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Extremal Bipartite Graphs with Given Parameters on the Resistance–Harary Index

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Abstract: Resistance distance is a concept developed from electronic networks. The calculation of resistance distance in various circuits has attracted the attention of many engineers. This report considers the resistance-based graph invariant, the Resistance–Harary index, which represents the sum of the reciprocal resistances of any vertex pair in the figure G , denoted by $RH(G)$. Vertex bipartiteness in a graph G is the minimum number of vertices removed that makes the graph G become a bipartite graph. In this study, we give the upper bound and lower bound of the RH index, and describe the corresponding extremal graphs in the bipartite graph of a given order. We also describe the graphs with maximum RH index in terms of graph parameters such as vertex bipartiteness, cut edges, and matching numbers.

Keywords: Resistance–Harary index; resistance distance; cut edges; bipartite graph; matching number; vertex bipartiteness

1. Introduction

There are graph invariants that describe certain properties of a graph, which we call topological indices. Various topological indices are proposed and researched by both theoretical chemists and mathematicians. Topological index is mainly used to study the quantitative relationship between structure and performance and between structure and activity. It would be helpful for describing partially biological and chemical properties. Some of them have been proved to be successful [1]. Recently, finding the extreme value for the topological indices, as well as the related problem of characterizing the extremal graphs, attracted the attention of many researchers, and many results were obtained.

Among these topological indices, one of most widely known topological description is the Wiener index, which was proposed in 1947 and represents the sum of the distances of all pairs of vertices in the graph, i.e.,

$$W(G) = \sum_{\{u,v\} \in V(G)} d_G(u,v).$$

Another graph invariant based on distance is called the Harary index, has been introduced independently by Placšić et al. [2] and by Ivanciuc et al. [3] in 1993, which is the sum of the reciprocal distances of any vertex pair in graph G , i.e.,

$$H(G) = \sum_{\{u,v\} \in V(G)} \frac{1}{d_G(u,v)}.$$

More results on the Harary index can be found in the literature [4–7].

Recently, graph invariants based on resistance distance have attracted the attention of theorists, such as the Kirchhoff index. The resistance distance is what Klein and Randić [8] came up with as a function of the distance of the graph. The resistance distance between two vertices u and v of G , denoted by $r_G(u, v)$, represents the effective resistance of two elements u and v in a circuit, and each edge in G means the cell resistance.

Similar to the distance in the path graph, the resistance distance is also closely related to the structure of the graph, and not only has good mathematics and physics characteristics [9,10], but also has widespread chemistry applications.

The Kirchhoff index is one of the most studied topological indices, which is defined as

$$kf(G) = \sum_{\{x,y\} \subseteq V(G)} r_G(x,y).$$

With the continuous development and improvement of electrical network theory, D.J. Klein and O. Ivanciuc [11] investigated the global cyclicity index $C(G)$, defined as

$$C(G) = \sum_{uv \in E(G)} \left[\frac{1}{r_G(u,v)} - \frac{1}{d_G(u,v)} \right],$$

Y. Yang [12] obtained some results on global cyclicity index.

Inspired by the Harary index, S. Chen et al. [13] modify the global cyclicity index and put forward the Resistance–Harary index, described as

$$RH(G) = \sum_{\{u,v\} \subseteq V(G)} \frac{1}{r_G(u,v)}.$$

In [14], the structure of the graph with maximum RH value is described among the connected graph with given order and cut edges.

All graphs considered here are connected and simple. Let G be a graph with vertex set $V(G)$ and edge set $E(G)$, and the degree of each vertex v is expressed as $d_G(v)$, which means the number of neighbors of v in G . $d_G(u, v)$ is the distance between u and v in G , the longest distance between any two vertices in the graph is called the *diameter*.

As usual, let C_n , S_n and P_n be a cycle, a star, and a path with n vertices, respectively. $G - uv$ represents the subgraph obtained by deleting an edge uv from graph G . Similarly, $G + uv$ represents the graph obtained by adding an edge uv to graph G . Let U and W be all the vertex sets of G . Where $W \subseteq U$, then $U \setminus W$ represents the complement of W in U . The *pendant vertex* of G refers to the vertex of graph G with degree 1. The *pendant edge* is the edge adjacent to the pendant vertex.

A *bipartite* graph (or *bigraph*) is a graph whose vertices can be divided into two disjoint and independent sets X and Y , such that every edge connects a vertex in X to one in Y . Vertex sets X and Y are usually called the parts of the graph. If a graph G is a bipartite graph, and all vertices in X are connected to all vertices in Y , then G is a *completed bipartite graph*.

If the number of vertices in each part of the completed bipartite is m and n , respectively, denoted it by $K_{m,n}$. The *cut vertex (edge)* will increase the number of branches of the graph if it is removed. Other terms not defined here are referred to [15].

A matching M in graph G is a set of non-adjacent edges, that is, no two edges share a common vertex. A maximum matching (also known as maximum-cardinality matching) is a matching that contains the largest possible number of edges. There may be many maximum matchings. The *matching number* of a graph G is the size of a maximum matching.

Inspired by the above results, it is natural to consider these extremal problems from the class of general connected graphs to the bipartite graphs. Our aim in this article is to study the extremal bipartite graphs with given parameters on Resistance–Harary index. First, we give the upper bound and lower bound of RH index, and describe the corresponding extremal graphs in the bipartite graph

of a given order. We also describe the graphs with maximum RH index in terms of graph parameters such as vertex bipartiteness v_b , (where $1 \leq v_b \leq n - 2$), cut edges, and matching numbers.

2. General Connected Bipartite Graphs

In this section, we give the upper bound and lower bound of RH index, and describe the corresponding extremal graphs in the bipartite graph of a given order. In the simple connected acyclic graph, the Resistance distance and distance from the two points in the graph are equal, that is, the Resistance–Harary index and the Harary index are the same in the acyclic graph. There is a formula for this scenario:

$$RH(P_n) = H(P_n) = 1 + n \sum_{i=2}^{n-1} \frac{1}{i}.$$

However, when the connected graph contains cycles, the resistance distance is different from the general distance. Our calculation is based on electrical network theory, given a fixed resistor on each edge, the shortest distance between two vertices represents the effective resistance of the corresponding two components in the circuit. Let $C_k = u_1u_2 \dots u_ku_1$ be the cycle on k vertices, where $k \geq 3$. By Ohm’s law, any two components in a circuit $u_s, u_t \in V(C_k)$ with $s < t$, we have

$$\frac{1}{r_{C_k}(u_s, u_t)} = \frac{1}{t - s} + \frac{1}{k - (t - s)},$$

then, we have

$$r_{C_k}(u_s, u_t) = \frac{(t - s)(k + s - t)}{k}.$$

We start with some useful lemmas.

Lemma 1 ([8]). w is the cut vertex of graph G , and let u and v be two vertices of different components of $G - w$. There must be $r_G(u, v) = r_G(u, w) + r_G(w, v)$.

Lemma 2 ([14]). Let G be a graph that is not complete. Add an edge from G and we get the graph G^* . So there is $RH(G^*) > RH(G)$. That is to say, $RH(G)$ increases with addition of edges.

Corollary 1. G is a connected graph with n vertices, and H is a connected spanning subgraph of G . Then $RH(H) \leq RH(G)$, the equal sign is true when $G \cong H$.

Lemma 3 ([13]). Let T be a tree on n vertices different from P_n and S_n . Then

$$RH(P_n) < RH(T) < RH(S_n).$$

Theorem 1. $K_{\lfloor \frac{n}{2} \rfloor, \lceil \frac{n}{2} \rceil}$ is the graph with maximum RH index among all connected bipartite graphs of order n .

Proof. Choose G^0 as the graph such that its Resistance–Harary index is as large as possible, let (X, Y) be its two divisions, where $|X| + |Y| = n$. We first prove the following two claims.

Claim 1. G^0 is a complete bipartite graph.

Suppose to the contrary that $G^0 = (X, Y)$ is a graph that is not complete. Thus we can add one edge from $u \in X$ to $v \in Y$ to form a new graph $G^0 + uv$. It is obvious that $G^0 + uv$ is still a bipartite graph. By Lemma 2, we know that $RH(G^0 + uv) > RH(G^0)$, which contradicts the maximality of G^0 .

Claim 2. $G^0 \cong K_{\lfloor \frac{n}{2} \rfloor, \lceil \frac{n}{2} \rceil}$.

From Claim 1, we denote G^0 as $K_{s,t}$. In a complete connected bipartite graph $K_{s,t}$, Klein [16] obtain that the resistance distance between vertices from X and Y , respectively, is $\frac{s+t-1}{st}$. The resistance

distance between any two vertices in X and in Y is $\frac{2}{t}$ and $\frac{2}{s}$, respectively, hence, by Lemma 1 and the definition of RH index, we can get that

$$\begin{aligned} RH(K_{s,t}) &= \frac{st}{s+t-1}st + \frac{s}{2} \binom{t}{2} + \frac{t}{2} \binom{s}{2}, \\ &= \frac{s^2t^2}{s+t-1} + \frac{st(t-1)}{4} + \frac{st(s-1)}{4}, \\ &= \frac{st(4st + (s+t)^2 - 3(s+t) + 2)}{4(s+t-1)}. \end{aligned}$$

$$RH(K_{s-1,t+1}) = \frac{(s-1)(t+1)(4(s-1)(t+1) + (s+t)^2 - 3(s+t) + 2)}{4(s+t-1)}.$$

Let $M = (s+t)^2 - 3(s+t) + 2$, if $s > t + 1$, then, we have

$$\begin{aligned} RH(K_{s-1,t+1}) - RH(K_{s,t}) &= \frac{[(s-1)(t+1)(4(s-1)(t+1) + M) - st(4st + M)]}{4(s+t-1)}, \\ &= \frac{4(s-1)^2(t+1)^2 + M(s-1)(t+1) - 4s^2t^2 - M \cdot st}{4(s+t-1)}, \\ &= \frac{4(s-t-1)(2st + s-t-1) + M(s-t-1)}{4(s+t-1)}, \\ &> 0. \end{aligned}$$

Then,

$$RH(K_{s-1,t+1}) > RH(K_{s,t}).$$

So $RH(K_{s,t})$ obtain the extremal value if and only if $K_{s,t} \cong K_{\lfloor \frac{n}{2} \rfloor, \lceil \frac{n}{2} \rceil}$. This completes the proof. \square

Theorem 2. For any bipartite graph G of order n , we have

$$1 + n \sum_{i=2}^{n-1} \frac{1}{i} \leq RH(G) \leq \frac{\lfloor \frac{n}{2} \rfloor \lceil \frac{n}{2} \rceil (4 \lfloor \frac{n}{2} \rfloor \lceil \frac{n}{2} \rceil + n^2 - 3n + 2)}{4(n-1)}.$$

Proof. By Lemma 3 and Corollary 1, we can deduce that P_n has minimal RH index in the bipartite graphs of order n . By Theorem 1, one can see that $K_{\lfloor \frac{n}{2} \rfloor, \lceil \frac{n}{2} \rceil}$ has the maximum Resistance–Harary index. By direct calculation, we have

$$RH(K_{\lfloor \frac{n}{2} \rfloor, \lceil \frac{n}{2} \rceil}) = \frac{\lfloor \frac{n}{2} \rfloor \lceil \frac{n}{2} \rceil (4 \lfloor \frac{n}{2} \rfloor \lceil \frac{n}{2} \rceil + n^2 - 3n + 2)}{4(n-1)}$$

and

$$RH(P_n) = H(P_n) = 1 + n \sum_{i=2}^{n-1} \frac{1}{i}.$$

This completes the proof. \square

3. Bipartite Graphs Given Number of Matchings

In this section, we are going to characterize the extremal bipartite graphs of order n with given matching number q for the Resistance–Harary index.

Lemma 4. *The function for $f(x) = \frac{x^2q^2}{x+q-1}$ for $q > 1$ and $x > q$ is strictly increasing.*

Proof. Now, let us compute the derivative of this function

$$\begin{aligned} f'(x) &= \frac{2xq^2(x+q-1) - x^2q^2}{(x+q-1)^2}, \\ &= \frac{x^2q^2 + 2xq^3 - 2xq^2}{(x+q-1)^2}, \\ &= \frac{x^2q^2 + 2xq^2(q-1)}{(x+q-1)^2}, \\ &> 0. \end{aligned}$$

This completes the proof. \square

Theorem 3. *Graph $K_{q,n-q}$ has the largest RH in the bipartite graphs of order n given matching number q .*

Proof. We assume that G is a bipartite graph of a given matching number q , and (U, W) is its vertex partition, and G has the largest RH index. Obviously, $q \leq \lfloor \frac{n}{2} \rfloor$, if $q = \lfloor \frac{n}{2} \rfloor$, by Lemma 2 and Theorem 1, the extremal graph happens to be isomorphic to $K_{\lfloor \frac{n}{2} \rfloor, \lceil \frac{n}{2} \rceil}$, as expected. We are going to prove that, $q < \lfloor \frac{n}{2} \rfloor$, naturally, we make $|W| \geq |U|$ and take $|M| = q$ as the maximal matching of G , by Lemma 2, the value of the Resistance–Harary index is increasing when we increase the number of edges. So if $|U| = q$, the extremal graph $G \cong K_{q,n-q}$. Next, we consider $|U| > q$. Let U_M, W_M be the vertex subset sets in U, W saturated with M , respectively. Then, $|U_M| = |W_M| = q$. By the maximality of M , we infer that there are no edges set between $U \setminus U_M$ and $W \setminus W_M$. Add as many edges between the vertices of U_M and W_M , U_M and $W \setminus W_M$, $U \setminus U_M$ and W_M as we can from G , we get the result graph G' . Note that $W \setminus W_M \neq \emptyset$ and $U \setminus U_M \neq \emptyset$ and G' has at least $q + 1$ matching number. So, $G \neq G'$ and by Lemma 2, we have $RH(G') > RH(G)$. We get another bipartite graph G'' by separating two vertices sets of $U \setminus U_M$ and W_M and associating two sets of $U \setminus U_M$ and U_M in graph G' . Obviously, G'' is isomorphic to the complete bipartite graph $K_{q,n-q}$, which has the matching number q . Next, we will prove that

$$RH(G'') > RH(G').$$

Let $|U \setminus U_M| = n_1$, $|W \setminus W_M| = n_2$. Suppose that $n_2 \geq n_1$, we partition $V_{G'} = V_{G''}$ into $U_M \cup W_M \cup (W \setminus W_M) \cup (U \setminus U_M)$ as shown in Figure 1. For all $x \in W \setminus W_M$ (rep. $y \in U_M, z \in W_M, w \in U \setminus U_M$), by computing immediately, we have

$$\begin{aligned}
 \sum_{\substack{x \in W \setminus W_M \\ y \in U_M}} \frac{1}{r_{G'}(x, y)} &= \sum_{\substack{x \in W \setminus W_M \\ y \in U_M}} \frac{1}{r_{G''}(x, y)} = \frac{n_2^2 q^2}{n_2 + q - 1}. \\
 \sum_{\substack{x \in W \setminus W_M \\ z \in W_M}} \frac{1}{r_{G'}(x, z)} &= \sum_{\substack{x \in W \setminus W_M \\ z \in W_M}} \frac{1}{r_{G''}(x, z)} = \frac{n_2 q^2}{2} + \frac{n_2^2 q}{2}. \\
 \sum_{\substack{y \in U_M \\ z \in W_M}} \frac{1}{r_{G'}(y, z)} &= \sum_{\substack{y \in U_M \\ z \in W_M}} \frac{1}{r_{G''}(y, z)} = \frac{q^4}{2q - 1}. \\
 \sum_{\substack{z \in W_M \\ w \in U \setminus U_M}} \frac{1}{r_{G'}(z, w)} &= \frac{n_1 q^2}{2} + \frac{q n_1^2}{2} \cdot \sum_{\substack{z \in W_M \\ w \in U \setminus U_M}} \frac{1}{r_{G''}(z, w)} = \frac{n_2^2 q^2}{n_2 + q - 1}. \\
 \sum_{\substack{y \in U_M \\ w \in U \setminus U_M}} \frac{1}{r_{G'}(y, w)} &= \frac{n_1^2 q^2}{n_1 + q - 1} \cdot \sum_{\substack{y \in U_M \\ w \in U \setminus U_M}} \frac{1}{r_{G''}(y, w)} = \frac{n_2 q^2}{2} + \frac{q n_2^2}{2}.
 \end{aligned}$$

For $x \in W \setminus W_M$ and $w \in U \setminus U_M$, the resistance distance between two vertices x and w is

$$r_{G'}(x, w) = 1 + 1 + \frac{2q - 1}{q^2} = \frac{2q^2 + 2q - 1}{q^2}.$$

Then, we have

$$\sum_{\substack{x \in W \setminus W_M \\ w \in U \setminus U_M}} \frac{1}{r_{G'}(x, w)} = \frac{q^2 n_1 n_2}{2q^2 + 2q - 1} \cdot \sum_{\substack{x \in W \setminus W_M \\ w \in U \setminus U_M}} \frac{1}{r_{G''}(x, w)} = \frac{n_1 n_2 q}{2}.$$

This gives

$$\begin{aligned}
 RH(G'') - RH(G') &= \left(\sum_{\substack{x \in W \setminus W_M \\ w \in U \setminus U_M}} \frac{1}{r_{G''}(x, w)} + \sum_{\substack{y \in U_M \\ w \in U \setminus U_M}} \frac{1}{r_{G''}(y, w)} + \sum_{\substack{z \in W_M \\ w \in U \setminus U_M}} \frac{1}{r_{G''}(z, w)} \right) \\
 &- \left(\sum_{\substack{x \in W \setminus W_M \\ w \in U \setminus U_M}} \frac{1}{r_{G'}(x, w)} + \sum_{\substack{y \in U_M \\ w \in U \setminus U_M}} \frac{1}{r_{G'}(y, w)} + \sum_{\substack{z \in W_M \\ w \in U \setminus U_M}} \frac{1}{r_{G'}(z, w)} \right). \\
 &= \left(\frac{n_1 n_2 q}{2} + \frac{n_2^2 q^2}{n_2 + q - 1} + \frac{n_2 q^2 + n_2^2 q}{2} \right) \\
 &- \left(\frac{q^2 n_1 n_2}{2q^2 + 2q - 1} + \frac{n_1^2 q^2}{n_1 + q - 1} + \frac{n_1 q^2 + n_1^2 q}{2} \right). \\
 &= n_1 n_2 \frac{2q^3 - q}{2(2q^2 + 2q - 1)} + \frac{q^2}{2} (n_2 - n_1) + \frac{q}{2} (n_2^2 - n_1^2) \\
 &+ \frac{n_2^2 q^2}{n_2 + q - 1} - \frac{n_1^2 q^2}{n_1 + q - 1}.
 \end{aligned}$$

where $n_2 - n_1 > 0$, $n_2^2 - n_1^2 > 0$ for $n_2 > n_1$. $\frac{2q^3 - q}{2(2q^2 + 2q - 1)} > 0$ for $q \geq 1$. By Lemma 4, the function $f(x) = \frac{x^2 q^2}{x + q - 1}$ for $q > 1$ and $x > q$ is strictly increasing. Thus when $n_2 \geq n_1 > q$, we have

$$\frac{n_2^2 q^2}{n_2 + q - 1} - \frac{n_1^2 q^2}{n_1 + q - 1} > 0.$$

According to the above analysis, we have $RH(G'') - RH(G') > 0$, thus

$$RH(G'') > RH(G').$$

This completes the proof. \square

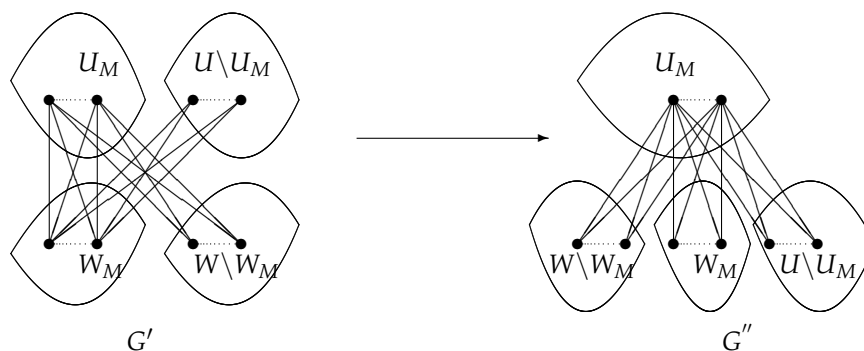


Figure 1. Two graphs G' and G'' in Theorem 3.

4. Graphs with Given Vertex Bipartiteness

In this section, we described the extremal graph with a given vertex bipartiteness for Resistance–Harary index. Let G_1 and G_2 be the graphs where any two vertices do not intersect. We obtain the joint graph of G_1 and G_2 through the correlation of every vertex of graph G_1 with every vertex of graph G_2 , denoted it by $G_1 \vee G_2$. The vertex bipartiteness of a graph G is the minimum number of vertices removed makes the graph G a bipartite graph, which is denoted by $v_b(G)$, see [17]. Let $G_{n,\delta}$ be the set of the graphs with n vertices and $v_b(G) \leq \delta$, where δ is the positive integer that does not exceed $n - 2$.

Lemma 5. *Let G be the graph in $G_{n,\delta}$. There is a pair of positive integers s and t that satisfies $s + t = n - \delta$, we have $RH(G) \leq RH(G^*)$ for all graphs $G \in G_{n,\delta}$, and the equality holds if and only if $G^* \cong K_\delta \vee K_{s,t}$.*

Proof. By Lemma 2, we know that RH is a topological index whose value increases with the number of edges. Let $G^* \in G_{n,\delta}$ be the graph with the largest RH index value, that is to say, $RH(G^*) \geq RH(G)$ for all graphs $G \in G_{n,\delta}$. Since $G^* \in G_{n,\delta}$, there are $v_1, v_2, \dots, v_k \in V(G^*)$ ($k \leq \delta$) such that $G^* - \{v_1, v_2, \dots, v_k\}$ is a bipartite graph, let (X, Y) be its vertex sets, and $|X| = s$ and $|Y| = t$. Thus, $s + t = n - k$. If $G^* - \{v_1, v_2, \dots, v_k\} \neq K_{s,t}$, then there exists two vertices u, v that are not adjacent and $u \in X, v \in Y$. We get another graph $G^* + e \in G_{n,\delta}$ by getting a new edge $e = uv$, then $RH(G^* + e) > RH(G^*)$, and we get the contradiction, so $G^* - \{v_1, v_2, \dots, v_k\} = K_{s,t}$. In addition, if there are two vertices that are not adjacent to each other and $u, v \in \{v_1, v_2, \dots, v_k\}$, then we get a new graph $G^* + uv \in G_{n,\delta}$, by adding a new edge uv into G^* , then $RH(G^* + uv) > RH(G^*)$, again, a contradiction. This suggests that the subgraph induced by $\{v_1, v_2, \dots, v_k\}$ is K_k , so $G^* \cong K_k \vee K_{s,t}$. At last, we prove that $k = \delta$. To the contrary, assume that $|X| = s \geq 2$ or $|Y| = t \geq 2$. Naturally, we set $t \geq 2$. Pick a vertex v from Y , and add the edges vv_i to $K_k \vee K_{s,t}$, where $v_i \in \{v_1, v_2, \dots, v_k\}$, the resulting graph is $K_{k+1} \vee K_{s,t-1} \in G_{n,\delta}$, and it has $t - 1 \geq 1$ edges more than graph G^* , implying that $RH(K_{k+1} \vee K_{s,t-1}) > RH(K_k \vee K_{s,t}) = RH(G^*)$, which is a contradiction. Therefore, $k = \delta$ and $G^* \cong K_\delta \vee K_{s,t}$. Complete the proof of the theorem. \square

Lemma 6. *Let $G \cong K_\delta \vee K_{s,t}$ and $G' \cong K_\delta \vee K_{s+1,t-1}$. If $s \leq t - 2$, then $RH(G') > RH(G)$.*

Proof. By the definition of the RH index and by Lemma 1, we have

$$\begin{aligned}
 RH(G) &= RH(K_\delta \vee K_{s,t}) \\
 &= RH(K_{s,t}) + RH(K_\delta) + \sum_{\substack{x \in V(K_{s,t}) \\ y \in V(K_\delta)}} \frac{1}{r_G(x,y)}, \\
 &= RH(K_{s,t}) + RH(K_\delta) \\
 &+ s\delta(1 + \frac{t(\delta-1)}{2} + \frac{(s-1)t}{3}) + t\delta(1 + \frac{s(\delta-1)}{2} + \frac{(t-1)s}{3}), \\
 &= \frac{st(4st + (s+t)^2 - 3(s+t) + 2)}{4(s+t-1)} + \frac{\delta^2(\delta-1)}{8}, \\
 &+ \frac{\delta(6s + 6t + 6st(\delta-1) + 2st(s+t-2))}{6},
 \end{aligned}$$

where $M = (s+t)^2 - 3(s+t) + 2$. We have

$$\begin{aligned}
 RH(G') &= RH(K_\delta \vee K_{s+1,t-1}) \\
 &= RH(K_{s+1,t-1}) + RH(K_\delta) + \sum_{\substack{x \in V(K_{s+1,t-1}) \\ y \in V(K_\delta)}} \frac{1}{r_G(x,y)}, \\
 &= \frac{4(s+1)^2(t-1)^2 + M(st+t-s-1)}{4(s+t-1)} + \frac{\delta^2(\delta-1)}{8}, \\
 &+ \frac{\delta(6s + 6t + 6(s+1)(t-1)(\delta-1) + 2(s+1)(t-1)(s+t-2))}{6}.
 \end{aligned}$$

where $M = (s+t)^2 - 3(s+t) + 2$. So

$$\begin{aligned}
 RH(G') - RH(G) &= \frac{4(t-s-1)(2st+t-s-1) + M(t-s-1)}{4(s+t-1)}, \\
 &+ \frac{\delta(t-s-1)(6(\delta-1) + 2(s+t-2))}{6}, \\
 &> 0.
 \end{aligned}$$

where $M = (s+t)^2 - 3(s+t) + 2$. Then $RH(G') > RH(G)$. This completes the proof. \square

Next, we describe the graphs with extremal Resistance–Harary index values in the graph with given vertex bipartiteness. The following conclusion is easy to deduce by applying Lemmas 2, 5, and 6.

Theorem 4. Let G be the graph of $G_{n,\delta}$. Where $1 \leq \delta \leq n - 2$, then

(a) If $n - m$ is even, then $RH(G^*) \geq RH(G)$ holds, where $G^* \cong K_\delta \vee K_{\frac{n-\delta}{2}, \frac{n-\delta}{2}}$.

(b) If $n - m$ is odd, then $RH(G^*) \geq RH(G)$ holds, where $G^* \cong K_\delta \vee K_{\lfloor \frac{n-\delta}{2} \rfloor, \lceil \frac{n-\delta+1}{2} \rceil}$.

5. Bipartite Graph with a Given Cut Edges

In this section, we determine bipartite graph given cut edges with maximum Resistance–Harary index.

Lemma 7. G_1 and G_2 are connected graphs whose vertices do not intersect, assume that $u \in G_1$ and $v \in G_2$. We connect u and v to get G , and if we identified two vertices u with v in G , we get graph G' . Let the new vertex be w , which is adjacent to a pendant vertex w_0 (see Figure 2). Then $RH(G') > RH(G)$.

Proof. By Lemma 1 and the definition of *RH* index, we have

$$RH(G) = \sum_{i=1}^2 RH(G_i) + \sum_{x \in V(G_1)} \frac{1}{r_{G_1}(x, u) + 1} + 1 + \sum_{y \in V(G_2)} \frac{1}{r_{G_2}(v, y) + 1} + \sum_{\substack{x \in V(G_1), \\ y \in V(G_2)}} \frac{1}{r_{G_1}(x, u) + r_{G_2}(y, v) + 1}.$$

$$RH(G') = \sum_{i=1}^2 RH(G_i) + \sum_{x \in V(G_1)} \frac{1}{r_{G_1}(x, u) + 1} + 1 + \sum_{y \in V(G_2)} \frac{1}{r_{G_2}(v, y) + 1} + \sum_{\substack{x \in V(G_1), \\ y \in V(G_2)}} \frac{1}{r_{G_1}(x, u) + r_{G_2}(y, v)}.$$

$$RH(G') - RH(G) = \sum_{\substack{x \in V(G_1), \\ y \in V(G_2)}} \left(\frac{1}{r_{G_1}(x, u) + r_{G_2}(y, v)} - \frac{1}{r_{G_1}(x, u) + r_{G_2}(y, v) + 1} \right) > 0.$$

Then $RH(G') > RH(G)$. This completes the proof. \square

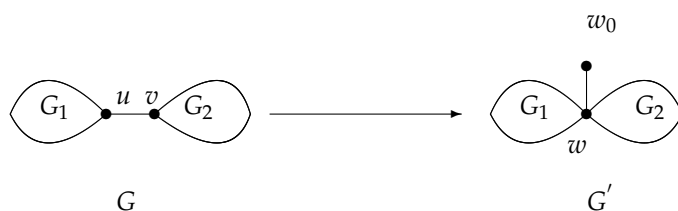


Figure 2. Graphs G and G' in Lemma 7.

Lemma 8 ([13]). Let G be a graph from a connect graph G_0 by attaching some pendant vertices. If u and v are two vertices in graph G_0 , pendant vertices u_1, u_2, \dots, u_a are attached to the vertex u and b pendant vertices v_1, v_2, \dots, v_b are attached to the vertex v . Let $G' = G - \{uv_1, uv_2, \dots, uv_b\} + \{uv_1, uv_2, \dots, uv_b\}$ and $G'' = G - \{uu_1, uu_2, \dots, uu_a\} + \{vu_1, vu_2, \dots, vu_a\}$. Then $RH(G') > RH(G)$ or $RH(G'') > RH(G)$.

Lemma 9. For bipartite graph $K_{r,s}^k$ with $r > s + 2$ and $k, s \geq 1$ (see Figure 3). One has $RH(K_{r,s}^k) < RH(K_{r-1,s+1}^k)$.

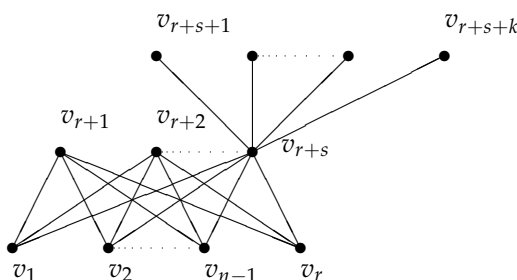


Figure 3. The graph $K_{r,s}^k$.

Proof. By Lemmas 1 and direct calculations, we can get the value of RH of $K_{r,s}^k$.

$$\begin{aligned} RH(K_{r,s}^k) &= RH(S_k) + RH(K_{r,s}) + \sum_{\substack{x \in V(S_k) \\ y \in V(K_{r,s})}} \frac{1}{r_G(x,y)} \\ &= \frac{k^2 + 3k}{4} + \frac{rs(4rs + (r+s)^2 - 3(r+s) + 2)}{4(r+s-1)} + k \left[\frac{rs+2}{r+2} + \frac{sr^2}{rs+r+s-1} \right]. \end{aligned}$$

Let $f(r,s) = \frac{rs(4rs+(r+s)^2-3(r+s)+2)}{4(r+s-1)}$. Then we know from the proof of Theorem 1, $f(r-1, s+1) > f(r,s)$. Similarly, let $g(r,s) = \frac{rs+2}{r+2} + \frac{sr^2}{rs+r+s-1}$, by comparison, we have $g(r-1, s+1) - g(r,s) > 0$. Thus, we have $RH(K_{r,s}^k) < RH(K_{r-1,s+1}^k)$. This completes the proof. \square

By Lemma 9, it is straightforward to see that

Corollary 2. Let \mathcal{G}_n^k be the bipartite graphs of order n with k cut edges obtained by identifying the center of K_{k+1} order star graph and one vertex of a complete graph with $n-k$ vertices. For $G \in \mathcal{G}_n^k$, we have $RH(G) \leq RH(K_{\lfloor \frac{n-k}{2} \rfloor \lceil \frac{n-k}{2} \rceil}^k)$, and equality is attained if and only if $G \cong K_{\lfloor \frac{n-k}{2} \rfloor \lceil \frac{n-k}{2} \rceil}^k$.

Let \mathcal{B}_n^k be the set of connected bipartite graphs with n order and k cut edges. For $k=0$, from Theorem 1, then the graph with maximum RH index is isomorphic to graph $K_{\lfloor \frac{n}{2} \rfloor \lceil \frac{n}{2} \rceil}$. For $k=n-1$, the bipartite graph is a tree, so the Resistance distance and distance between the vertices in the tree are equal, that is, the Resistance–Harary index in the tree was the same as the Harary index. So the maximum Resistance–Harary index is obtained uniquely at S_n .

Next, we focus on the case $1 \leq k \leq n-4$.

Theorem 5. In all connected bipartite graphs with n order and k cut edges, where $1 \leq k \leq n-4$, the maximum Resistance–Harary index is founded at $K_{\lfloor \frac{n-k}{2} \rfloor \lceil \frac{n-k}{2} \rceil}^k$.

Proof. Let G_0 be the graph having the maximum RH index value in \mathcal{B}_n^k and E_1 be the set of cut edges of G_0 . Where G_0 and $G_0 - E_1$ are bipartite graphs, then by Lemma 2, we can know that each component of $G_0 - E_1$ is a complete bipartite graph. In addition, by Lemma 7, every edge of E_1 must be pendant edges. Hence, G_0 must be the graph constructed from $K_{m,n-m-k}$ by hanging k pendant edges. Finally, by Lemma 8, all these pendant edges in G_0 must be attached to one common vertex. That is to say, G_0 must be one of the graph \mathcal{G}_n^k , furthermore, by Corollary 2, we get that $G_0 \cong K_{\lfloor \frac{n-k}{2} \rfloor \lceil \frac{n-k}{2} \rceil}^k$. This completes the proof. \square

6. Discussion

Chemical graph theory is the topology branch of mathematical chemistry which applies graph theory to mathematical modelling of chemical phenomena. In chemical graph theory, vertices represent atoms and edges represent the connections between atoms. The topological exponent of a graph is a function defined on a (molecular) graph regardless of the labeling of its vertices. The Resistance–Harary index is a topological descriptor that has been correlated with the relationship between structure and performance and between structure and activity molecular descriptors. To correlate with electrical network theory and real analysis, the Resistance–Harary index has much better predictive power than that of the global cyclicity index.

7. Conclusions

In this paper, we first present a structural of the extremal graphs for Resistance–Harary index over all bipartite graphs with n vertices, then characterize the extremal graphs given vertex bipartiteness on the RH index. Moreover, we optimize the extremal structure of bipartite graphs with given cut edges

and bipartite graphs with given matching numbers. Along this line, some other interesting extremal problems on bipartite graphs with given parameters are valuable to be considered. In the future we can also characterize extremal bipartite graphs with fixed diameter on the Resistance–Harary index.

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Sample Availability: Samples of the compounds are available from the authors.



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