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The Extremal Values of Some Monotonic Topological Indices in Graphs with Given Vertex Bipartiteness*

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Abstract

Let $I(G)$ be a topological index of a graph G. If $I(G+e) < I(G)$ (or $I(G+e) > I(G)$, respectively) for each edge $e \notin G$, then $I(G)$ decreases (or increases, respectively) with addition of edges. The vertex bipartiteness of a graph is the minimum number of vertices whose deletion from G results in a bipartite graph. In this paper, we determine the extremal values of some monotonic topological indices and characterize the corresponding extremal graphs among all graphs with a given vertex bipartiteness.

1 Introduction

The structural invariants of a (molecular) graph are numerical parameters of a graph which characterize its topology and are usually called topological indices in chemical graph theory. They are the final results of a logical and mathematical procedure which transforms chemical information encoded within a symbolic representation of a molecule into a useful number or the result of some standardized experiment, and have been shown to be useful in modeling many physicochemical properties in numerous QSAR and QSPR studies [21]. Some of the most famous topological indices are based on the graph-distances (the Wiener index, the Harary index, the Kirchhoff index, the detour index, etc.), the edge contributions (the Randić index, the Zagreb index, the Szeged index, the PI-index,

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etc.) and a variety of quantities to describe the structure of graphs (the energy, the matching energy, the Estrada index, the Hosoya index, the Merrifield-Simmons index, etc.), respectively.

On the other hand, many important topological indices have the monotonicity, i.e., decrease (or increase, respectively) with addition of edges, including the Wiener index, the Kirchhoff index, the Hosoya index, the matching energy, the Zagreb index, etc. In [2,38], we determined the extremal values of some monotonic topological indices in all bipartite graphs with a given matching number, and the extremal values of some monotonic topological indices in terms of the number of cut vertices, or cut edges, or the vertex connectivity, or edge connectivity, respectively. In [26], Liu and Pan obtained the minimum Kirchhoff index among graphs with a fixed number of vertices and fixed vertex bipartiteness. In [32], Robbiano, Morales and San provided an upper bound of the spectral radius and signless Laplacian spectral radius in terms of the vertex bipartiteness of a graph.

Motivated from [2,26,32,38], we continue to study the mathematical properties of the monotonic topological indices and concentrate on the extremal values of some monotonic topological indices with a given vertex bipartiteness.

2 Basic properties

Throughout this paper we consider only simple and connected graphs. First, we consider the effect of edge addition (or deletion) on topological indices.

Let $I(G)$ be a topological index of a graph G. If $I(G+e) < I(G)$ (or $I(G+e) > I(G)$, respectively) for each edge $e \notin G$, then $I(G)$ decreases (or increases, respectively) with addition of edges.

For example, the Wiener index and the Merrifield-Simmons index decrease with addition of edges, the spectral radius, the first and second Zagreb indices, the Hosoya index and the matching energy increase with addition of edges.

In this section, we discuss the property of graphs with the minimum or maximum topological indices decrease or increase with addition of edges among all graphs with a given vertex bipartiteness.

Let $G = (V, E)$ be a graph with vertex set $V = V(G)$ and edge set $E = E(G)$. For a vertex $v \in V(G)$, denote by $N_G(v)$ the neighborhood of v in G and by $d_G(v) = |N_G(v)|$ the degree of v in G.

A bipartite graph is a graph G whose vertex set can be divided into two disjoint set

X, Y such that every edge has an end vertex in X and the other one in Y. The set (X, Y) is called a bipartition of G. A complete bipartite graph $K_{s,t}$ is a bipartite graph with a bipartition (X, Y), where $|X| = s$ and $|Y| = t$ and such that each vertex in X is joined to each vertex in Y.

The distance $d_G(u, v)$ between vertices u and v in G is the length of any shortest path in G connecting u and v. The eccentricity $\varepsilon(v)$ of a vertex v is the maximum distance from v to any other vertex. When the graph is clear from the context, we will omit the subscript G from the notation.

The vertex-disjoint union of the graphs G and H is denoted by $G \cup H$. The join of the graphs G and H is the graph $G \vee H$ such that $V(G \vee H) = V(G) \cup V(H)$ and $E(G \vee H) = E(G) \cup E(H) \cup \{uv : u \in V(G) \text{ and } v \in V(H)\}$. Let K_n be the complete graph with n vertices. For $S \subset V(G)$, let $G - S$ be the graph formed from G by deleting the vertices in S and the edges incident with them.

The minimum number of vertices whose deletion yields a bipartite graph from G is called the vertex bipartiteness of G and it is denoted $v_b(G)$, see [7]. Let $\mathcal{G}_{n,\delta}$ be the set of the graphs with n vertices and $v_b(G) \leq \delta$, where δ is a natural number such that $\delta \leq n-2$.

Recently, many literatures [24, 37] etc. have been involved in the research of the extremal value for some topological indices in terms of some given parameters, such as, the graphs (bipartite graphs) with given matching number, the graphs with given diameters, the graphs with given connectivity, the graphs with given cut vertices (edges), etc.

In fact, all topological indices in these literatures above are monotonic, and the extremal graphs for these indices have some common structural characteristics over all graphs with n vertices and a given parameter [2, 38]. The following result shows a common structural characteristic of the extremal graphs for monotonic topological indices over all graphs with n vertices and a vertex bipartiteness.

Proposition 1. *Let $G \in \mathcal{G}_{n,\delta}$. Then there are positive integers s and t such that $s + t = n - \delta$ and*
(i) $I(G) \geq I(K_\delta \vee K_{s,t})$ for the topological index I which decreases with addition of edges;
(ii) $I(G) \leq I(K_\delta \vee K_{s,t})$ for the topological index I which increase with addition of edges.

Proof. Without loss of generality, we assume I is a topological index which decreases with addition of edges. Let $G_0 \in \mathcal{G}_{n,\delta}$ be a graph with the minimum value of I, i.e., $I(G_0) \leq I(G)$ for any $G \in \mathcal{G}_{n,\delta}$. Since $G_0 \in \mathcal{G}_{n,\delta}$, there are $v_1, v_2, \ldots, v_k \in V(G_0)$ $(k \leq \delta)$ such that $G_0 \backslash \{v_1, v_2, \ldots, v_k\}$ is a bipartite graph with a bipartition (X, Y). Let $|X| = s$

and $|Y| = t$. Hence $s + t = n - k$.

If $G_0 \backslash \{v_1, v_2, \ldots, v_k\} \neq K_{s,t}$, then there exist two vertices $x \in X$ and $y \in Y$ such that x and y are not adjacent. By adding a new edge $e = xy$, we will get a new graph $G_0 + e \in \mathcal{G}_{n,\delta}$, and $I(G_0 + e) < I(G_0)$, a contradiction. So, $G_0 \backslash \{v_1, v_2, \ldots, v_k\} = K_{s,t}$.

On the other hand, if there exist two vertices $v_i, v_j \in \{v_1, v_2, \ldots, v_k\}$ such that v_i and v_j are not adjacent, then we can also obtain a new graph $G_0 + v_iv_j \in \mathcal{G}_{n,\delta}$ by adding a new edge v_iv_j into G_0, and $I(G_0 + v_iv_j) < I(G_0)$, a contradiction again. This implies the subgraph induced by $\{v_1, v_2, \ldots, v_k\}$ is K_k. So, $G_0 = K_k \vee K_{s,t}$.

Finally, we show that $k = \delta$. Assume the opposite, namely that $k \leq \delta - 1$ and $s + t = n - k \geq n - \delta + 1 \geq 3$. Thus $s + t \geq 3$, implying $|X| = s \geq 2$ or $|Y| = t \geq 2$. Without loss of generality, we assume $|Y| = t \geq 2$. By taking a vertex y from Y, and adding all edges yv_i into $K_k \vee K_{s,t}$, where $v_i \in \{v_1, v_2, \ldots, v_k\}$, we obtain a new graph $K_{k+1} \vee K_{s,t-1} \in \mathcal{G}_{n,\delta}$ and $I(K_{k+1} \vee K_{s,t-1}) < I(K_k \vee K_{s,t})$, a contradiction. Therefore, $k = \delta$ and $G_0 = K_\delta \vee K_{s,t}$. ■

3 Applications

In this section, using Proposition 1 above, we will give the extremal values of some topological indices with vertex bipartiteness at most δ.

3.1 The extremal values of the Kirchhoff index and the number of spanning trees over graphs with a given vertex bipartiteness

The Kirchhoff index was introduced by Klein and Randić [23], defined as

$$Kf(G) = \sum_{\{u,v\} \subseteq V(G)} r_G(u, v)$$

where $r_G(u, v)$ is the effective resistance between vertices u and v computed with Ohm's law when the edges of the graph are supposed to have unit resistances.

The following Lemmas 2, 3 and 4 are well known, see [15, 27].

Lemma 2. *Let G be a connected graph but not complete. Then, for each $e \notin E(G)$, we have (i) [27] $Kf(G + e) < Kf(G)$; (ii) $\tau(G + e) > \tau(G)$.*

Let $\tau(G)$ denote the number of spanning trees of a connected graph G and $0 = \mu_1 < \mu_2 \leq \cdots \leq \mu_n$ the Laplacian eigenvalues of G. There are famous relationships between the Laplacian eigenvalues, $Kf(G)$ and $\tau(G)$.

Lemma 3. *[15] Let G be a connected graph of order n. Then $Kf(G) = n\sum_{i=2}^{n}\frac{1}{\mu_i}$ and $\tau(G) = \frac{1}{n}\prod_{i=2}^{n}\mu_i$, where $0 = \mu_1 < \mu_2 \leq \cdots \leq \mu_n$ are the Laplacian eigenvalues of G.*

Lemma 4. *[29] If $0 = \alpha_1 \leq \alpha_2 \leq \cdots \leq \alpha_s$ are the Laplacian eigenvalues of G_1 and $0 = \beta_1 \leq \beta_2 \leq \cdots \leq \beta_t$ are the Laplacian eigenvalues of G_2, then the Laplacian eigenvalues of $G_1 \vee G_2$ are $0, \alpha_2 + t, \cdots, \alpha_r + t, \beta_2 + s, \cdots, \beta_s + s, s + t$.*

Note that the Laplacian eigenvalues of the complete K_δ are $0, \delta, \cdots, \delta$, by Lemma 4, the Laplacian eigenvalues of $K_{s,t} = K_s^c \vee K_t^c$ are $0, s, \cdots, s, t, \cdots, t, s+t$, and the Laplacian eigenvalues of $K_\delta \vee K_{s,t}$ are $0, \delta+s+t, \cdots, \delta+s+t, s+\delta, \cdots, s+\delta, t+\delta, \cdots, t+\delta, s+t+\delta, s+t+\delta$. So, $Kf(K_\delta \vee K_{s,t}) = (\delta+s+t)(\frac{1}{\delta+s+t} \times (\delta+1) + \frac{1}{s+\delta} \times (t-1) + \frac{1}{t+\delta} \times (s-1)) = \delta + s + t - 1 + \frac{t(t-1)}{s+\delta} + \frac{s(s-1)}{t+\delta}$ and $\tau(K_\delta \vee K_{s,t}) = (\delta + s + t)^\delta (s+\delta)^{t-1}(t+\delta)^{s-1}$.

Lemma 5. *Let $G = K_\delta \vee K_{s,t}$ and $G' = K_\delta \vee K_{s+1,t-1}$. If $s \leq t-2$, then (i) $Kf(G') < Kf(G)$ and (ii) $\tau(G') > \tau(G)$.*

Proof. Since $Kf(K_\delta \vee K_{s,t}) = \delta + s + t - 1 + \frac{t^2-t}{s+\delta} + \frac{s^2-s}{t+\delta}$, we have

$$\begin{aligned}
Kf(G') - Kf(G) &= \frac{(t-1)(t-2)}{s+1+\delta} + \frac{s(s+1)}{t-1+\delta} - \frac{t^2-t}{s+\delta} - \frac{s^2-s}{t+\delta} \\
&= \frac{(s+1)^3 + (t-1)^3 - (s+1)^2 - (t-1)^2 + ((s+1)^2 + (t-1)^2 - s - t)\delta}{(s+1+\delta)(t-1+\delta)} \\
&- \frac{s^3 + t^3 - s^2 - t^2 + (s^2 + t^2 - s - t)\delta}{(s+\delta)(t+\delta)} \\
&< \frac{(s+1)^3 + (t-1)^3 - (s+1)^2 - (t-1)^2 + ((s+1)^2 + (t-1)^2 - s - t)\delta}{(s+1+\delta)(t-1+\delta)} \\
&- \frac{s^3 + t^3 - s^2 - t^2 + (s^2 + t^2 - s - t)\delta}{(s+1+\delta)(t-1+\delta)} \\
&= \frac{3s^2 - 3t^2 + s + t - 2 + (2s - 2t + 2)\delta}{(s+1+\delta)(t-1+\delta)} < 0
\end{aligned}$$

and

$$\begin{aligned}
\frac{\tau(G')}{\tau(G)} &= \frac{(s+1+\delta)^{t-2}(t-1+\delta)^s}{(s+\delta)^{t-1}(t+\delta)^{s-1}} \\
&= \left(\frac{s+1+\delta}{t+\delta}\right)^{s-1} (s+1+\delta)^{t-s-1} \left(\frac{t-1+\delta}{s+\delta}\right)^s \frac{1}{(s+\delta)^{t-s-1}} \\
&= \left(\frac{s+1+\delta}{t+\delta} \times \frac{t-1+\delta}{s+\delta}\right)^{s-1} \left(\frac{t-1+\delta}{s+\delta}\right) \left(\frac{s+1+\delta}{s+\delta}\right)^{t-s-1} > 1
\end{aligned}$$

Thus, $Kf(G') < Kf(G) < 0$ and $\tau(G') > \tau(G)$. ■

The following result shows the extremal values and the corresponding extremal graphs of the Kirchhoff index and the number of spanning trees over graphs with a given vertex bipartiteness.

Theorem 6. *Let $G \in \mathcal{G}_{n,\delta}$, $1 \le \delta \le n-2$. Then*

$$(i)\quad [26]\ Kf(G) \ge \begin{cases} \delta+1+\frac{n(n-\delta-3)}{n+\delta+1}+\frac{n(n-\delta-1)}{n+\delta-1}, & \text{if } n-\delta \text{ is odd;} \\ \delta+1+\frac{2n(n-\delta-2)}{n+\delta}, & \text{if } n-\delta \text{ is even} \end{cases}$$

with equality if and only if $G \cong K_\delta \vee K_{\lfloor \frac{n-\delta}{2} \rfloor, \lceil \frac{n-\delta}{2} \rceil}$.

$$(ii)\ \tau(G) \le \begin{cases} n^\delta \left(\frac{n+\delta-1}{2}\right)^{\frac{n-\delta-1}{2}} \left(\frac{n+\delta+1}{2}\right)^{\frac{n-\delta-3}{2}}, & \text{if } n-\delta \text{ is odd;} \\ n^\delta \left(\frac{n+\delta}{2}\right)^{n-\delta-2}, & \text{if } n-\delta \text{ is even} \end{cases}$$

with equality if and only if $G \cong K_\delta \vee K_{\lfloor \frac{n-\delta}{2} \rfloor, \lceil \frac{n-\delta}{2} \rceil}$.

Proof. (i) It is easy to see that

$$Kf(K_\delta \vee K_{\lfloor \frac{n-\delta}{2} \rfloor, \lceil \frac{n-\delta}{2} \rceil}) = \begin{cases} \delta+1+\frac{n(n-\delta-3)}{n+\delta+1}+\frac{n(n-\delta-1)}{n+\delta-1}, & \text{if } n-\delta \text{ is odd;} \\ \delta+1+\frac{2n(n-\delta-2)}{n+\delta}, & \text{if } n-\delta \text{ is even} \end{cases}$$

Let G be a graph with the minimum Kirchhoff index among all graphs with n vertices and vertex bipartiteness at most δ. By Lemma 2 and Proposition 1, there are positive integers s and t, such that $s+t = n-\delta$ and $G \cong K_\delta \vee K_{s,t}$. From Lemma 5, we have $|t-s| \le 1$, and $G \cong K_\delta \vee K_{\lfloor \frac{n-\delta}{2} \rfloor, \lceil \frac{n-\delta}{2} \rceil}$.

(ii) It can be proved by the same way as in (i). ■

3.2 The extremal value of the modified-Wiener index over graphs with a given vertex bipartiteness

The modified-Wiener index [11] is defined as

$$W_\lambda(G) = \sum_{\{u,v\} \subseteq V(G)} d_G(u,v)^\lambda$$

where $\lambda \ne 0$ is a real number, and in particular, $W_\lambda(G)$ is the Wiener index [18] and the Harary index [20, 31] for $\lambda = 1$ and $\lambda = -1$, respectively.

The following lemma is the direct consequence of the definitions of the Modified-Wiener index.

Lemma 7. *Let G be a connected graph but not complete. Then, for each $e \notin E(G)$, we have (i) $W_\lambda(G+e) < W_\lambda(G)$ for $\lambda > 0$; (ii) $W_\lambda(G+e) > W_\lambda(G)$ for $\lambda < 0$.*

Lemma 8. *Let $G = K_\delta \vee K_{s,t}$ and $G' = K_\delta \vee K_{s+1,t-1}$. If $s \le t-2$, then (i) $W_\lambda(G') < W_\lambda(G)$ for $\lambda > 0$; (ii) $W_\lambda(G') > W_\lambda(G)$ for $\lambda < 0$.*

Proof. By the definition of the modified-Wiener index, we have

$$\begin{aligned}W_\lambda(G') - W_\lambda(G) =& 2^\lambda\left(\frac{s(s+1)}{2} + \frac{(t-1)(t-2)}{2}\right) + (s+1)(t-1)\\ &- 2^\lambda\left(\frac{s(s-1)}{2} + \frac{t(t-1)}{2}\right) - st\\ =&(1-2^\lambda)(t-s-1).\end{aligned}$$

Thus, $W_\lambda(G') - W_\lambda(G) < 0$ for $\lambda > 0$ and $W_\lambda(G') - W_\lambda(G) > 0$ for $\lambda < 0$. ■

The following result shows the extremal values and the corresponding extremal graphs of the modified-Wiener index over graphs with a given vertex bipartiteness.

Theorem 9. *Let $G \in \mathcal{G}_{n,\delta}$, $1 \le \delta \le n-2$. Then*
(i) For $\lambda > 0$,

$$W_\lambda(G) \ge \begin{cases} \frac{1}{4}[n^2 + 3\delta^2 - 2\delta n - 2\delta - 1 + 2^\lambda(3\delta - 2n - \delta n + n^2 + 1)], & \text{if } n-\delta \text{ is odd;}\\ \frac{1}{4}[n^2 + 3\delta^2 - 4\delta + 2^\lambda(n-\delta)(n-\delta-2)], & \text{if } n-\delta \text{ is even}\end{cases}$$

with equality if and only if $G \cong K_\delta \vee K_{\lfloor\frac{n-\delta}{2}\rfloor,\lceil\frac{n-\delta}{2}\rceil}$.
(ii) For $\lambda < 0$,

$$W_\lambda(G) \le \begin{cases} \frac{1}{4}[n^2 + 3\delta^2 - 2\delta n - 2\delta - 1 + 2^\lambda(3\delta - 2n - \delta n + n^2 + 1)], & \text{if } n-\delta \text{ is odd;}\\ \frac{1}{4}[n^2 + 3\delta^2 - 4\delta + 2^\lambda(n-\delta)(n-\delta-2)], & \text{if } n-\delta \text{ is even}\end{cases}$$

with equality if and only if $G \cong K_\delta \vee K_{\lfloor\frac{n-\delta}{2}\rfloor,\lceil\frac{n-\delta}{2}\rceil}$.

Proof. It is easy to see that

$$W_\lambda(K_\delta \vee K_{\lfloor\frac{n-\delta}{2}\rfloor,\lceil\frac{n-\delta}{2}\rceil}) =$$
$$\begin{cases} \frac{1}{4}[n^2 + 3\delta^2 - 2\delta n - 2\delta - 1 + 2^\lambda(3\delta - 2n - \delta n + n^2 + 1)], & \text{if } n-\delta \text{ is odd;}\\ \frac{1}{4}[n^2 + 3\delta^2 - 4\delta + 2^\lambda(n-\delta)(n-\delta-2)], & \text{if } n-\delta \text{ is even}\end{cases}$$

Let G be a graph with the maximum modified-Wiener index for $\lambda < 0$ (or, the minimum modified-Wiener index for $\lambda > 0$, respectively) among all graphs with n vertices and vertex bipartiteness at most δ. By Lemma 7 and Proposition 1, there are positive integers s and t, such that $s + t = n - \delta$ and $G \cong K_\delta \vee K_{s,t}$. From Lemma 8, we have $|t-s| \le 1$, and $G \cong K_\delta \vee K_{\lfloor\frac{n-\delta}{2}\rfloor,\lceil\frac{n-\delta}{2}\rceil}$. ■

In addition, the extremal values and the corresponding extremal graphs of the hyper-Wiener index [37] and the multiplicative Wiener index [13,14] for graphs with n vertices and vertex bipartiteness at most δ, can also be obtained similarly.

3.3 The extremal values of the Zagreb indices over graphs with a given vertex bipartiteness

One of the oldest graph invariants is the well-known Zagreb indices introduced by Gutman and Trinajestić [17], where Gutman and Trinajstć examined the dependence of total π-electron energy on molecular structure, and it was elaborated in [16]. For a (molecular) graph G, the first Zagreb index $M_1(G)$ and the second Zagreb index $M_2(G)$ are, respectively, defined as follows:

$$M_1(G) = \sum_{uv\in E(G)} (d_G(u) + d_G(v)) = \sum_{u\in V(G)} d_G(u)^2 \text{ and } M_2(G) = \sum_{uv\in E(G)} d_G(u)\cdot d_G(v)$$

Two fairly new indices [35, 36] with higher prediction ability than their classical versions, named the multiplicative Zagreb indices [12], are given by

$$\Pi_1(G) = \prod_{u\in V(G)} d_G(u)^2 \text{ and } \Pi_2(G) = \prod_{uv\in E(G)} d_G(u)\cdot d_G(v) = \prod_{v\in V(G)} d_G(v)^{d_G(v)}$$

Some recent results on the Zagreb indices can be found in [4, 5, 7, 34].

The following lemma is the direct consequence of the definition.

Lemma 10. *Let G be a connected graph but not complete. Then, for each $e \notin E(G)$, we have (i) $M_1(G+e) > M_1(G)$ and $M_2(G+e) > M_2(G)$; (ii) $\Pi_1(G+e) > \Pi_1(G)$ and $\Pi_2(G+e) > \Pi_2(G)$.*

Lemma 11. *Let $G = K_\delta \vee K_{s,t}$ and $G' = K_\delta \vee K_{s+1,t-1}$. If $s \le t-2$, then (i) $M_1(G') > M_1(G)$ and $M_2(G') > M_2(G)$; (ii) $\Pi_1(G') > \Pi_1(G)$ and $\Pi_2(G') > \Pi_2(G)$.*

Proof. (i) By the definition of the Zagreb indices, we have

$$\begin{aligned} M_1(G') - M_1(G) =&(s+1)(\delta+t-1)^2 + (t-1)(\delta+s+1)^2 - s(\delta+t)^2 - t(\delta+s)^2 \\ =&(t-s-1)(4\delta+s+t) > 0 \end{aligned}$$

and

$$\begin{aligned} &M_2(G') - M_2(G) \\ &= (\delta+t-1)(\delta+s+1)(s+1)(t-1) + (n-1)(\delta+s+1)\delta(t-1) \\ &+ (n-1)(\delta+t-1)\delta(s+1) - (\delta+t)(\delta+s)st - (n-1)(\delta+s)\delta t - (n-1)(\delta+t)\delta s \\ &= [(\delta+t-1)(\delta+s+1)(s+1)(t-1) - (\delta+t)(\delta+s)st] \\ &+ \delta(n-1)[(\delta+s+1)(t-1) + (\delta+t-1)(s+1) - (\delta+s)t - (\delta+t)s] \\ &> [(\delta+t-1)(\delta+s+1) - (\delta+t)(\delta+s)]st + 2\delta(n-1)(t-s-1) \\ &= (t-s-1)st + 2\delta(n-1)(t-s-1) > 0. \end{aligned}$$

(ii) For the multiplicative Zagreb indices, we have

$$\begin{aligned}\frac{\Pi_1(G')}{\Pi_1(G)} &= \frac{(\delta+t-1)^{2(s+1)}(\delta+s+1)^{2(t-1)}}{(\delta+t)^{2s}(\delta+s)^{2t}}\\ &= \left(\frac{\delta+t-1}{\delta+t}\right)^{2s}\left(\frac{\delta+s+1}{\delta+s}\right)^{2t}\left(\frac{\delta+t-1}{\delta+s+1}\right)^{2}\\ &> \left(\frac{(\delta+t-1)(\delta+s+1)}{(\delta+t)(\delta+s)}\right)^{2s} > 1\end{aligned}$$

and

$$\begin{aligned}\frac{\Pi_2(G')}{\Pi_2(G)} &= \frac{(\delta+s+1)^{(\delta+s+1)(t-1)}(\delta+t-1)^{(\delta+t-1)(s+1)}}{(\delta+s)^{(\delta+s)t}(\delta+t)^{(\delta+t)s}}\\ &= \left(\frac{\delta+s+1}{\delta+s}\right)^{(\delta+s)t}\left(\frac{\delta+t-1}{\delta+t}\right)^{(\delta+t)s}\frac{(\delta+t-1)^{\delta+t-s-1}}{(\delta+s+1)^{\delta+s-t+1}}\\ &> \left(\frac{\delta+s+1}{\delta+s}\right)^{(\delta+s)t}\left(\frac{\delta+t-1}{\delta+t}\right)^{(\delta+t)s} > \left(\frac{(\delta+s+1)(\delta+t-1)}{(\delta+s)(\delta+t)}\right)^{(\delta+t)s} > 1.\end{aligned}$$

Thus, the proof is complete. ■

The following results show the extremal values and the corresponding extremal graphs of the Zagreb indices over graphs with a given vertex bipartiteness. They can be proved by Lemma 10, Proposition 1 and Lemma 11, similar to the proof of Theorem 9.

Theorem 12. *Let $G \in \mathcal{G}_{n,\delta}$, $1 \le \delta \le n-2$. Then*

(i)

$$M_1(G) \le \begin{cases} \delta(n-1)^2 + \frac{1}{4}(n^3+\delta n^2-\delta^2 n-n-\delta^3-3\delta), & \text{if } n-\delta \text{ is odd;}\\ \delta(n-1)^2 + \frac{1}{4}(n^3+\delta n^2-\delta^2 n-\delta^3), & \text{if } n-\delta \text{ is even}\end{cases}$$

and

$$M_2(G) \le \begin{cases} \frac{1}{2}\delta(\delta-1)(n-1)^2 + \frac{1}{16}[((n+\delta)^2-1)((n-\delta)^2-1) \\ +4\delta(n-1)(2n^2-2\delta^2-2)], & \text{if } n-\delta \text{ is odd;}\\ \\ \frac{1}{2}\delta(\delta-1)(n-1)^2 + \frac{1}{16}(n^2-\delta^2)(n^2-\delta^2+8\delta n-8\delta), & \text{if } n-\delta \text{ is even}\end{cases}$$

with equality if and only if $G \cong K_\delta \vee K_{\lfloor\frac{n-\delta}{2}\rfloor,\lceil\frac{n-\delta}{2}\rceil}$.

(ii)

$$\Pi_1(G) \le \begin{cases} 2^{2(\delta-n)}(n-1)^{2\delta}(n+\delta+1)^{n-\delta-1}(n+\delta-1)^{n-\delta+1}, & \text{if } n-\delta \text{ is odd;}\\ 2^{2(\delta-n)}(n-1)^{2\delta}(n+\delta)^{2(n-\delta)}, & \text{if } n-\delta \text{ is even}\end{cases}$$

and

$$\Pi_2(G) \le \begin{cases} (n-1)^{\delta(n-1)}\left(\frac{n+\delta-1}{2}\right)^{\frac{1}{4}(n^2-\delta^2+2\delta-1)}\left(\frac{n+\delta+1}{2}\right)^{\frac{1}{4}(n^2-\delta^2-2\delta-1)}, & \text{if } n-\delta \text{ is odd;}\\ (n-1)^{\delta(n-1)}\left(\frac{n+\delta}{2}\right)^{\frac{1}{2}(n^2-\delta^2)}, & \text{if } n-\delta \text{ is even}\end{cases}$$

with equality if and only if $G \cong K_\delta \vee K_{\lfloor\frac{n-\delta}{2}\rfloor,\lceil\frac{n-\delta}{2}\rceil}$.

3.4 The extremal values of the connective eccentricity index, the eccentric distance sum index and the adjacent eccentric distance sum index over graphs with a given vertex bipartiteness

The connective eccentricity index (CEI) [9] of a graph G is defined as

$$\xi^{ce}(G) = \sum_{uv\in E(G)} \left(\frac{1}{\varepsilon_G(u)} + \frac{1}{\varepsilon_G(v)}\right) = \sum_{v\in V(G)} \frac{d_G(v)}{\varepsilon_G(v)}$$

where $\varepsilon_G(v)$ is the eccentricity of v in G.

The eccentricity distance sum (EDS) [10] of a graph G is defined as

$$\xi^d(G) = \sum_{\{u,v\}\in V(G)} (\varepsilon_G(u) + \varepsilon_G(v))d(u, v) = \sum_{v\in V(G)} \varepsilon_G(v) \cdot D_G(v)$$

where $D_G(v) = \sum\limits_{u\in V(G)} d_G(u, v)$.

As a novel topological descriptor, the adjacent eccentric distance sum index was put forward by Sardana and Madan [33], which is defined to be

$$\xi^{sv}(G) = \sum_{v\in V(G)} \frac{\varepsilon_G(v) \cdot D_G(v)}{d_G(v)}$$

Since the degree of some vertices will increase, the distance sum $D_G(v)$ of at least vertex $v \in V(G)$ will decrease and the eccentricity ε_G will not increase by adding new edges in a graph G, we can get the following result.

Lemma 13. *Let G be a connected graph but not complete. Then, for each $e \notin E(G)$, we have (i) $\xi^{ce}(G + e) > \xi^{ce}(G)$; (ii) $\xi^d(G + e) < \xi^d(G)$; (iii) $\xi^{sv}(G + e) < \xi^{sv}(G)$.*

Lemma 14. *Let $G = K_\delta \vee K_{s,t}$ and $G' = K_\delta \vee K_{s+1,t-1}$. If $s \le t - 2$, then (i) $\xi^{ce}(G') > \xi^{ce}(G)$; (ii) $\xi^d(G') < \xi^d(G)$; (iii) $\xi^{sv}(G') < \xi^{sv}(G)$.*

Proof. (i) By the definition of the connective eccentricity index, we have

$$\begin{aligned}\xi^{ce}(G') - \xi^{ce}(G) =& \frac{(\delta + t - 1)(s + 1)}{2} + \frac{(\delta + s + 1)(t - 1)}{2} - \frac{(\delta + t)s}{2} - \frac{(\delta + s)t}{2}\\ =& t - s - 1 > 0.\end{aligned}$$

(ii) For the eccentricity distance sum (EDS), we have

$$\begin{aligned}\xi^d(G') - \xi^d(G) =& 2(s + 1)(\delta + 2s + t - 1) + 2(t - 1)(\delta + 2t + s - 3)\\ & - 2s(\delta + 2s + t - 2) - 2t(\delta + 2t + s - 2)\\ =& 4(s - t + 1) < 0.\end{aligned}$$

(iii) Similarly, we have

$$\begin{aligned}
\xi^{sv}(G') - \xi^{sv}(G) =& \frac{2(s+1)(\delta+2s+t-1)}{\delta+t-1} + \frac{2(t-1)(\delta+2t+s-3)}{\delta+s+1} \\
& - \frac{2s(\delta+2s+t-2)}{\delta+t} - \frac{2t(\delta+2t+s-2)}{\delta+s} \\
=& \frac{(2s+2)(\delta+t)(\delta+2s+t-1) - 2s(\delta+t-1)(\delta+2s+t-2)}{(\delta+t)(\delta+t-1)} \\
& - \frac{2t(\delta+s+1)(\delta+s+2t-2) - (2t-2)(\delta+s)(\delta+s+2t-3)}{(\delta+s)(\delta+s+1)} \\
<& \frac{(2s+2)(\delta+t)(\delta+2s+t-1) - 2s(\delta+t-1)(\delta+2s+t-2)}{(\delta+s)(\delta+s+1)} \\
& - \frac{2t(\delta+s+1)(\delta+s+2t-2) - (2t-2)(\delta+s)(\delta+s+2t-3)}{(\delta+s)(\delta+s+1)} \\
=& \frac{2(2\delta+s+t)(s-t+1)}{(\delta+s)(\delta+s+1)} < 0.
\end{aligned}$$

Therefore, the proof is complete. ■

From Lemma 13, Proposition 1 and Lemma 14, the following results can be proved by the same way in Theorem 9, which show the extremal values and the corresponding extremal graphs of CEI, EDS and the adjacent eccentric distance sum index over graphs with a given vertex bipartiteness.

Theorem 15. *Let $G \in \mathcal{G}_{n,\delta}$, $1 \le \delta \le n-2$. Then*

(i)

$$\xi^{ce}(G) \le \begin{cases} \delta(n-1) + \frac{1}{4}(n^2-\delta^2-1), & \text{if } n-\delta \text{ is odd;} \\ \delta(n-1) + \frac{1}{4}(n^2-\delta^2), & \text{if } n-\delta \text{ is even} \end{cases}$$

with equality if and only if $G \cong K_\delta \vee K_{\lfloor \frac{n-\delta}{2} \rfloor, \lceil \frac{n-\delta}{2} \rceil}$.

(ii)

$$\xi^{d}(G) \ge \begin{cases} \delta^2 - 3\delta n + 3\delta + 3n^2 - 4n + 1, & \text{if } n-\delta \text{ is odd;} \\ \delta^2 - 3\delta n + 3\delta + 3n^2 - 4n, & \text{if } n-\delta \text{ is even} \end{cases}$$

with equality if and only if $G \cong K_\delta \vee K_{\lfloor \frac{n-\delta}{2} \rfloor, \lceil \frac{n-\delta}{2} \rceil}$.

(iii)

$$\xi^{sv}(G) \ge \begin{cases} \delta + \frac{(n-\delta-1)(3n-\delta-5)}{n+\delta+1} + \frac{(n-\delta+1)(3n-\delta-3)}{n+\delta-1}, & \text{if } n-\delta \text{ is odd;} \\ \delta + \frac{2(n-\delta)(3n-\delta-4)}{n+\delta}, & \text{if } n-\delta \text{ is even} \end{cases}$$

with equality if and only if $G \cong K_\delta \vee K_{\lfloor \frac{n-\delta}{2} \rfloor, \lceil \frac{n-\delta}{2} \rceil}$.

3.5 The extremal value of the general zeroth-order Randić index over graphs with a given vertex bipartiteness

The general zeroth-order Randić index [25], denoted by ${}^0R_\alpha$, is defined by

$${}^0R_\alpha(G) = \sum_{u \in V(G)} d_G(u)^\alpha$$

where $\alpha \neq 0$ is a real number, and ${}^0R_\alpha$ is the zeroth-Randić index [22], the first Zagreb index [30], the forgotten index [8] and the inverse degree [6] of a graph for $\alpha = -1/2$, $\alpha = 2$, $\alpha = 3$ and $\alpha = -1$, respectively.

By the definition of the general zeroth-order Randić index, we can get

Lemma 16. *Let G be a connected graph but not complete. Then, for each $e \notin E(G)$, we have (i) ${}^0R_\alpha(G+e) > {}^0R_\alpha(G)$ for $\alpha > 0$; (ii) ${}^0R_\alpha(G+e) < {}^0R_\alpha(G)$ for $\alpha < 0$.*

Lemma 17. *Let $G = K_\delta \vee K_{s,t}$ and $G' = K_\delta \vee K_{s+1,t-1}$. If $s \leq t-2$, then (i) ${}^0R_\alpha(G) < {}^0R_\alpha(G')$ for $0 < \alpha \leq 1$; (ii) ${}^0R_\alpha(G) > {}^0R_\alpha(G')$ for $\alpha < 0$.*

Proof. (i) For $0 < \alpha \leq 1$, we have

$$\begin{aligned}
&{}^0R_\alpha(G') - {}^0R_\alpha(G) = (s+1)(\delta+t-1)^\alpha + (t-1)(\delta+s+1)^\alpha - s(\delta+t)^\alpha - t(\delta+s)^\alpha \\
&= s[(\delta+t-1)^\alpha - (\delta+t)^\alpha] + (t-1)[(\delta+s+1)^\alpha - (\delta+s)^\alpha] + (\delta+t-1)^\alpha - (\delta+s)^\alpha \\
&> s[(\delta+t-1)^\alpha - (\delta+t)^\alpha + (\delta+s+1)^\alpha - (\delta+s)^\alpha] \\
&= s[\phi(\delta+t) - \phi(\delta+s+1)] \\
&\geq 0 \qquad (\text{since } \delta+t > \delta+s+1)
\end{aligned}$$

where $\phi(x) = (x-1)^\alpha - x^\alpha$, and $\phi'(x) = \alpha[(x-1)^{\alpha-1} - x^{\alpha-1}] \geq 0$ for $0 < \alpha \leq 1$ and $x > 1$.

(ii) Similarly, for $\alpha < 0$, we have

$$\begin{aligned}
&{}^0R_\alpha(G') - {}^0R_\alpha(G) = (s+1)(\delta+t-1)^\alpha + (t-1)(\delta+s+1)^\alpha - s(\delta+t)^\alpha - t(\delta+s)^\alpha \\
&= s[(\delta+t-1)^\alpha - (\delta+t)^\alpha] + (t-1)[(\delta+s+1)^\alpha - (\delta+s)^\alpha] + (\delta+t-1)^\alpha - (\delta+s)^\alpha \\
&< (t-1)[(\delta+t-1)^\alpha - (\delta+t)^\alpha + (\delta+s+1)^\alpha - (\delta+s)^\alpha] \\
&= (t-1)[\phi(\delta+t) - \phi(\delta+s+1)] \\
&< 0 \qquad (\text{since } \delta+t > \delta+s+1)
\end{aligned}$$

where $\phi(x) = (x-1)^\alpha - x^\alpha$, and $\phi'(x) = \alpha[(x-1)^{\alpha-1} - x^{\alpha-1}] < 0$ for $\alpha < 0$ and $x > 1$. ■

From Lemma 16, Proposition 1 and Lemma 17, the following result can be proved by the same way in Theorem 9, which show the extremal values and the corresponding extremal graphs of the general zeroth-order Randić index over graphs with a given vertex bipartiteness.

Theorem 18. *Let $G \in \mathcal{G}_{n,\delta}$, $1 \leq \delta \leq n-2$. Then*

(i) For $0 < \alpha \leq 1$, we have

$${}^0R_\alpha(G) \leq \begin{cases} \delta(n-1)^\alpha + \frac{n-\delta-1}{2}\left(\frac{n+\delta+1}{2}\right)^\alpha + \frac{n-\delta+1}{2}\left(\frac{n+\delta-1}{2}\right)^\alpha, & \text{if } n-\delta \text{ is odd;} \\ \delta(n-1)^\alpha + (n-\delta)\left(\frac{n+\delta}{2}\right)^\alpha, & \text{if } n-\delta \text{ is even} \end{cases}$$

with equality if and only if $G \cong K_\delta \vee K_{\lfloor \frac{n-\delta}{2} \rfloor, \lceil \frac{n-\delta}{2} \rceil}$.
(ii) For $\alpha < 0$, *we have*

$$ {}^0R_\alpha(G) \geq \begin{cases} \delta(n-1)^\alpha + \frac{n-\delta-1}{2}\left(\frac{n+\delta+1}{2}\right)^\alpha + \frac{n-\delta+1}{2}\left(\frac{n+\delta-1}{2}\right)^\alpha, & \text{if } n-\delta \text{ is odd;} \\ \delta(n-1)^\alpha + (n-\delta)\left(\frac{n+\delta}{2}\right)^\alpha, & \text{if } n-\delta \text{ is even} \end{cases} $$

with equality if and only if $G \cong K_\delta \vee K_{\lfloor \frac{n-\delta}{2} \rfloor, \lceil \frac{n-\delta}{2} \rceil}$.

In view of the result above, an interesting problem is valuable to be considered.

Problem. For $\alpha > 1$, how to determine the graph with the general zeroth-order Randić index ${}^0R_\alpha$ over graphs with a given vertex bipartiteness?

3.6 The extremal values of the additively weighted and multiplicative weighted Harary indices over graphs with a given vertex bipartiteness

The additively weighted Harary index $H^+(G)$ and the multiplicative weighted Harary index $H^*(G)$ of a graph G are defined as

$$ H^+(G) = \sum_{\{u,v\}\subseteq V(G)} \frac{d(u)+d(v)}{d(u,v)} \quad \text{and} \quad H^*(G) = \sum_{\{u,v\}\subseteq V(G)} \frac{d(u)\cdot d(v)}{d(u,v)}. $$

$H^+(G)$ is also called the reciprocal sum-degree distance of G, introduced independently by Alizadeh et al. [1] and Hua and Zhang [19]. It was shown that the reciprocal degree distance can be used as an efficient measuring tool in the study of complex networks Alizadeh et al. [1]. Deng et al [3] determined the extremal values of the multiplicatively weighted Harary indices for some familiar classes of graphs and characterize the corresponding extremal graphs.

Lemma 19. *[19] Let* G *be a connected graph but not complete. Then, for each* $e \notin E(G)$, *we have (i)* $H^+(G+e) > H^+(G)$; *(ii)* $H^*(G+e) > H^*(G)$.

Lemma 20. *Let* $G = K_\delta \vee K_{s,t}$ *and* $G' = K_\delta \vee K_{s+1,t-1}$. *If* $s \leq t-2$, *then (i)* $H^+(G') > H^+(G)$; *(ii)* $H^*(G') > H^*(G)$.

Proof. By the definition of the additively weighted Harary index, we have

$$ \begin{aligned} H^+(G) =& \delta s[(n-1)+(\delta+t)] + \delta t[(n-1)+(\delta+s)] + st(2\delta+t+s) \\ &+ \frac{1}{2}s(s-1)(\delta+t) + \frac{1}{2}t(t-1)(\delta+s) + \delta(\delta-1)(n-1) \end{aligned} $$

and

$$\begin{aligned}H^+(G') =&\delta(s+1)[(n-1)+(\delta+t-1)]+\delta(t-1)[(n-1)+(\delta+s+1)]\\&+(s+1)(t-1)(2\delta+t+s)+\frac{1}{2}s(s+1)(\delta+t-1)\\&+\frac{1}{2}(t-1)(t-2)(\delta+s+1)+\delta(\delta-1)(n-1)\end{aligned}$$

So,

$$H^+(G')-H^+(G)=\frac{1}{2}(t-s-1)(6\delta+3s+3t-2)>0.$$

Similarly,

$$\begin{aligned}H^*(G) =&\delta s(n-1)(\delta+t)+\delta t(n-1)(\delta+s)+st(\delta+t)(\delta+s)+\frac{1}{4}s(s-1)(\delta+t)^2\\&+\frac{1}{4}t(t-1)(\delta+s)^2+\frac{1}{2}\delta(\delta-1)(n-1)^2\end{aligned}$$

$$\begin{aligned}H^*(G') =&\delta(s+1)(n-1)(\delta+t-1)+\delta(t-1)(n-1)(\delta+s+1)\\&+(s+1)(t-1)(\delta+s+1)(\delta+t-1)+\frac{1}{4}s(s+1)(\delta+t-1)^2\\&+\frac{1}{4}(t-1)(t-2)(\delta+s+1)^2+\frac{1}{2}\delta(\delta-1)(n-1)^2.\end{aligned}$$

And we have

$$H^*(G')-H^*(G)=\frac{1}{4}(t-s-1)(5t-7s-12\delta+8\delta n+6\delta t+12st+2\delta^2-6)>0.$$

■

The following results show the extremal values and the corresponding extremal graphs of the additively weighted and multiplicative weighted Harary indices over graphs with a given vertex bipartiteness. They can be proved by Lemma 19, Proposition 1 and Lemma 20.

Theorem 21. *Let $G\in\mathcal{G}_{n,\delta}$, $1\le\delta\le n-2$. Then*

(i)

$$H^+(G)\le\begin{cases}\delta(\delta-1)(n-1)+\frac{1}{8}[5n^3+3\delta n^2-5\delta^2 n-8\delta n-2n^2-5n-3\delta^3+10\delta^2-\delta+2], & \text{if } n-\delta \text{ is odd;}\\ \delta(\delta-1)(n-1)+\frac{1}{8}(n-\delta)[3n^2-2n-3\delta^2-2\delta+4\delta(n-\delta)(3n+\delta-2)], & \text{if } n-\delta \text{ is even}\end{cases}$$

with equality if and only if $G \cong K_\delta \vee K_{\lfloor \frac{n-\delta}{2} \rfloor, \lceil \frac{n-\delta}{2} \rceil}$.

(ii)

$$H^*(G) \leq \begin{cases} \frac{1}{32}[(16\delta+3)n^3 + (10\delta^2 - 34\delta - 6)n^2 - (16\delta^3 + 30\delta^2 - 16\delta - 2)n \\ +3\delta^4 + 18\delta^3 + 18\delta^2 + 6\delta + 3], \\ \hfill \text{if } n-\delta \text{ is odd;} \\ \frac{1}{16}(n^2-\delta^2)[n^2-\delta^2-(n+\delta)(n-\delta-2)-8\delta(n-1)] + \frac{1}{2}\delta(\delta-1)(n-1)^2, \\ \hfill \text{if } n-\delta \text{ is even} \end{cases}$$

with equality if and only if $G \cong K_\delta \vee K_{\lfloor \frac{n-\delta}{2} \rfloor, \lceil \frac{n-\delta}{2} \rceil}$.

3.7 The extremal value of the Merrifield-Simmons index over graphs with a given vertex bipartiteness

The Merrifield-Simmons index of a graph G, denoted by $i(G)$, was introduced by Merrifield and Simmons [28], which is defined as the total number of independent vertex sets of G, including the empty vertex set. The following result is well-known.

Lemma 22. *Let G be a graph and uv be an edge of G. Then*

$$i(G) = i(G-uv) - i(G - N_G(u) \cup N_G(v)).$$

By Lemma 22, we have

Lemma 23. *Let G be a connected graph but not complete. Then $i(G+e) < i(G)$ for each $e \notin E(G)$.*

Lemma 24. *Let $G = K_\delta \vee K_{s,t}$ and $G' = K_\delta \vee K_{s+1,t-1}$. If $s \leq t-2$, then $i(G') < i(G)$.*

Proof. By the definition of the Merrifield-Simmons index, we have

$$\begin{aligned} i(G) =& \binom{n}{0} + \binom{n}{1} + \binom{s}{2} + \binom{s}{3} + \cdots + \binom{s}{s} + \binom{t}{2} + \binom{t}{3} + \cdots + \binom{t}{t} \\ =& 1 + n + (2^s - s - 1) + (2^t - t - 1) \end{aligned}$$

and

$$\begin{aligned} i(G') =& \binom{n}{0} + \binom{n}{1} + \binom{s+1}{2} + \binom{s+1}{3} + \cdots + \binom{s+1}{s+1} \\ &+ \binom{t-1}{2} + \binom{t-1}{3} + \cdots + \binom{t-1}{t-1} \\ =& 1 + n + (2^{s+1} - s - 2) + (2^{t-1} - t). \end{aligned}$$

So,

$$\begin{aligned} i(G') - i(G) =& (2^{s+1} - s - 2) + (2^{t-1} - t) - (2^s - s - 1) - (2^t - t - 1) \\ =& 2^s - 2^{t-1} < 0. \end{aligned}$$

■

Using Lemma 23, Proposition 1 and Lemma 24, we can prove the following result, which shows the extremal values and the corresponding extremal graphs of the Merrifield–Simmons index over graphs with a given vertex bipartiteness.

Theorem 25. *Let $G \in \mathcal{G}_{n,\delta}$, $1 \leq \delta \leq n-2$. Then*

$$i(G) \geq \begin{cases} 2^{\frac{n-\delta-1}{2}} + 2^{\frac{n-\delta+1}{2}} + \delta - 1, & \text{if } n-\delta \text{ is odd;} \\ 2^{\frac{n-\delta+2}{2}} + \delta - 1, & \text{if } n-\delta \text{ is even} \end{cases}$$

with equality if and only if $G \cong K_\delta \vee K_{\lfloor \frac{n-\delta}{2} \rfloor, \lceil \frac{n-\delta}{2} \rceil}$.

4 Conclusions

In this paper, we give a common characterization of a graph with the extremal value for a monotonic topological index among all graphs of order n with vertex bipartiteness at most δ, and determine the extremal values of some monotonic topological indices (including the Wiener index, the Harary index, the Zagreb index, the connective eccentricity index, the eccentricity distance sum, the Merrifield-Simmons index etc.).

As future work, we will study the extremal values of other monotonic topological indices, such as the Hosoya index, the matching energy, the Estrada index, the distance spectral radius, the distance signless Laplacian spectral radius, the Harary spectral radius etc, over graphs with a given vertex bipartiteness.

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