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ON THE NON-BACKTRACKING SPECTRAL RADIUS OF GRAPHS*

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Abstract. Given a graph G with $m \geq 1$ edges, the non-backtracking spectral radius of G is the spectral radius of its non-backtracking matrix $B(G)$ defined as the $2m \times 2m$ matrix where each edge uv is represented by two rows and two columns, one per orientation: (u, v) and (v, u), and the entry of $B(G)$ in row (u, v) and column (x, y) is given by $\delta_{vx}(1 - \delta_{uy})$, with δ_{ij} being the Kronecker delta. A tight upper bound is given for the non-backtracking spectral radius in terms of the spectral radius of the adjacency matrix and minimum degree, and those connected graphs that maximize the non-backtracking spectral radius are determined if the connectivity (edge connectivity, bipartiteness, respectively) is given.

Key words. Non-backtracking matrix, Non-backtracking spectral property, Non-backtracking spectral radius, Non-backtracking walk.

AMS subject classifications. 05C50, 15A18.

1. Introduction.

Non-backtracking walks in a graph have been studied in several contexts, including finding a Moore bound for irregular graphs [2], mixing times [1], and Alon's second eigenvalue conjecture [8]. Let G be a graph with vertex set $V(G)$ and edge set $E(G)$. For a vertex v of G, denote by $N_G(v)$ the set of neighbors of v, and $d_G(v)$ the degree of v, i.e., $d_G(v) = |N_G(v)|$. A vertex v of a graph G is a pendant vertex if $d_G(v) = 1$. A non-backtracking walk in a graph G is a walk $v_1 \ldots v_k$ in G such that $v_{j+1} \neq v_{j-1}$ for all j with $2 \leq j \leq k - 1$.

Given a graph G with at least one edge, the non-backtracking-directed graph $\widehat{G}$ of G is a directed graph whose vertices are the directed edges obtained by replacing each edge uv of G by two directed edges (u, v) and (v, u) and there is a directed edge from (u, v) to (x, y) in $\widehat{G}$ if and only if $x = v$ and $u \neq y$. A non-backtracking walk $v_1 \ldots v_k$ in G corresponds naturally to an equivalent walk $e_1 \ldots e_{k-1}$ in $\widehat{G}$, where $e_j = (v_j, v_{j+1})$ for $j = 1, \ldots, k-1$. The non-backtracking matrix $B(G) = (b_{(u,v),(x,y)})$ of a graph G is defined to be the adjacency matrix of $\widehat{G}$. That is,

$$b_{(u,v),(x,y)} = \begin{cases} 1 & \text{if } v = x \text{ and } u \neq y, \\ 0 & \text{otherwise,} \end{cases}$$

where $(u, v), (x, y) \in V(\widehat{G})$. The non-backtracking matrix of a graph is indexed by its directed edges and can be used to count non-backtracking walks of a given length. Denote by $A(G)$ the adjacency matrix of G. As the entries of powers of the adjacency matrix, $A(G)^\ell$, count the number of walks of length ℓ from one vertex to another, the entries of $B(G)^\ell$ count the number of non-backtracking walks of length ℓ from one vertex to another in $\widehat{G}$, or the number of non-backtracking walks of $\ell + 1$ directed edges from one directed edge to another in $\widehat{G}$.

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For a graph G, denote by $D(G)$ the diagonal degree matrix of G. We use I_n to denote the unit matrix of order n. The spectrum of the non-backtracking matrix is called the non-backtracking spectrum of the graph. In the literature, the non-backtracking spectral properties received much attention. For instance, the non-backtracking spectrum of a graph may be computed from Ihara's Theorem [12, 13, 18]. Here we use an equivalent form.

Theorem 1.1 (Ihara's Theorem). *Let G be a graph with n vertices and m edges, where $m \geq 1$. Then,*

$$\det(\lambda I_{2m} - B(G)) = (\lambda^2 - 1)^{m-n} \det(\lambda^2 I_n - \lambda A(G) + D(G) - I_n).$$

The non-backtracking spectrum of regular graphs may be completely determined by Ihara's Theorem. Kotani and Sunada [13] determined the non-backtracking spectrum of bipartite biregular graphs. Angel et al. [3] studied the non-backtracking spectral properties of the universal cover of a graph. More related work may be found in [16, 20]. Very recently, Glover and Kempton [9] showed how to obtain eigenvectors of the non-backtracking matrix in terms of eigenvectors of a smaller matrix and gave an expression for the eigenvalues of the non-backtracking matrix in terms of the eigenvalues of the adjacency matrix and nonorthogonal eigenvectors of the adjacency matrix and a smaller matrix when they exist.

For a square real matrix M, let $\rho(M)$ denote the spectral radius of M, that is, the maximum modulus of the eigenvalues of M. Suppose that M is nonnegative. Then, the spectral radius $\rho(M)$ is also called the maximal eigenvalue of M in [15]. By the well-known Perron-Frobenius theorem for nonnegative matrices, $\rho(M)$ is an eigenvalue of M, and if M is irreducible, then there is a unique positive eigenvector of M associated with $\rho(M)$ up to a multiplicative constant, see Theorems 4.1, 4.2 and 4.3 in [15, pp. 11–14]. For a graph G, the spectral radius of $A(G)$ is known as the adjacency spectral radius of G, which is denoted by $\rho_A(G)$, and the spectral radius of $B(G)$ is called the non-backtracking spectral radius of G, which is denoted by $\rho_B(G)$.

We present a sharp upper bound of the non-backtracking spectral radius of a graph in terms of the adjacency spectral radius and determine the unique graphs with maximum non-backtracking spectral radius among graphs with fixed vertex connectivity, fixed edge connectivity, and fixed number of pendant vertices, respectively.

2. Preliminaries.

For a real square matrix M, denote by $\sigma(M)$ the spectrum of M.

Let G be a graph of order n. Define

$$X(G) = \begin{pmatrix} A(G) & D(G) - I_n \\ -I_n & O \end{pmatrix}.$$

Then, $\det(\lambda I_{2n} - X(G)) = \det(\lambda^2 I_n - \lambda A(G) + D(G) - I_n)$. So, for a graph G on $n \geq 4$ vertices with $m \geq n$ edges, we have by Theorem 1.1 that $\sigma(X(G)) \subseteq \sigma(B(G))$.

In the following, we use $\rho_X(G)$ to denote $\rho(X(G))$.

For a graph G, denote by $\delta(G)$ the minimum degree of G and $\Delta(G)$ the maximum degree of G.

The proofs of Lemmas 2.1, 2.2 and 2.3 appear in [9], see Proposition 5.2 (i) and (ii), Proposition 2.3, Lemma 5.6 in [9], respectively.

Lemma 2.1. *Let G be a graph. Then, every eigenvector of $X(G)$ associated with $\mu \in \sigma(X(G))$ is of the form* $\begin{pmatrix} -\mu \mathbf{y} \\ \mathbf{y} \end{pmatrix}$, *and $1 \in \sigma(X(G))$.*

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Lemma 2.2. *Let G be a connected graph that is not a cycle and $\delta(G) \geq 2$. Then, $B(G)$ is irreducible.*

Lemma 2.3. *Let G be a connected graph that is not a cycle and $\delta(G) \geq 2$. For an eigenvector of $X(G)$ with the form $\begin{pmatrix} -\rho_X(G)\mathbf{y} \\ \mathbf{y} \end{pmatrix}$ associated with $\rho_X(G)$, $\mathbf{y}$ can be chosen to be positive.*

Lemma 2.4. *Let G be a graph G on $n \geq 4$ vertices with $m \geq n$ edges. Then, $\rho_B(G) = \rho_X(G) \in \sigma(X(G))$.*

Proof. As $m \geq n$, we have by Lemma 2.1 that $1 \in \sigma(X(G)) \subseteq \sigma(B(G))$. So, by Theorem 1.1, each positive eigenvalue of $B(G)$ is also an eigenvalue of $X(G)$. By Perron-Frobenius Theorem, $\rho_B(G)$ is a positive eigenvalue of $B(G)$. Therefore, we have $\rho_B(G) = \rho_X(G) \in \sigma(X(G))$. □

For two disjoint graphs G and H, let $G \cup H$ be the graph with vertex set $V(G) \cup V(H)$ and edge set $E(G) \cup E(H)$, $G \vee H$ be the graph obtained from $G \cup H$ by adding edges between each vertex of G and each vertex of H.

For a set V_1 of vertices of a graph G with $\varnothing \neq V_1 \neq V(G)$, we denote by $G - V_1$ the graph obtained from G by deleting all vertices of V_1, and $G[V_1]$ the subgraph of G induced by V_1. Similarly, for a set E_1 of edges of a graph G, we denote by $G - E_1$ the graph obtained from G by deleting all edges of E_1.

Let S_n and K_n be the star and complete graph on n vertices, respectively. Let $K_{a,b}$ be the complete bipartite graph with two partite sets of cardinalities a and b.

For a graph H, denote by $P(H)$ the set of vertices of degree one in H. Let G be a connected graph with at least one cycle and at least one vertex of degree one. Let $G_0 = G$ and $G_{i+1} = G_i - P(G_i)$ for $i \geq 1$. Then, there is a smallest $s \geq 1$ with $P(G_s) = \varnothing$, so the minimum degree of G_s is at least two, and every vertex lies on some cycle in G_s. We call G_s the 2-core of G, denoted by $C(G)$.

The following lemma follows from previous works that vertices outside the 2-core of a graph (which includes the vertices of degree one) do not affect the non-zero part of the non-backtracking spectrum, see [19, Corollary 3.3]. For completeness, however, we include a proof here.

If G is a nontrivial tree, then $\rho_B(G) = 0$.

Lemma 2.5. *Let G be a connected graph. Suppose that G is not a tree and v is a vertex of degree one in G. Then, $\rho_B(G) = \rho_B(G - v)$, so $\rho_B(G) = \rho_B(C(G))$.*

Proof. Let u be the neighbor of v in G. Then, each entry of the row of $B(G)$ corresponding to (u, v) is 0. In the submatrix of B by deletion of row and column corresponding to (u, v), each entry of the column corresponding to (v, u) is zero. Let $m = |E(G)|$. Then,

$$\det(\rho I_{2m} - B(G)) = \rho^2 \det(\rho I_{2(m-1)} - B(G - v)).$$

So $\rho_B(G) = \rho_B(G - v)$, which implies that $\rho_B(G) = \rho_B(C(G))$. □

The follow lemma is Theorem 5.1 in [15, p. 19], which serves as part of Perron-Frobenius theorem.

Lemma 2.6 ([15, p. 19]). *The spectral radius of an irreducible nonnegative matrix is greater than the spectral radius of any its principal submatrix.*

Lemma 2.7. *Let G be a nontrivial connected graph with nonadjacent distinct vertices u and v. Then, $\rho_B(G) < \rho_B(G + uv)$.*

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Proof. Let $H = G + uv$. It is evident that the degree of u (v, respectively) is at least two in H. As G is connected, u, v must lie on some cycle in H.

By Lemma 2.5, we may assume that the minimum degree of H is at least two, as otherwise we may consider $C(H)$.

Suppose first that H is a cycle. Then, $\widehat{H}$ consists of two directed cycles, so $\rho_B(H) = 1$. Note that $G = H - uv$ is a path, so $\rho_B(G) = 0$. It thus follows that $\rho_B(G) < \rho_B(H)$.

Suppose next that H is not a cycle. By Lemma 2.2, $B(H)$ is irreducible. As $\widehat{G}$ is obtained from $\widehat{H}$ by removing two vertices (u, v) and (v, u) together with incident directed edges, $B(G)$ is a principal submatrix of $B(H)$. By Lemma 2.6, we have $\rho_B(G) < \rho_B(H)$. ∎

The follow lemma is part of Theorem 1.1 in [15, p. 24].

LEMMA 2.8. *Let $M = (m_{ij})$ be an $n \times n$ nonnegative matrix. Let R_j be the j-th row sum for $j = 1, \dots, n$. Then,*

$$\min\{R_j : j = 1, \dots, n\} \le \rho(M) \le \max\{R_j : j = 1, \dots, n\}.$$

3. Bounding the spectral radius of the non-backtracking matrix. First, we present an upper bound on the spectral radius of the non-backtracking matrix using the adjacency spectral radius.

First, we recall some known facts. For a graph G with minimum degree δ, $\rho_A(G) \ge \delta$ by Lemma 2.8, so $\rho_A(G)^2 \ge \delta^2 \ge 4(\delta - 1)$. If G is connected and H is an induced subgraph of G, then $\rho_A(H) \le \rho_A(G)$ with equality if and only if $H = G$. This follows from the interlacing theorem or the Perron-Frobenius theorem.

THEOREM 3.1. *Let G be a nontrivial connected graph with minimum degree δ. Then,*

$$\rho_B(G) \le \frac{\rho_A(G) + \sqrt{\rho_A(G)^2 - 4(\delta - 1)}}{2},$$

with equality if and only if G is regular and $\delta \ge 2$.

Proof. Suppose that $\delta \ge 2$. It is trivial if G is a cycle. Suppose that G is not a cycle. Then, $\rho_B(G) \ge \delta - 1 \ge 1$. Let $n = |V(G)|$ and $m = |E(G)|$. By Theorem 1.1 and Lemma 2.1, $\det(\lambda I_{2m} - B(G)) = (\lambda^2 - 1)^{m-n} \det(\lambda I_{2n} - X(G))$ and $1 \in \sigma(X(G))$. So $\rho_B(G) = \rho_X(G)$.

By Lemma 2.3, we may choose a positive $\mathbf{y}$ for the eigenvector $\begin{pmatrix} -\rho_X(G)\mathbf{y} \\ \mathbf{y} \end{pmatrix}$. So

$$\rho_X(G)^2\mathbf{y} - \rho_X(G)A(G)\mathbf{y} + (D(G) - I_n)\mathbf{y} = 0. \tag{3.1}$$

As G is connected, $A(G)$ is irreducible, so we have by the Perron-Frobenius theorem that there is a positive eigenvector $\mathbf{x}$ such that $A(G)\mathbf{x} = \rho_A(G)\mathbf{x}$. Since both $\mathbf{x}$ and $\mathbf{y}$ are positive, we have $\mathbf{x}^\top\mathbf{y} > 0$. Left-multiplying by $\mathbf{x}^\top$ for (3.1), we have

$$\rho_X(G)^2\mathbf{x}^\top\mathbf{y} - \rho_X(G)\mathbf{x}^\top A(G)\mathbf{y} + \mathbf{x}^\top(D(G) - I_n)\mathbf{y} = 0,$$

i.e.,

$$\rho_X(G)^2\mathbf{x}^\top\mathbf{y} - \rho_X(G)\rho_A(G)\mathbf{x}^\top\mathbf{y} + \mathbf{x}^\top(D(G) - I_n)\mathbf{y} = 0.$$

As both $\mathbf{x}$ and $\mathbf{y}$ are positive, we have

$$\mathbf{x}^\top(D(G) - I_n)\mathbf{y} \ge \mathbf{x}^\top(\delta - 1)I_n\mathbf{y} = (\delta - 1)\mathbf{x}^\top\mathbf{y},$$

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with equality if and only if G is regular. It follows that

$$\rho_X(G)^2 - \rho_A(G)\rho_X(G) + \delta - 1 \leq 0,$$

with equality if and only if G is regular. Recall that $\rho_A(G)^2 \geq \delta^2 \geq 4(\delta - 1)$. Then,

$$\rho_X(G) \leq \frac{\rho_A(G) + \sqrt{\rho_A(G)^2 - 4(\delta-1)}}{2},$$

with equality if and only if G is regular. That is,

$$\rho_B(G) \leq \frac{\rho_A(G) + \sqrt{\rho_A(G)^2 - 4(\delta-1)}}{2},$$

with equality if and only if G is regular.

Next, suppose that $\delta = 1$. If G is a tree, then $\rho_B(G) = 0$, and $\rho_A(G) \geq \delta = 1$, so the result follows. Suppose that G is not a tree. As $C(G)$ is an induced subgraph, we have $\rho_A(C(G)) \leq \rho_A(G)$. By Lemma 2.5 and the result in Case 1, we have

$$\begin{aligned}
\rho_B(G) &= \rho_B(C(G)) \\
&\leq \frac{\rho_A(C(G)) + \sqrt{\rho_A(C(G))^2 - 4(\delta(C(G)) - 1)}}{2} \\
&< \rho_A(C(G)) \\
&\leq \rho_A(G) \\
&= \frac{\rho_A(G) + \sqrt{\rho_A(G)^2 - 4(\delta-1)}}{2}.
\end{aligned}$$

This completes the proof. □

We remark that the upper bound for the non-backtracking spectral radius in the above theorem has already been reported by Glover and Kempton in [9] under the technical condition that

$$\rho_A(G) \geq 2\sqrt{\mathbf{x}^\top (D(G) - I_n)\mathbf{y}},$$

where $\mathbf{x}$ and $\mathbf{y}$ are the eigenvectors in the proof.

Though the vertices of degree one in a graph do not affect the non-backtracking spectral radius, we still evaluate the case when the minimum degree is one. This is because the vertices of degree one in a graph affect the adjacency spectral radius and we are working on a upper bound on the non-backtracking spectral radius in terms of the adjacency spectral radius.

Corollary 3.2. *Let G be a connected graph that is not a tree. Then,*

$$\rho_B(G) \leq \frac{\rho_A(C(G)) + \sqrt{\rho_A(C(G))^2 - 4(\delta(C(G)) - 1)}}{2},$$

with equality if and only if $C(G)$ is regular.

Proof. By Lemma 2.5, $\rho_B(G) = \rho_B(C(G))$. The result follows by applying Theorem 3.1 to $C(G)$. □

As pointed out in [9], upper bounds for the adjacency spectral radius lead to upper bounds for the non-backtracking spectral radius by Theorem 3.1.

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Corollary 3.3. *Let G be a connected graph with $n \geq 2$ vertices, m edges, and minimum degree δ. Then,*

$$\rho_B(G) \leq \frac{\sqrt{2m-n+1}+\sqrt{2m-n-4\delta+5}}{2},$$

with equality if and only if G is the complete graph with $n \geq 3$.

Proof. The result follows from Theorem 3.1 as

$$\rho_A(G) \leq \sqrt{2m-n+1},$$

with equality if and only if G is the star or the complete graph [11]. ◻

Corollary 3.4. *Let G be a connected graph with $n \geq 2$ vertices, m edges, maximum degree Δ, and minimum degree δ. Let $a = 2m - \delta(n-1)$. Then,*

$$\rho_B(G) \leq \frac{\sqrt{a+(\delta-1)\Delta}+\sqrt{a+(\delta-1)(\Delta-4)}}{2},$$

with equality if and only if G is a regular graph with $n \geq 3$.

Proof. The result follows from Theorem 3.1 as

$$\rho_A(G) \leq \sqrt{2m-\delta(n-1)+(\delta-1)\Delta},$$

with equality if and only if G is a regular graph [5]. ◻

4. Maximizing the non-backtracking spectral radius over classes of graphs with fixed parameters. Let M, N, P, and Q be respectively $p \times p$, $p \times q$, $q \times p$, and $q \times q$ matrices, where Q is invertible. It is well known that

$$\det \begin{pmatrix} M & N \\ P & Q \end{pmatrix} = \det Q \, \det(M - NQ^{-1}P). \tag{4.2}$$

Let $J_{s,t}$ be the $s \times t$ all-one matrix. We write J_s for $J_{s \times s}$.

Let G be a connected graph that is not complete. By a vertex cut of G, we mean a set S of vertices of G such that $G - S$ is disconnected. The connectivity $\kappa(G)$ is the cardinality of a minimum vertex cut. If $G \cong K_n$, then $\kappa(G)$ is defined to be $n-1$. It is evident that $\kappa(G) \leq n-2$ if G is a connected graph that is not complete.

Theorem 4.1. *Over all connected graphs on n vertices with connectivity κ, where $n \geq 4$ and $1 \leq \kappa \leq n-2$, $K_\kappa \vee (K_{n-1-\kappa} \cup K_1)$ uniquely maximizes the non-backtracking spectral radius, which is equal to the largest real root of $\widetilde{f}_{n,\kappa}(t) = 0$, where*

$$\widetilde{f}_{n,\kappa}(t) = t^5 - t^4(n-4) - t^2(n^2-6n+\kappa^2-2\kappa+10) - t(\kappa^2-2\kappa+1) - \kappa n^2 + n^2 + 5\kappa n - 5n - 6\kappa + 6.$$

Proof. Suppose that G is a connected graph on n vertices with connectivity κ that maximizes the non-backtracking spectral radius.

Denote by S a vertex cut of G with $|S| = \kappa$. Then, $G - S$ is not connected. Let G_1 be a component of $G - S$ and let $G_2 = G[V(G) \setminus (S \cup V(G_1))]$. By Lemma 2.7, adding edges to a connected graph increases the non-backtracking spectral radius, so $G[S]$, G_1 and G_2 are all complete. Assume that $|V(G_1)| \geq |V(G_2)|$.

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Let $a=|V(G_1)|$. Then, $G\cong K_\kappa\vee(K_a\cup K_{n-\kappa-a})$, where $\frac{n-\kappa}{2}\le a\le n-\kappa-1$. With respect to the vertex set partition $V(G)=S\cup V(G_1)\cup V(G_2)$, we have

$$A(G)=\begin{pmatrix} J_\kappa-I_\kappa & J_{\kappa,a} & J_{\kappa,n-a-\kappa}\\ J_{a,\kappa} & J_a-I_a & O\\ J_{n-a-\kappa,\kappa} & O & J_{n-a-\kappa}-I_{n-a-\kappa}\end{pmatrix},$$

and

$$D(G)=\begin{pmatrix}(n-1)I_\kappa & O & O\\ O & (\kappa+a-1)I_a & O\\ O & O & (n-a-1)I_{n-a-\kappa}\end{pmatrix}.$$

By Lemma 2.4, we have $\rho_B(G)=\rho_X(G)\in\sigma(X(G))$. To determine $\rho_B(G)$, we calculate the characteristic polynomial of $X(G)$. Applying (4.2) and the definition of $X(G)$, we have

$$\begin{aligned}\det(\rho I_{2n}-X(G))&=\det(\rho I_n)\det\left(\rho I_n-A(G)-(D(G)-I_n)\cdot\left(\rho^{-1}I_n\right)\cdot(-I_n)\right)\\&=\rho^n\det\left(\rho I_n-A(G)+\rho^{-1}(D(G)-I_n)\right).\end{aligned}$$

So, it suffices to calculate $\det\left(\rho I_n-A(G)+\rho^{-1}(D(G)-I_n)\right)$. Let $b=n-a-\kappa$. Then,

$$\begin{aligned}&\det\left(\rho I_n-A(G)+\rho^{-1}(D(G)-I_n)\right)\\&=\det\begin{pmatrix}\frac{\rho^2+\rho+n-2}{\rho}I_\kappa-J_\kappa & -J_{\kappa,a} & -J_{\kappa,b}\\ -J_{a,\kappa} & \frac{\rho^2+\rho+\kappa+a-2}{\rho}I_a-J_a & O\\ -J_{b,\kappa} & O & \frac{\rho^2+\rho+n-a-2}{\rho}I_b-J_b\end{pmatrix}.\end{aligned}$$

Subtracting the k-th row from the 1-st, …, $(\kappa-1)$-th row, respectively, adding the 1-st, …, $(\kappa-1)$-th column to the κ-th column, and expanding the resulted determinant according to the first $\kappa-1$ rows, we have

$$\begin{aligned}&\det\left(\rho I_n-A(G)+\rho^{-1}(D(G)-I_n)\right)\\&=\left(\frac{\rho^2+\rho+n-2}{\rho}\right)^{\kappa-1}\det\begin{pmatrix}\frac{\rho^2+\rho+n-2}{\rho}-\kappa & -J_{1,a} & -J_{1,b}\\ -\kappa J_{a,1} & \frac{\rho^2+\rho+\kappa+a-2}{\rho}I_a-J_a & O\\ -\kappa J_{b,1} & O & \frac{\rho^2+\rho+n-a-2}{\rho}I_b-J_b\end{pmatrix}.\end{aligned}$$

Similarly, we have

$$\begin{aligned}&\det\left(\rho I_n-A(G)+\rho^{-1}(D(G)-I_n)\right)\\&=\left(\frac{\rho^2+\rho+n-2}{\rho}\right)^{\kappa-1}\left(\frac{\rho^2+\rho+\kappa+a-2}{\rho}\right)^{a-1}\left(\frac{\rho^2+\rho+n-a-2}{\rho}\right)^{b-1}\\&\quad\times\det\begin{pmatrix}\frac{\rho^2-\rho(\kappa-1)+n-2}{\rho} & -a & -(n-a-\kappa)\\ -\kappa & \frac{\rho^2-\rho(a-1)+\kappa+a-2}{\rho} & 0\\ -\kappa & 0 & \frac{\rho^2-\rho(n-a-\kappa-1)+n-a-2}{\rho}\end{pmatrix}.\end{aligned}$$

So

$$\begin{aligned}&\det\left(\rho I_n-A(G)+\rho^{-1}(D(G)-I_n)\right)\\&=\left(\frac{\rho^2+\rho+n-2}{\rho}\right)^{\kappa-1}\left(\frac{\rho^2+\rho+\kappa+a-2}{\rho}\right)^{a-1}\left(\frac{\rho^2+\rho+n-a-2}{\rho}\right)^{b-1}\rho^{-3}(\rho-1)f_a(\rho).\end{aligned}$$

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where

$$f_a(\rho) = \rho^5 - \rho^4(n-4) + \rho^3(a-1)(n-a-\kappa-1) - \rho^2(n^2 - a\kappa n - 6n + \kappa n + a\kappa^2 + a^2\kappa - 3\kappa + 10) \\ - \rho(n^2 - an^2 + a^2 n - 4n + 3an + a\kappa^2 + a^2\kappa - 3a\kappa - 3a^2 + 4) + (n-2)(a-n+2)(a+\kappa-2).$$

Now it follows that

$$\begin{aligned}\det(\rho I_{2n} - X(G)) &= \rho^n \det\left(\rho I_n - A(G) + \rho^{-1}(D(G) - I_n)\right) \\ &= (\rho^2+\rho+n-2)^{\kappa-1}(\rho^2+\rho+\kappa+a-2)^{a-1}(\rho^2+\rho+n-a-2)^{n-a-\kappa-1}(\rho-1)f_a(\rho).\end{aligned}$$

From the expression for the characteristic polynomial of $X(G)$, we see that the spectrum of $X(G)$ consists of 1 with multiplicity 1, $\frac{-1\pm i\sqrt{4n-9}}{2}$ with multiplicity $\kappa-1$, $\frac{-1\pm i\sqrt{4\kappa+4a-9}}{2}$ with multiplicity $a-1$, $\frac{-1\pm i\sqrt{4(n-a)-9}}{2}$ with multiplicity $b-1$ and the roots of $f_a(\rho)=0$. By a simple calculation, the maximum modulus of eigenvalues of $X(G)$ different from the roots of $f_a(\rho)=0$ is $\left|\frac{-1-i\sqrt{4n-9}}{2}\right| = \sqrt{n-2}$. So $\rho_B(G) \geq \sqrt{n-2}$ and $\rho_B(G) = r_a$, where $\rho = r_a$ is the largest real root of $f_a(\rho)=0$.

Suppose that $a < n-\kappa-1$. From the above expression for $f_a(\rho)$, we have

$$f_a(\rho) - f_{a+1}(\rho) = (\rho^3 + \kappa\rho^2 + n\rho + \kappa\rho - 3\rho - n + 2)(2a+\kappa-n+1) > 0,$$

for $\rho \geq \sqrt{n-2}$. So

$$f_{a+1}(r_a) = -\left(f_a(r_a) - f_{a+1}(r_a)\right) < 0.$$

This, together with the fact $f_{a+1}(\rho) \geq 0$ for $\rho \geq r_{a+1}$, implies that $r_{a+1} > r_a$. This is a contradiction. It thus follows that $a = n-\kappa-1$. That is, $G \cong K_\kappa \vee (K_{n-1-\kappa} \cup K_1)$. Let $\widetilde{f}_{n,\kappa}(t) = f_{n-\kappa-1}(t)$. Then, $\rho_B(G)$ is the largest real root of $\widetilde{f}_{n,\kappa}(t) = 0$. ∎

Let G be a nontrivial connected graph. An edge cut of G is a set E' of edges such that $G - E'$ is disconnected. The edge connectivity $\lambda(G)$ of G is the cardinality of a minimum edge cut, and we define $\lambda(K_1) = 0$.

It is well known that $\lambda(G) \leq \delta(G)$ for any graph G. So, for a connected graph G on n vertices, we have $\lambda(G) \leq n-1$ with equality if and only if G is complete.

Theorem 4.2. *Over all connected graphs on n vertices with edge connectivity λ, where $n \geq 4$ and $1 \leq \lambda \leq n-2$, $K_\lambda \vee (K_{n-1-\lambda} \cup K_1)$ uniquely maximizes the non-backtracking spectral radius, which is equal to the largest real root of $\widetilde{f}_{n,\lambda}(t) = 0$, where*

$$\widetilde{f}_{n,\lambda}(t) = t^5 - t^4(n-4) + t^2(-n^2 + 6n - \lambda^2 + 2\lambda - 10) - t(\lambda-1)^2 - n^2\lambda + n^2 + 5n\lambda - 5n - 6\lambda + 6.$$

Proof. From the proof of Theorem 4.1, $\rho_B(K_\lambda \vee (K_{n-1-\lambda} \cup K_1))$ is the largest real root of $\widetilde{f}_{n,\lambda}(t) = 0$. As

$$\widetilde{f}_{n,\lambda}(n-3) = -\lambda(n-2)(n-3)(\lambda-1) \leq 0,$$

one has $\rho_B(K_\lambda \vee (K_{n-1-\lambda} \cup K_1)) \geq n-3$.

Suppose that G is a connected graph on n vertices with edge connectivity λ that maximizes the non-backtracking spectral radius. As the edge connectivity of $K_\lambda \vee (K_{n-1-\lambda} \cup K_1)$ is λ, we have $\rho_B(G) \geq \rho_B(K_\lambda \vee (K_{n-1-\lambda} \cup K_1)) \geq n-3$.

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Note that $\lambda \leq \delta(G)$. Suppose that $\lambda < \delta(G)$. Let E_c be an edge cut with cardinality λ of G, and G_1 and G_2 be the components of $G - E_c$. Let $n_i = |V(G_i)|$ for $i = 1, 2$. By Lemma 2.7, we have $G_i \cong K_{n_i}$ for $i = 1, 2$. Assume that $n_1 \leq n_2$. If $n_1 \leq \lambda$, then there exists a vertex w in $V(G_1)$ such that

$$d_G(w) \leq n_1 - 1 + \frac{\lambda}{n_1} \leq (n_1 - 1)\frac{\lambda}{n_1} + \frac{\lambda}{n_1} = \lambda,$$

which is contradiction. If $n_1 = \lambda + 1$, then there exists a vertex w in $V(G_1)$ such that

$$d_G(w) \leq n_1 - 1 = \lambda,$$

which is also a contradiction. So $n_2 \geq n_1 \geq \lambda + 2$. Note that the maximum row sum of $B(G)$ is at most $n_2 - 2 + \lambda$. By Lemma 2.8, $\rho(B(G)) \leq n_2 - 2 + \lambda \leq n_2 - 2 + n_1 - 2 = n - 4 < \rho(B(G))$, which is a contradiction. Thus $\lambda = \delta(G)$.

Let u be a vertex of degree λ in G. Then, $\{uw : w \in N_G(u)\}$ is an edge cut of cardinality λ in G. By Lemma 2.7, we have $G - \{u\} \cong K_{n-1}$. So $G \cong K_\lambda \vee (K_{n-1-\lambda} \cup K_1)$. $\square$

The vertex bipartiteness of a graph G is the minimum number of vertices whose deletion from G results in a bipartite graph [7].

Theorem 4.3. *Over connected graphs on n vertices with vertex bipartiteness γ, where $n \geq 4$ and $1 \leq \gamma \leq n-2$, $K_\gamma \vee K_{\lceil (n-\gamma)/2 \rceil, \lfloor (n-\gamma)/2 \rfloor}$ uniquely maximizes the non-backtracking spectral radius, which is equal to the largest real root of $\widetilde{h}_{n,\gamma}(t) = 0$, where*

$$\begin{aligned}\widetilde{h}_{n,\gamma}(t) = &(2t^2 + t(n-k) + n + k - 2)^2(t - n + 2) + (2t^2 + t(n-k) + n + k - 2)(t(n-k)(n-k-2) + 1)\\ &+ (t^2 - 1)(t + \gamma) - 2,\end{aligned}$$

if $n - \gamma$ is odd, and

$$\widetilde{h}_{n,\gamma}(t) = (2t^2 + t(n-\gamma) + n + \gamma - 2)(t - n + 2) + t(n-\gamma)(n-\gamma-2),$$

if $n - \gamma$ is even.

Proof. Suppose that G is a connected graph on n vertices with bipartiteness γ that maximizes the non-backtracking spectral radius.

Let S be a subset of $V(G)$ with cardinality γ such that $G - S$ is a bipartite graph. Let U_1 and U_2 be the partite sets of $G - S$ of cardinalities a and $n - \gamma - a$, respectively. Suppose without loss of generality that $n - \gamma - a \leq a$. Then, $\frac{n-\gamma}{2} \leq a \leq n - \gamma - 1$. By Lemma 2.7, $G[S] \cong K_\gamma$ and $G[U_1 \cup U_2] = K_{a,n-\gamma-a}$, so $G \cong K_\gamma \vee K_{a,n-\gamma-a}$. With respect to the partition $V(G) = U \cup X \cup Y$, we have

$$A(G) = \begin{pmatrix} J_\gamma & J_{\gamma,a} & J_{\gamma,n-\gamma-a} \\ J_{a,\gamma} & O & J_{a,n-\gamma-a} \\ J_{n-\gamma-a,\gamma} & J_{n-\gamma-a,a} & O \end{pmatrix},$$

and

$$D(G) = \begin{pmatrix} (n-1)I_\gamma & O & O \\ O & (n-a)I_a & O \\ O & O & (a+\gamma)I_{n-\gamma-a} \end{pmatrix}.$$

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By Lemma 2.4, $\rho_B(G) = \rho_X(G) \in \sigma(X(G))$. By similar argument as in the proof of Theorem 4.1, we have

$$\begin{aligned}
\det(\rho I_{2n} - X(G)) &= \rho^n \det\left(\rho I_n - A(G) + \rho^{-1}(D(G) - I_n)\right) \\
&= \rho^n \det \begin{pmatrix} \left(\rho + 1 + \frac{n-2}{\rho}\right) I_\gamma - J_\gamma & -J_{\gamma,a} & -J_{\gamma,n-\gamma-a} \\ -J_{a,\gamma} & \left(\rho + \frac{n-a-1}{\rho}\right) I_a & -J_{a,n-\gamma-a} \\ -J_{n-\gamma-a,\gamma} & -J_{n-\gamma-a,a} & \left(\rho + \frac{\gamma+a-1}{\rho}\right) I_{n-\gamma-a} \end{pmatrix} \\
&= \rho^3 \left(\rho^2 + \rho + n - 2\right)^{\gamma-1} \left(\rho^2 + n - a - 1\right)^{a-1} \left(\rho^2 + n - \gamma - 1\right)^{n-\gamma-a-1} \\
&\quad \times \det \begin{pmatrix} \frac{\rho^2 - \rho(\gamma-1) + n - 2}{\rho} & -a & -(n-\gamma-a) \\ -\gamma & \frac{\rho^2 + n - a - 1}{\rho} & -(n-\gamma-a) \\ -\gamma & -a & \frac{\rho^2 + \gamma + a - 1}{\rho} \end{pmatrix} \\
&= \left(\rho^2 + \rho + n - 2\right)^{\gamma-1} \left(\rho^2 + n - a - 1\right)^{a-1} \left(\rho^2 + n - \gamma - 1\right)^{n-\gamma-a-1} (\rho - 1) h_a(\rho),
\end{aligned}$$

where

$$\begin{aligned}
h_a(t) = t^5 &- t^4(\gamma - 2) + t^3(-an - \gamma n + 2n + a^2 + a\gamma + \gamma^2 - 2) \\
&- t^2(2an + a\gamma n + 2\gamma n - 3n - a^2\gamma - 2a^2 - a\gamma^2 - 2a\gamma - 3\gamma + 4) \\
&- t((a + \gamma - 1)n^2 - (2a\gamma + a + \gamma + \gamma^2 + a^2 - 2)n + a^2\gamma + a^2 + a\gamma^2 + a\gamma + \gamma^2 - 1) \\
&- an^2 + n^2 - \gamma n^2 + a\gamma n - 3n + 2an + 3\gamma n + a^2 n - 2a^2 - 2a\gamma - 2\gamma + 2.
\end{aligned}$$

Then, the spectrum of $X(G)$ consists of 1 with multiplicity 1, $\frac{-1 \pm i\sqrt{4n-9}}{2}$ with multiplicity $\gamma - 1$, $\pm i\sqrt{n-a-1}$ with multiplicity $a-1$, $\pm i\sqrt{n-\gamma-1}$ with multiplicity $n-\gamma-a-1$, and the roots of $h_a(t) = 0$. By Lemma 2.4, $\rho_B(G)$ is the largest real eigenvalue of $X(G)$. As $\rho_B(G) \geq \left|\frac{-1 \pm i\sqrt{4n-9}}{2}\right| = \sqrt{n-2} > 1$, we have $\rho_B(G) = s_a$, where $t = s_a$ is the largest real root of $h_a(t) = 0$.

Suppose that $a \geq \lceil \frac{n-\gamma}{2} \rceil + 1$. Then,

$$h_{a-1}(t) - h_a(t) = -q(t)(2a + \gamma - n - 1),$$

where $q(t) = t^3 + t^2(\gamma + 2) + t(n - 1 - \gamma) + n - 2$. For $t \in [1, +\infty)$, as $q(t)$ is strictly increasing, one has

$$h_{a-1}(s_a) = h_{a-1}(s_a) - h_a(s_a) \leq -q(1)(2a + \gamma - n - 1) = -2n(2a + \gamma - n - 1) < 0.$$

This, together with the fact that $h_{a-1}(t) \geq 0$ for $t \geq s_{a-1}$, implies that $s_{a-1} > s_a$, which is a contradiction. Thus $a = \lceil \frac{n-\gamma}{2} \rceil$, i.e., $G \cong K_\gamma \vee K_{\lceil (n-\gamma)/2 \rceil, \lfloor (n-\gamma)/2 \rfloor}$.

Finally, we determine the value of $\rho_B(G)$.

If $n - \gamma$ is odd, then by above argument, $\rho_B(G)$ is the largest real root of $h_{\lceil (n-\gamma)/2 \rceil}(t) = 0$, or the largest real root of $\widetilde{h}_{n,\gamma}(t) = 0$ as $h_{\lceil (n-\gamma)/2 \rceil}(t) = \frac{1}{4}\widetilde{h}_{n,\gamma}(t)$. Suppose that $n - \gamma$ is even. Then, $\rho_B(G)$ is the largest real root of $h_{\lceil (n-\gamma)/2 \rceil}(t) = 0$, where

$$h_{\lceil (n-\gamma)/2 \rceil}(t) = \frac{1}{4}(2t^2 + t(n - \gamma) + n + \gamma - 2)\widetilde{h}_{n,\gamma}(t).$$

If $(n-\gamma)^2 < 8(n+\gamma-2)$, then the roots of $2t^2 + t(n-\gamma) + n + \gamma - 2 = 0$ are not real, and so by Lemma 2.4, $\rho_B(G)$ is the largest real root of $\widetilde{h}_{n,\gamma}(t) = 0$. If $(n-\gamma)^2 \geq 8(n+\gamma-2)$, then the roots, say t_1 and t_2 with $t_1 \leq t_2$ of $2t^2 + t(n-\gamma) + n + \gamma - 2 = 0$ are real and negative, and $\rho_B(G)$ is positive, so $\rho_B(G)$ is also the largest real root of $\widetilde{h}_{n,\gamma}(t) = 0$. $\square$

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THEOREM 4.4. *Let G be a connected graph on n vertices with p pendant vertices, where $n \geq 4$ and $1 \leq p \leq n-3$. Then, $\rho_B(G) \leq n-p-2$, with equality if and only if G' is a complete graph, where G' is obtained from G by deleting all pendant vertices.*

Proof. By Lemma 2.5, $\rho_B(G) = \rho_B(G')$. Thus, $\rho_B(G) \leq n-p-2$, with equality if and only if G' is a complete graph. ∎

5. Concluding remarks. In this paper, we gave tight upper bounds for the non-backtracking spectral radius for graphs with fixed connectivity, edge connectivity, and bipartiteness, respectively, and characterized the extremal graphs.

By Lemma 2.7, adding edges to a connected graph results in the increase of the non-backtracking spectral radius. This fact is also true for the adjacency spectral radius [17]. Because of this fact, one may think that graphs with certain conditions maximizing the non-backtracking spectral radius will be the same families that maximize the adjacency spectral radius. There are indeed such examples but it is not always the case.

From the results in [14] and Theorem 4.1, we find that $K_\kappa \vee (K_{n-1-\kappa} \cup K_1)$ uniquely maximizes both the adjacency and non-backtracking spectral radii among all connected graphs on n vertices with connectivity κ, where $n \geq 4$ and $1 \leq \kappa \leq n-2$. However, it should be noted that the adjacency spectral radius has no immediate connections with the non-backtracking spectral radius, so one cannot get the result on the non-backtracking spectral radius from the result on the adjacency spectral radius. We also note that quite different techniques are needed to maximize the adjacency spectral radius and non-backtracking spectral radius, respectively. In the literature, in showing that graphs maximizing the adjacency spectral radius have a particular structure, one supposes the graph does not have the structure and perform graft operations to obtain a graph for which the adjacency spectral radius is increased, and there are lots of graft operations, apart from adding edges [6, 17]. In the process, Perron-Frobenius theorem is important. In showing that graphs maximizing the non-backtracking spectral radius have a particular structure, one can use Lemma 2.7 only at present so that the graph has a roughly particular structure and then calculates the characteristic polynomial of an auxiliary but larger matrix $X(G)$ that is neither nonnegative nor symmetric and maximizes the largest real eigenvalue of this matrix by somewhat algebraic techniques.

There are families of graphs in which the graphs maximizing the adjacency spectral radius are different from the ones maximizing the non-backtracking spectral radius. We list some examples:

(i) among all trees of order $n \geq 2$, the star uniquely maximizes the adjacency spectral radius, while all trees have non-backtracking spectral radius 0;
(ii) among all unicyclic graphs of order $n \geq 3$, the graph formed from the star by adding an edge uniquely maximizes the adjacency spectral radius, while all unicyclic graphs have non-backtracking spectral radius 1;
(iii) among all connected graphs of order n with p pendant vertices, where $1 \leq p \leq n-3$, the graph consisting of a complete graph of order $n-p$ and p pendant vertices at a common vertex uniquely maximizes the adjacency spectral radius, while all graphs consisting of a complete graph of order $n-p$ and p pendant vertices that are not necessarily at a common vertex maximize the non-backtracking spectral radius (see Theorem 4.4).

Recently, Huang et al. [10] determined the unique graph that maximizes the adjacency spectral radius in the set of all k-connected graphs of order n with diameter D. One may also consider the non-backtracking

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version of this class of graphs. Apart from Lemma 2.7, one needs more other different techniques and heavy calculations. Actually, there are lots of other families of graphs that may be considered to maximize the non-backtracking spectral radius, see [17] and references cited therein.

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