( G \) by adding vertex \( v \notin V_G \) or edge \( uv \notin E_G \), respectively (note, if a vertex \( v \) is added to \( G \), then its neighbours in \( G \) should be specified somehow). For \( v \in V_G \), let \( N_G(v) \) (or \( N(v) \) for short) denote the set of all the adjacent vertices of \( v \) in \( G \).

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 \( G \). Let \( M \) be a matching of \( G \). The vertex \( v \) in \( G \) is \( M \)-saturated if \( v \) is incident with an edge in \( M \); 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 matching number \( q \) of \( G \) is the cardinality of a maximum matching of \( G \). Denoted by \( \mathcal{C}_{n,q} \) the set of cacti with \( n \) vertices and matching number \( q \).

The spectrum of a graph arises in a variety of applications in organic chemistry, where the energy levels of certain molecules (such as polycyclic hydrocarbons) are essentially the eigenvalues of the graph of molecule [28]. It also plays an important role in modelling virus propagation in networks [24]. It is well known that the spectrum of a graph does provide a wealth of information about the graph. The spectral radius of a graph is an important invariant related to the structure. The investigation of the spectral radii of graphs is an important topic in the theory of graph spectra, and it is directly related with several parameters (the chromatic number, cut edges, cut vertices, pendants, diameter, maximal degree and the clique number, etc.) of graph; see [1, 10, 14, 15, 19, 27, 31, 30].

Recently, the problem concerning maximal spectral radii of graph(s) with perfect matching (resp. maximum matching) has attracted much attention in the literature. Feng, Yu and Zhang [13] determined the spectral radius of graphs with a given matching number. Chang and Xu [6, 32], respectively, studied the spectral radius of trees with perfect matchings, while Chang [5] determined the bounds on the second largest eigenvalue of a tree with a perfect matching. Chang and Tian [7] studied the spectral radius of unicyclic graphs with perfect matching, whereas Chang, Tian and Yu [8] studied the spectral radius of bicyclic graphs with perfect matchings. Geng and one of the present authors [17] characterized the spectral radius of tricyclic graphs with perfect matchings. Hou and Li [22] studied the spectral radius of trees with a given matching number; while Yu and Tian [33, 34] studied the spectral radius of unicyclic graphs (resp. bicyclic graphs) each with a given size of maximal matching. Geng and one of the present authors studied the spectral radius of tricyclic graphs with a maximum matching; see [16]. On the other hand, cacti are a class of polycyclic graphs in which any two of its cycles have at most one common vertex and studied extensively [2, 9, 18, 31, 26]. Motivated by these facts, we will generalize the results to the polycyclic graphs.

In this paper, we will determine the first and second largest spectral radii together with the corresponding graphs among cacti with \( n \) vertices and matching number \( q \).

2. Preliminaries. Let \( T_v^{s,t} \) (resp. \( H_t^s \)) denote the \( n \)-vertex tree (resp. cactus) as shown in Figure 1, where \( s \) and \( t \) are nonnegative integers satisfying \( 2s + t + 1 = n \).
$G_1$-$G_6$ are $n$-vertex graphs as depicted in Figure 2, which will be used in this section and the subsequent sections. It is easy to see that each of them is in $\mathcal{C}_{n,q}$.

Further on we will need the following lemmas.

**Lemma 2.1.** ([10, 29]) Let $G$ be a simple graph. Denote by $\mathcal{C}(v)$ (resp. $\mathcal{C}(e)$) the set of all cycles in $G$ containing a vertex $v$ (resp. an edge $e=uv$). Then

\[
\phi(G) = x\phi(G-v) - \sum_{w \in N_G(v)} \phi(G-v-w) - 2 \sum_{Z \in \mathcal{C}(v)} \phi(G-V_Z); \quad (1)
\]

\[
\phi(G) = \phi(G-e) - \phi(G-u-v) - 2 \sum_{Z \in \mathcal{C}(e)} \phi(G-V_Z). \quad (2)
\]

We assume that $\phi(G) = 1$ if $G$ is the empty graph (i.e. with no vertices).

**Lemma 2.2.** Let $G$ and $G'$ be two graphs.

(i) If $G'$ is a proper spanning subgraph of a connected graph $G$, then $\phi(G';x) > \phi(G;x)$ for $x \geq \rho(G)$ (see ([25])).
(ii) If $\phi(G''; x) > \phi(G; x)$ for $x \geq \rho(G)$, then $\rho(G) > \rho(G')$ (see ([10, 11])).

**Lemma 2.3.** ([27, 30]) Let $G$ be a connected graph. Suppose that $u, v \in V$ and $v_1, v_2, \ldots, v_s \in N(v) \setminus N(u) (1 \leq s \leq d(v))$ and $x = (x_{v_1}, x_{v_2}, \ldots, x_{v_n})^T$ is the Perron vector of $A_G$, where $x_{v_i}$ corresponds to the vertex $v_i (1 \leq i \leq n)$. Let $G^*$ be the graph obtained from $G$ by deleting the edges $uu_i$ and adding the edges $uv_i (1 \leq i \leq s)$. If $x_u > x_v$, then $\rho(G) < \rho(G^*)$.

**Proof.** We use $x_u$ and $x_v$ to denote the components of the Perron vector of $G$ corresponding to $u$ and $v$. Suppose that $N(u) = \{v, v_1, \ldots, v_s\}$ and $N(v) = \{u, u_1, \ldots, u_t\}$. Since $e = uv$ is a non-pendant edge of $G$, it follows that $s, t \geq 1$.

If $x_u \geq x_v$, let $G' = G - \{vv_1, \ldots, vv_t\} + \{uu_1, \ldots, uu_t\}$; otherwise, let $G'' = G - \{vv_1, \ldots, vv_t\} + \{uv_1, \ldots, uv_s\}$. Obviously, $G' \cong G^* \cong G''$. By Lemma 2.3, we have $\rho(G) < \rho(G^*)$, as desired.

**Lemma 2.5.** Given a connected graph $G$ as depicted in Figure 3, where $uv \in E_G, N(u) \cap N(v) = \emptyset$ and $d_G(u), d_G(v) \geq 3$. Let $G^*$ be the graph obtained from $G$ by deleting the edges $uv, uu_0$ and $vv_0$, identifying $u$ with $v$, and adding a new edge and a path of length 2 to $u$; see Figure 3. Then $\rho(G) < \rho(G^*)$.

![Graphs G and G*](image)

**Figure 3: Graphs G and G*.**

**Proof.** We use $x_u$ and $x_v$ to denote the components of the Perron vector of $G$ corresponding to $u$ and $v$. Suppose that $N(u) = \{v, u_0, u_1, \ldots, u_t\}$, $N(v) = \{u, v_0, v_1, \ldots, v_t\}$. Note that $d_G(u), d_G(v) \geq 3$, it follows that $s \geq 1, t \geq 1$.

If $x_u \geq x_v$, let $G' = G - \{vv_1, vv_2, \ldots, vv_t\} + \{uu_1, uu_2, \ldots, uu_t\}$; otherwise, let $G'' = G - \{uu_1, uu_2, \ldots, uu_t\} + \{uv_1, uv_2, \ldots, uv_s\}$. Obviously, $G' \cong G^* \cong G''$. Thus, by Lemma 2.3, we have $\rho(G) < \rho(G^*)$, as required.

**Remark 1.** We refer to the procedures of obtaining $G^*$ from $G$, described in Lemmas 2.4 and 2.5, as Operation I and Operation II on the graph $G$, respectively.

**Lemma 2.6.** Let $H_1$ and $H_2$ be the graphs as depicted in Figure 4, where $H$ is a connected graph with at least two vertices. Then $\rho(H_1) < \rho(H_2)$.
By direct calculation, we have \( \phi(P_2) = x^2 - 1 \). By direct computing (based on Equation (2)) we get
\[
\phi(H_1) = (x^4 - 3x^2 + 1)\phi(H) - (2x^3 + 2x^2 - 2x)\phi(H - u), \\
\phi(H_2) = (x^4 - 2x^2 + 1)\phi(H) - (3x^3 + 2x^2 - 3x - 2)\phi(H - u).
\]
This gives
\[
\phi(H_1) - \phi(H_2) = (x^3 - x - 2)\phi(H - u) - x^2\phi(H).
\]
As \( H - u \) is a proper subgraph of \( H \), by Lemma 2.2(i), we have \( \phi(H - u) > \phi(H) \) for any \( x \geq \rho(H_2) > \rho(H) \). Note that \( x^3 - x - 2 > x^2 \) holds for \( x > \rho(H_2) > \rho(C_3) = 2 \). Hence, for any \( x > \rho(H_2) \), we have \( \phi(H_1) > \phi(H_2) \). Then by Lemma 2.2(ii), we have \( \rho(H_1) < \rho(H_2) \).

This completes the proof. \( \square \)

**Lemma 2.7.** Let \( H_{q-1}^{n-2q+1} \) and \( G_1 \) be the \( n \)-vertex graphs as depicted in Figure 1 and Figure 2, respectively. Then we have \( \rho(G_1) < \rho(H_{q-1}^{n-2q+1}) \).

**Proof.** Consider the Perron-vector \( \mathbf{x} = (x_{v_0}, x_{v_1}, x_{v_2}, \ldots, x_{v_{n-1}})^T \) of \( A_{G_1} \). If \( x_{v_0} \geq x_{v_2} \), let \( G' = G_1 - v_2v_3 + v_0v_3 \); otherwise, let
\[
G^* = G_1 - \{v_0v_i | v_i \in N(v_0) \setminus \{v_1, v_2\}\} + \{v_2v_i | v_i \in N(v_0) \setminus \{v_1, v_2\}\}.
\]
Obviously, \( G' \cong H_{q-1}^{n-2q+1} \cong G^* (q \geq 1) \). Then by Lemma 2.3, we have \( \rho(G_1) < \rho(H_{q-1}^{n-2q+1}) \), as desired. \( \square \)

**Lemma 2.8.** Let \( G_1, G_2, G_3 \) and \( G_5 \) be the \( n \)-vertex graphs as shown in Figure 2, then \( \rho(G_i) < \rho(G_1) \) holds for \( i = 2, 3, 5 \).

**Proof.** It is easy to see that \( G_2 \) is a proper subgraph of \( G_1 \). Hence, by Lemma 2.2, we have \( \rho(G_2) < \rho(G_1) \).

Consider the Perron-vector \( \mathbf{x} = (x_{v_0}, x_{v_1}, x_{v_2}, \ldots, x_{v_{n-1}})^T \) of \( A_{G_3} \). If \( x_{v_0} \geq x_{v_2} \), then let \( G' = G_3 - v_2v_3 + v_0v_3 \); otherwise, let \( G'' = G_3 - \{v_0w | w \in N(v_0) \setminus \{v_1\}\} + \{v_2w | w \in N(v_0) \setminus \{v_1\}\} \).
Lemma 2.9. Let $G_1$ and $G_4$ be the $n$-vertex graphs as shown in Figure 2 with $n \geq 2q + 1$, then $\rho(G_4) < \rho(G_1)$.

Proof. Consider the Perron-Vector $x = (x_{v_0}, x_{v_1}, x_{v_2}, \ldots, x_{v_{n-1}})^T$ of $A_{G_4}$. If $x_{v_2} \geq x_{v_3}$, let $G' = G_4 - \{v_3\} + \{v_2\}$; otherwise, let $G' = G_4$. Obviously, $G' \cong G''$. In view of Lemma 2.3, we get $\rho(G_3) < \rho(G_1)$.

By carrying Operation I on the edge $v_2v_3$, we may transform $G_5$ into $G_1$. In view of Lemma 2.4, we have $\rho(G_5) < \rho(G_1)$.

This completes the proof. □

Lemma 2.10. Let $G_1$ and $G_6$ be the $n$-vertex graphs as shown in Figure 2 with $n \geq 6, q \geq 3$, then $\rho(G_6) \leq \rho(G_1)$ with equality if and only if $n = 6, q = 3$.

Proof. When $n = 6, q = 3$, $G_6 \cong G_1$. For $n \geq 7, q \geq 3$, by direct computing (based on Equations (1) and (2)), we have $\phi(H_1^n) = x^4 - 4x^2 - 2x + 1$ and

\[
\phi(G_6) = x\phi(G_6 - v_0) - (n - 2q + 1)x^{n-2q}\phi(P_2)^{q-3}\phi(H_1^n)
\]

\[
- 2q - 3)x^{n-2q+2}\phi(P_2)^{q-4}\phi(H_1^n) - \phi(G_6 - v_0 - v_1) - \phi(G_6 - v_0 - v_2)
\]

\[
- 2(q - 3)x^{n-2q+1}\phi(P_2)^{q-4}\phi(H_1^n) - 2\phi(G_6 - v_0 - v_1 - v_2)
\]

\[
= x^{n-2q+2}\phi(P_2)^{q-3}\phi(H_1^n) - (n - 2q + 1)x^{n-2q}\phi(P_2)^{q-3}\phi(H_1^n)
\]

\[
- 2(q - 3)x^{n-2q+2}\phi(P_2)^{q-4}\phi(H_1^n) - x^{n-2q+1}\phi(P_2)^{q-3}\phi(C_3)
\]

\[
- x^{n-2q+2}\phi(P_2)^{q-2} - 2(q - 3)x^{n-2q+1}\phi(P_2)^{q-4}\phi(H_1^n) - 2x^{n-2q+1}\phi(P_2)^{q-2}
\]

\[
x^{n-2q}\phi(P_2)^{q-4}[x^2(x^2 - 1)(x^4 - 4x^2 - 2x + 1)
\]

\[- (n - 2q + 1)(x^2 - 1)(x^4 - 4x^2 - 2x + 1) - (2q - 6)x^2(x^4 - 4x^2 - 2x + 1)
\]

\[- x(x^2 - 1)(x^3 - 3x - 2) - x^3(x^2 - 1)^2 - (2q - 6)x(x^4 - 4x^2 - 2x + 1)
\]

\[- 2x(x^2 - 1)^2].
\]

Similarly, we have

\[
\phi(G_1) = x^{n-2q}\phi(P_2)^{q-3}[x(x^3 - 2x)(x^2 - 1) - (n - 2q)(x^2 - 2)(x^2 - 1)
\]

\[- (2q - 4)x(x^3 - 2x) - (x^2 - 1)^2 - x^3(x^2 - 1) - 2x(x^2 - 1)
\]

\[- (2q - 4)(x^3 - 2x)].
\]
Together with Equation (2), we have
\[ \phi(G_6) - \phi(G_1) = \phi(P_2)^q - x^{n-2q}(x+1)^3[(n-6)x-n+2q]. \]

Note that \( n \geq 7 \), hence \( g(x) = (n-6)x-n+2q \) is increasing for \( x \geq \rho(G_1) \geq 2.3028 > 2 \). Thus, \( g(x) > g(2) > 0 \). It follows that \( \phi(G_6) > \phi(G_1) \) for \( x \geq \rho(G_1) > 2 \). Then by Lemma 2.2(ii), we have \( \rho(G_1) > \rho(G_6) \). \( \square \)

3. Main results. In this section, we determine the spectral radius of graphs in \( \mathcal{C}_{n,q} \). The corresponding graphs are also characterized.

**Theorem 3.1.** Let \( G \) be a cactus in \( \mathcal{C}_{n,q} \) with \( q \geq 2 \). Then

\[ \rho(G) \leq \begin{cases} 
  r_1, & n \neq 2q+1; \\
  r_2, & n = 2q+1 
\end{cases} \tag{3a, 3b} \]

where \( r_1 \) and \( r_2 \) are, respectively, the largest roots of the equations

\[
\begin{align*}
  f(x) &= x^4 - nx^2 - 2(q-1)x + n - 2q + 1 = 0, \\
  g(x) &= x^3 - (2q+1)x - 2q = 0.
\end{align*}
\]

The equality in (3a) holds if and only if \( G \cong H_{q-1}^{n-2q+1} \), whereas the equality holds in (3b) if and only if \( G \cong H_q^0 \).

**Proof.** We choose \( G \in \mathcal{C}_{n,q} \) such that the spectral radii of \( G \) is as large as possible. Let \( x = (x_{v_1}, x_{v_2}, \ldots, x_{v_n})^T \) be the Perron vector of \( A_G \).

Let \( M \) be a maximum matching of \( G \). Then \( |M| = q \) and there are three cases for a non-pendant edge \( e = uv \) in \( G \): (1) \( e = uv \) is an \( M \)-saturated edge; (2) \( e = uv \) has exactly one \( M \)-saturated vertex; (3) \( e = uv \) is not an \( M \)-saturated edge but both \( u \) and \( v \) are \( M \)-saturated vertices. Now the following facts play a crucial role:

**Fact 1.** All cycles of \( G \) are of length 3.

**Proof.** We assume, on the contrary, that there exists a cycle, say \( C^0 = v_0v_1 \ldots v_{l-1}v_0 \), in \( G \) such that its length is greater than 3, that is \( l \geq 4 \).

If there exits an edge on \( C^0 \) of case (1) or (2), by taking Operation I once, we may get a new graph \( G' \) such that \( \rho(G) < \rho(G') \), a contradiction to the choice of \( G \).

Thus, all edges on \( C^0 \) are of case (3). Hence, \( v_i (i = 0, 1, 2, \ldots, l-1) \) is adjacent to a vertex \( p_i \), respectively, such that \( v_i p_i \in M \) and \( p_i \neq v_{i-1}, p_i \neq v_{i+1} \) (if \( i = l-1, v_{i+1} = v_0; \) if \( i = 0, v_{i-1} = v_{l-1} \)). Let

\[ G' = \begin{cases} 
  G - v_2v_3 + v_1v_3, & \text{if } x_{v_1} \geq x_{v_2}; \\
  G - v_1v_0 + v_2v_0, & \text{if } x_{v_1} < x_{v_2}.
\end{cases} \]

By Lemma 2.3, we have \( \rho(G) < \rho(G') \), a contradiction to the choice of \( G \).

This completes the proof of Fact 1. \( \square \)
FACT 2. If \( G \) contains a pendant tree attached to a vertex on some cycle of \( G \), then the pendant tree is a star.

Proof. On the contrary, suppose that the pendant tree \( T_{k_0} \) attached to \( v_{k_0} \) is not a star. Hence, there must exist a path \( P' \) of length 2 in \( T_{k_0} \) and \( v_{k_0} \) is an end-vertex of \( P' \). Let \( P' = v_{k_0}u_1u_2 \). Obviously, \( G + v_{k_0}u_2 \in \mathcal{C}_{n,q} \). By Lemma 2.2, we have \( \rho(G) < \rho(G + v_{k_0}u_2) \), a contradiction. This completes the proof. \( \square \)

FACT 3. Any two cycles of \( G \) have a common vertex.

Proof. Assume to the contrary, there are two cycles, say \( C^1 \) and \( C^2 \), have no common vertex. Then, there exists a path \( P = v_1v_2 \ldots v_p \) of length \( p - 1 \) \((p \geq 2)\) connecting \( C^1 \) and \( C^2 \), where \( V_P \cap V_{C^1} = \{v_1\} \) and \( V_P \cap V_{C^2} = \{v_p\} \). In view of Fact 1, let \( C^1 = v_1w_1w_2v_1, C^2 = v_pw_1u_2v_p \). In what follows we show that there exists a \( q \)-matching, say \( M' \), such that \( \{w_1v_1, w_2v_1, u_1v_p, u_2v_p\} \cap M' = \emptyset \). Here we only show that \( \{w_1v_1, w_2v_1\} \cap M' = \emptyset \). Similarly, we can also show that \( \{u_1v_p, u_2v_p\} \cap M' = \emptyset \), which is omitted here.

In fact, if \( w_1v_1, w_2v_1 \notin M \), let \( M' := M \), then our result holds. Otherwise, without loss of generality, we assume that \( w_2v_1 \in M \). First we consider that \( w_1 \) is not saturated by \( M \). Let \( M' := M - w_2v_1 + w_1w_2 \). It is easy to see that \( M' \) is a \( q \)-matching of \( G \) and \( \{w_1v_1, w_2v_1\} \cap M' = \emptyset \) holds in this case. Now we consider that \( w_1 \) is saturated by \( w_1t_1 \) in \( M \). Note that in this case, \( d_G(w_1) \geq 3 \).

If \( x_{w_1} \geq x_{v_1} \), then let \( G' = G - \{v_1x : x \in N_G(v_1) \setminus \{w_1, w_2\}\} + \{w_1x : x \in N_G(v_1) \setminus \{w_1, w_2\}\} \). It is easy to see that \( G' \in \mathcal{C}_{n,q} \). By Lemma 2.3, \( \rho(G) < \rho(G') \), a contradiction.

If \( x_{w_1} < x_{v_1} \), then let \( G' = G - \{v_1x : x \in N_G(v_1) \setminus \{w_2, v_1\}\} + \{v_1x : x \in N_G(v_1) \setminus \{w_2, v_1\}\} \). In this case, \( G' \) contains a \( q \)-matching \( M' := M - w_2v_1 - w_1t_1 + w_1w_2 + v_1t_1 \). Hence, \( G' \in \mathcal{C}_{n,q} \). By Lemma 2.3, \( \rho(G) < \rho(G') \), a contradiction.

Thus, we obtain that there exists a \( q \)-matching \( M' \) of \( G \) such that \( w_1v_1, w_2v_1, u_1v_p, u_2v_p \) are not in \( M' \). Let

\[
G'' = \begin{cases} G - \{v_1w_1, v_1w_2\} + \{v_pw_1, v_pw_2\}, & \text{if } x_{v_p} > x_{v_1}; \\ G - \{v_pu_1, v_pu_2\} + \{v_1u_1, v_1u_2\}, & \text{otherwise}. \end{cases}
\]

It is routine to check that \( G'' \in \mathcal{C}_{n,q} \). By Lemma 2.3, \( \rho(G) < \rho(G'') \), a contradiction.

This completes the proof of Fact 3. \( \square \)

By Facts 1 and 3, each of the cycles contained in \( G \) is of length 3 and all the cycles contained in \( G \) have just one vertex in common. Denote the common vertex by \( v_0 \).

FACT 4. If \( G \) contains pendant tree(s), then all the pendant trees are attached to \( v_0 \).
Proof. Based on Fact 2 we assume, on the contrary, that there exists a cycle, say $v_0v_1v_2v_0$, in $G$ such that $v_1$ (resp. $v_2$) is adjacent to $i$ (resp. $j$) pendant vertices, where $i, j \geq 0$ and $i + j \geq 1$.

**Case 1.** $i \geq 1, j = 0$ or $i = 0, j \geq 1$. Here we only consider the former, similarly we may consider the latter, which is omitted here.

- There exists a pendant edge, say $v_1v_1'$, attached to $v_1$ being in $M$. If $x_{v_0} \geq x_{v_1}$, then let $G' = G - \{v_1x : x \in N_G(v_1) \setminus \{v_0, v_2\}\} + \{v_0x : x \in N_G(v_1) \setminus \{v_0, v_2\}\}$. Set $M' := M - v_2v_0 + v_1v_2$ if $v_2v_0 \in M$ and $M' := M - v_1v_1' + v_1v_2$ otherwise. It is easy to see that $M'$ is a $q$-matching of $G'$. By Lemma 2.3, $\rho(G) < \rho(G')$, a contradiction. If $x_{v_0} < x_{v_1}$, then let $G' = G - \{v_0x : x \in N_G(v_0) \setminus \{v_1, v_2\}\} + \{v_1x : x \in N_G(v_0) \setminus \{v_1, v_2\}\}$. Set $M' := M$ if $v_0$ is not saturated by $M$ or $v_0$ is saturated by $v_0v_2$ and $M' := M - v_1v_1' + v_0v_2$ otherwise. It is easy to see that $M'$ is a $q$-matching of $G'$. By Lemma 2.3, $\rho(G) < \rho(G')$, a contradiction.

- Each of the pendant edges attached to $v_1$ is not in $M$. If $x_{v_0} \geq x_{v_1}$, then let $G' = G - \{v_1x : x \in N_G(v_1) \setminus \{v_0, v_2\}\} + \{v_0x : x \in N_G(v_1) \setminus \{v_0, v_2\}\}$. It is easy to see that $G' \notin \mathcal{E}_{n,q}$. By Lemma 2.3, $\rho(G) < \rho(G')$, a contradiction. So we consider $x_{v_0} < x_{v_1}$ in what follows. In this subcase, let $G' = G - \{v_0x : x \in N_G(v_0) \setminus \{v_1, v_2\}\} + \{v_1x : x \in N_G(v_0) \setminus \{v_1, v_2\}\}$ and $M' := M - v_1v_2 + v_0v_2$ if $v_1v_2 \in M$ and $M' := M$ otherwise. It is obvious that $M'$ is a $q$-matching of $G'$. By Lemma 2.3, $\rho(G) < \rho(G')$, a contradiction.

**Case 2.** $i, j \geq 2$. Without loss of generality, we assume that $x_{v_1} \geq x_{v_2}$. It is easy to see that there exists a pendant edge, say $v_2v_2'$, such that $v_2v_2' \notin M$. Let $G' = G - v_2v_2' + v_1v_2'$, its routine to check that $M$ is also a $q$-matching of $G'$. Hence, $G' \notin \mathcal{E}_{n,q}$. By Lemma 2.3, $\rho(G) < \rho(G')$, a contradiction.

**Case 3.** $i \geq 2, j = 1$ or $i = 1, j \geq 2$. Here we only consider the former, similarly we may consider the latter, which is omitted here. In fact, it is easy to see that there exists a pendant edge, say $v_1v_1'$, not in $M$. Denote the only pendant edge attached to $v_2$ by $v_2v_2'$. Let $G_1 = G - v_2v_2' + v_1v_2'$ if $x_{v_1} \geq x_{v_2}$ and $G_1' = G - v_1v_1' + v_2v_2'$ if $x_{v_1} < x_{v_2}$.

- $v_2v_2' \notin M$. It is easy to see that $G_1 \notin \mathcal{E}_{n,q}$. By Lemma 2.3, $\rho(G) < \rho(G_1)$, a contradiction.

- $v_2v_2' \in M$. In this subcase, if $v_1$ is saturated by $v_0v_1 \in M$, then let $M' := M - \{v_2v_2', v_1v_0\} + \{v_1v_1', v_2v_0\}$. Hence, $M'$ is a $q$-matching of $G_1$. By Lemma 2.3, $\rho(G) < \rho(G_1)$, a contradiction. If $v_1$ is saturated by a pendant edge, say $v_1v_1'$, in $M$, then let $G' = G_1' + v_1v_1'$, which contains $M' := M - \{v_2v_2', v_1v_1'\} + \{v_1v_1', v_2v_2'\}$ as its $q$-matching. It is easy to see that $\rho(G) < \rho(G_1') < \rho(G')$, a contradiction.

**Case 4.** $i = j = 1$. Let $v_1v_1'$ (resp. $v_2v_2'$) be the only pendant edge attached to $v_1$ (resp. $v_2$).

- $v_1v_1', v_2v_2' \notin M$. By a similar discussion as in the proof of Case 2, there exists a graph $G'$ in $\mathcal{E}_{n,q}$ such that $\rho(G) < \rho(G')$, a contradiction.
It is easy to see that $M$ and $\rho_1$ are both in $M$. Let $G' = G - \{v_1'v_1', v_2'v_2\} + \{v_0v_1', v_0v_2', v_1v_2'\}$ and $M' := M - \{v_1'v_1', v_2'v_2\} + \{v_1v_1', v_2v_2\}$. It is easy to see that $M'$ is a $q$-matching of $G'$ and $\rho(G) < \rho(G')$, a contradiction.

- $v_1v_1' \in M$, $v_2v_2' \notin M$, or $v_1v_1' \notin M$, $v_2v_2' \in M$. Here we only consider the former and omit the procedure for the latter. If $x_{v_1} \geq x_{v_2}$, let $G' = G - v_2v_2' + v_1v_1'$. It is easy to see that $G'$ is in $\mathcal{C}_{n,q}$ and $\rho(G) < \rho(G')$, a contradiction. If $x_{v_1} < x_{v_2}$, let $G' = G - v_1v_1' + v_2v_2'$. Furthermore, if $v_2v_0 \notin M$, it is easy to see that $G'$ is in $\mathcal{C}_{n,q}$ and $\rho(G) < \rho(G')$, a contradiction. If $v_2v_0 \in M$, then let $M' := M - v_2v_0 + v_1v_0$. Obviously, $M'$ is a $q$-matching of $G'$. Hence, by Lemma 2.3, $\rho(G) < \rho(G')$, a contradiction.

This completes the proof of Fact 4.

Hence, in view of Facts 1–4 and Lemma 2.2, we have $G \cong H_n^{q-1} + 1$ if $n \neq 2q + 1$; and $G \cong H_0^n$ if $n = 2q + 1$.

By direct computing (based on Lemma 2.1), we get

\[
\phi(H_n^{q-1} + 1) = x^{2q-2q+1} - 2(q-1)x + n - 2q + 1, \\
\phi(H_0^n) = (x^2 - 1)^q - 1 - (2q + 1)x - 2q.
\]

It is easy to see that $\rho(H_n^{q-1} + 1), \rho(H_0^n) > 1$, hence our results hold immediately.

This completes the proof of Theorem 3.1.

**Theorem 3.2.** Let $G$ be a cactus in $\mathcal{C}_{n,q}$ with $q \geq 2$. Then

(i) If $G \in \mathcal{C}_{n,q} \setminus \{H_n^{q-1} + 1\}$ with $n \neq 2q + 1$. Then $\rho(G) \leq r_3$, the equality holds if and only if $G \cong G_1$ (see Figure 1), where $r_3$ is the largest root of the equation

\[
h_1(x) = x^5 - x^4 - nx^3 + (n - 2q + 2)x^2 + (2n - 5)x - (2n - 4q + 1) = 0. (6)
\]

(ii) If $G \in \mathcal{C}_{n,q} \setminus \{H_0^n\}$ with $n = 2q + 1$. Then $\rho(G) \leq \min\{r_4, r_5\}$, the equality holds if and only if $G \cong H_0^{q-1}$ or $H_4$ (see Figure 5), where $r_4, r_5$ are, respectively, the largest roots of equations

\[
h_2(x) = x^3 - 2q + 2 = 0, \quad (7)
\]
\[
h_3(x) = x^5 - 2q^2 + 2q^3 + (2q + 2)x^2 + (6q + 6)x - 2q = 0. (8)
\]

**Proof.** (i) For any graph $G \in \mathcal{C}_{n,q} \setminus \{H_n^{q-1} + 1\}$, by the proof of Theorem 3.1, it is easy to see that $G$ can be transformed into $H_n^{q-1} + 1$ by carrying Operation I and Operation II, and applying Lemmas 2.2, 2.3 and 2.6, repeatedly.

In $\mathcal{C}_{n,q} \setminus \{H_n^{q-1} + 1\}$, let $\mathcal{X}$ denote the set of cacti which can be transformed into $H_n^{q-1} + 1$ by applying Lemma 2.2 once; let $\mathcal{Y}$ denote the set of cacti which can be transformed into $H_n^{q-2q+1}$ by applying Lemma 2.3 once. Note that by applying Operation II (resp. Lemma 2.5) once, we can not transform any graph into
Thus, from Lemmas 2.2-2.4, the cacti with the second largest spectral radius in $\mathcal{C}_{n,q}$ must be in $\mathcal{A} \cup \mathcal{D}$.

From the definition of $\mathcal{A}$, we know that $\mathcal{A} = \{G_2\}$. And by Lemma 2.8, we have $\rho(G_2) < \rho(G_1)$.

For any $G \in \mathcal{D}$, from the definition of $\mathcal{D}$, $G$ must be isomorphic to $G_4$, $G_5$, $\langle i, j \rangle G_{s,t}(s, t)$ (see Figure 5) with $i \geq 1, j \geq 1, s = 0$ or $t = 0, i + j = q - 1, s + t = n - 2q$; or $\langle i, j \rangle \tilde{G}_{s,t}(s, t)$ (see Figure 5) with $i \geq 0, j \geq 0, s \geq 0, t \geq 0, i + j = q - 2, s + t = n - 2q + 1, i + s \neq 0, j + t \neq 0$.

If $G \cong G_4$ (resp., $G \cong G_5$), by Lemma 2.9 (resp., Lemma 2.8), we have $\rho(G) < \rho(G_1)$; if $G \cong \langle i, j \rangle G_{s,t}(s, t)$ with $i \geq 1, j \geq 1, s = 0$ or $t = 0, i + j = q - 1, s + t = n - 2q$, without loss of generality, suppose that $s = 0$. By applying Lemma 2.3, we may transform $G$ into $G_3$ such that $\rho(G) \leq \rho(G_3)$ with the equality if and only if $G \cong G_3$. Then by Lemma 2.8, we have $\rho(G) < \rho(G_3) < \rho(G_1)$.

Finally we consider $G \cong \langle i, j \rangle \tilde{G}_{s,t}(s, t)$ with $i \geq 0, j \geq 0, s \geq 0, t \geq 0, i + j = q - 2, s + t = n - 2q + 1, i + s \neq 0, j + t \neq 0$.

If $i = 0$, then $j = q - 2$, $s \geq 1$. Suppose that $x_{v_1} \geq x_{v_2}$, by Lemma 2.3, we may transform $G$ into $G_6$ such that $\rho(G) < \rho(G_6)$. Together with Lemma 2.10, we have $\rho(G) < \rho(G_6) < \rho(G_1)$. So we consider that $x_{v_1} < x_{v_2}$. By Lemma 2.3, we transform $G$ into $G_1$ such that $\rho(G) < \rho(G_1)$ with the equality if and only if $s = 1$, i.e. $G \cong G_1$.

Similarly, if $j = 0$, we have $\rho(G) < \rho(G_1)$ with the equality if and only if $G \cong G_1$.

If $i \geq 1, j \geq 1$, applying Lemma 2.3, we can transform $G$ into $G_6$ such that $\rho(G) \leq \rho(G_6)$ with the equality if and only if $G \cong G_6$. In view of Lemma 2.10, we have $\rho(G) < \rho(G_6) < \rho(G_1)$.

Now we consider $G \cong \langle i, j \rangle G_{s,t}(s, t)$ with $i \geq 1, j \geq 1, s = 0$ or $t = 0, i + j = q - 1, s + t = n - 2q$, or $G \cong G_4$. By a similar discussion as the proof of $G \in \mathcal{D}$, we as well get $\rho(G) < \rho(G_1)$.

Note that $\rho(G_1) > 1$, hence in view of Equation (3) and by an elementary calculation, we know that $\rho(G_1)$ is the largest root of the equation $h_1(x) = 0$ in (6).

(ii) For any graph $G \in \mathcal{C}_{2q+1,q} \setminus \{H_q^0\}$, by the proof of Theorem 3.1, it is easy to see that $G$ can be transformed into $H_q^0$ by carrying Operation I and Operation II, and applying Lemmas 2.2, 2.3 and 2.6, repeatedly.
In \(\mathcal{C}_{2q+1,q}\setminus\{H_q^0\}\), let \(\mathcal{A}'\) denote the set of cacti which can be transformed into \(H_q^0\) by applying Lemma 2.2 once; and let \(\mathcal{D}'\) denote the set of cacti which can be transformed into \(H_q^0\) by applying Lemma 2.3 once. Note that by applying Operation I (resp. Operation II, Lemma 2.5) once, we can not transform any graph into \(H_q^0\). Thus, from Lemmas 2.2 and 2.3, the cacti with the second largest spectral radius in \(\mathcal{C}_{2q+1,q}\) must be in \(\mathcal{A}' \cup \mathcal{D}'\).

From the definition of \(\mathcal{A}'\), we know that \(\mathcal{A}' = \{H_{2q-1}^0, H_3\}\). Note that we can transform \(H_3\) into \(H_{2q-1}^0\) by carrying Operation I once. By Lemma 2.4, we have \(\rho(H_3) < \rho(H_{2q-1}^0)\). From the definition of \(\mathcal{D}'\), we get that \(\mathcal{D}' = \{H_4\}\).

Thus, for any \(G \in \mathcal{C}_{2q+1,q}\setminus\{H_q^0\}\), we have \(\rho(G) \leq \min\{\rho(H_{2q-1}^0), \rho(H_4)\}\). By direct computing (based on Lemma 2.1), we have

\[
\phi(H_4) = (x^2 - 1)^q - 2x^4 + (2q + 2)x^3 + (6q + 6)x - 2q,
\]

\[
\phi(H_{2q-1}^0) = x(x^2 - 1)^q - 2x(x^3 - 2q - 2q + 2).
\]

Note that \(\rho(H_4), \rho(H_{2q-1}^0) > 1\), hence by an elementary calculation, we have \(\rho(H_4), \rho(H_{2q-1}^0)\) are, respectively, the largest roots of the equations (7) and (8).

This completes the proof of Theorem 3.2. \(\square\)

In [23], the unique graph with the maximum spectral radius among 2q-vertex cacti with perfect matchings was characterized. According to Theorems 3.1 and 3.2 in this paper, the unique graph with the largest (resp. the second largest) eigenvalue among 2q-vertex cacti with perfect matchings are also determined.

**Corollary 3.3.** If \(G\) is a 2q-vertex cactus graph with perfect matchings \(q \geq 2\), then

(i) \(\rho(G) < \rho(G_1) < \rho(H_{q-1}^1)\), for any \(G \notin \{H_{q-1}^1, G_1\}\);

(ii) \(\rho(G_1)\) is the largest root of the equation \(p(x) = 0\) and \(\rho(H_{q-1}^1)\) is the largest root of equation \(q(x) = 0\), where

\[
p(x) = x^5 - x^4 - 2qx^3 + 2x^2 + (4q - 5)x - 1,
\]

\[
q(x) = x^3 - x^2 - (2q - 1)x + 1.
\]

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**References**


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