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On the Resistance–Harary Index of Unicyclic Graphs

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Abstract

In this paper, we study a new graph invariant named Resistance-Harary index, defined as $RH(G) = \sum\limits_{\{u,v\}\subseteq V(G)} \dfrac{1}{r_G(u,v)}$, where $r_G(u,v)$ is the resistance distance between vertices u and v of a connected graph G. We establish that S_n^3 and P_n^3 are the graphs with the maximal and minimal Resistance-Harary index among all unicyclic graphs on n vertices, respectively.

1 Introduction

Topological indices are numbers associated with molecular structures which serve for quantitative relationships between chemical structures and properties. The first such index was published by Wiener [1], but the name topological index was invented by Hosoya [2]. Many of them are based on the graph distance [3], the vertex degree [4]. In addition, several graph invariants are based on both the vertex degree and the graph distance [5].

All graphs considered in this paper are both connected and simple. For any $v \in V(G)$, $d(v)$ is the degree of vertex v, the distance between vertices u and v, denoted by $d(u,v)$, is the length of a shortest path between them. Wiener index was introduced by American

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chemist H. Wiener in [5], defined as

$$W(G) = \sum_{\{u,v\} \subseteq V(G)} d(u,v) \tag{1}$$

Another distance-based graph invariant *Harary index*, has been introduced independently by D. Plavšić et al. [6] and by O. Ivanciuc et al. [7] in 1993 for the characterization of molecular graphs. It has been named in honor of Professor Frank Harary on the occasion of his 70th birthday. The Harary index $H(G)$ is defined as the sum of reciprocals of distances between all pairs of vertices of the graph G, i.e.

$$H(G) = \sum_{\{u,v\} \subseteq V(G)} \frac{1}{d(u,v)} \tag{2}$$

I. Gutman in [8] and K. Xu in [9] investigated the Harary index of trees, they showed that for any n-vertex tree T, $H(P_n) \leq H(T) \leq H(S_n)$ with left equality holding if and only if $T \cong P_n$, and right equality holding if and only if $T \cong S_n$. More results related to Harary index, please refer to [10].

In 1993, Klein and Randić [11] introduced a distance function named *resistance distance* on the basis of electrical network theory. They viewed a graph G as an electrical network N such that each edge of G is assumed to be a unit resistor. The resistance distance between the vertices u and v, are denoted by $r_G(u,v)$ ($r(u,v)$ for short), is defined to be the effective resistance between nodes u, $v \in N$, which is computed by the methods of the theory of resistive electrical networks based on Ohm's and Kirchhoff's laws. The Kirchhoff index $Kf(G)$ of a graph G is defined as [11, 12]

$$Kf(G) = \sum_{\{u,v\} \subseteq V(G)} r(u,v) \tag{3}$$

The Kirchhoff index is an important molecular structure descriptor [11], it has been well studied in both mathematical and chemical literatures, see recent papers [12-17] and references therein.

The reciprocal resistance distance is also called electrical conductance, D. J. Klein and O. Ivanciuc in [18] investigated QSAR and QSPR molecular descriptors computed from the resistance distance and electrical conductance matrices, and they proposed the global cyclicity index $C(G)$ as

$$C(G) = \sum_{u \sim v} \left[\frac{1}{r(u,v)} - \frac{1}{d(u,v)} \right] \tag{4}$$

where $u \sim v$ means u, v are adjacent and the sum is over all edges of G. Since $d(u,v) = 1$ for $u \sim v$, $C(G)$ can also be rewritten as

$$C(G) = \sum_{u \sim v} \frac{1}{r(u,v)} - |E(G)| \tag{5}$$

In [19], Y. Yang using techniques from graph theory, electrical network theory and real analysis, obtained some results on global cyclicity index.

Analogous to the relationship between Winer index and Harary index, we introduce here a new graph invariant reciprocal to Kirchhoff index, named *Resistance-Harary index*, as

$$RH(G) = \sum_{\{u,v\} \subseteq V(G)} \frac{1}{r(u,v)} \tag{6}$$

Obviously, the Resistance-Harary index is a generalization of global cyclicity index.

A graph G is called a unicyclic graph if it contains exactly one cycle, the unique cycle $C_l = v_1 v_2 \cdots v_l v_1$ in a unicyclic graphs, simply denoted as $G = U(C_l; T_1, T_2, \cdots, T_l)$, where T_i is the components of G. $E(C_l)$ containing $v_i, 1 \leq i \leq l$, T_i is a tree rooted at v_i. Let P_n^l denote the graph obtained by identifying one end-vertex of P_{n-l+1} with any vertex of C_l, S_n^l denote the graph obtained from cycle C_l by adding $n-l$ pendant edges to a vertex of C_l. Obviously, $P_n^n = S_n^n = C_n$. Let $\mathcal{U}(n;l)$ be the set of unicyclic graphs with n vertices and the unique cycle C_l, $\mathscr{U}(n)$ be the set of unicyclic graphs with n vertices.

For a graph G with $v \in V(G)$, $G - v$ denotes the graph resulting from G by deleting v (and its incident edges). For an edge uv of the graph G (the complement of G, respectively), $G - uv$ ($G + uv$, respectively) denotes the graph resulting from G by deleting (adding, respectively) uv.

In this paper, we determine firstly that among $\mathcal{U}(n,l)$, S_n^l has the maximal Resistance-Harary index. Secondly, we determine the graph with the maximum and minimum Resistance-Harary index among all unicyclic graphs.

The paper is organized as follows, in Section 2 we state some preparatory results, whereas in Section 3 we state our main results.

2 Preliminary Results

Let $R_G(u) = \sum_{v\in V(G)\setminus\{u\}} \frac{1}{r(u,v)}$, then $RH(G) = \sum_{v\in V(G)} R_G(v)$. Let C_g be the cycle on $g \geq 3$ vertices, for any two vertices $v_i, v_j \in V(C_g)$ with $i < j$, by Ohm's law, one has

$$r_{C_g}(v_i, v_j) = \frac{(j-i)(g+i-j)}{g} .$$

For any vertex $v \in V(C_g)$, it is easy to see that $R_{C_g}(v) = 2\sum_{i=1}^{g-1} \frac{1}{i}$, and the Resistance-Harary index of C_n is $RH(C_n) = \sum_{v\in V(C_n)} R_{C_g}(v) = n\sum_{i=1}^{n-1} \frac{1}{i}$.

Lemma 2.1([11]). Let x be a cut vertex of a connected graph and a and b be vertices occurring in different components which arise upon deletion of x. Then

$$r_G(a,b) = r_G(a,x) + r_G(x,b) . \tag{7}$$

Let v be a vertex of degree $p+1$ in a graph G, such that $vv_1, vv_2, \cdots, vv_p$ are pendant edges incident with v, and u is the neighbor of v distinct from $v_1, v_2, \cdots, v_p$, and $G' = \sigma(G,v)$ by removing the edges $vv_1, vv_2, \cdots, vv_p$ and adding new edges $uv_1, uv_2, \cdots, uv_p$, see Figure 1.

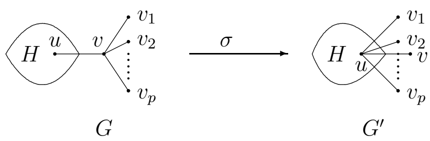

Figure 1. The σ-transformation at v

Lemma 2.2. Let $G' = \sigma(G,v)$ be a graph transformed from the graph G, $d(u) \geq 1$ described in Figure 1. Then $RH(G) \leq RH(G')$, with equality holds if and only if G is a star with v as its center.

Proof. Let $V_1 = \{v, v_1, v_2, \cdots, v_p\}$ in G, and $V_2 = \{v, v_1, v_2, \cdots, v_p\}$ in G'. By the definition of Resistance-Harary index, one has

$$\begin{aligned} RH(G) &= \sum_{x,y\in V(H)} \frac{1}{r(x,y)} + \sum_{x,y\in V(G_1)} \frac{1}{r(x,y)} + \sum_{x\in V(H),y\in V(G_1)} \frac{1}{r(x,y)} \\ &= RH(H) + p + \frac{1}{2}\binom{p}{2} + \sum_{x\in V(H)} \frac{1}{r(x,u)+1} + p\sum_{x\in V(H)} \frac{1}{r(x,u)+2}, \\ RH(G') &= RH(H) + \frac{1}{2}\binom{p+1}{2} + (p+1)\sum_{x\in V(H)} \frac{1}{r(x,u)+1} . \end{aligned}$$

Thus,

$$RH(G) - RH(G') = \frac{p}{2} + p(\sum_{x\in V(H)} \frac{1}{r(x,u)+2} - \sum_{x\in V(H)} \frac{1}{r(x,u)+1})$$
$$= p \sum_{x\in V(H)-u} (\frac{1}{r(x,u)+2} - \frac{1}{r(x,u)+1}) < 0 \ .$$

The proof is completed.

Let u, v be two vertices in a graph G, such that $u_1, u_2, \cdots, u_s$ are pendants incident with u, $v_1, v_2, \cdots, v_t$ are pendants incident with v in $G_0 \subseteq G$, respectively. G' and G'' are two graphs β-transformed from G, such that $G' = G - \{vv_1, vv_2, \cdots, vv_t\} + \{uv_1, uv_2, \cdots, uv_t\}$, $G'' = G - \{uu_1, uu_2, \cdots, uu_s\} + \{vu_1, vu_2, \cdots, vu_s\}$, see Figure 2.

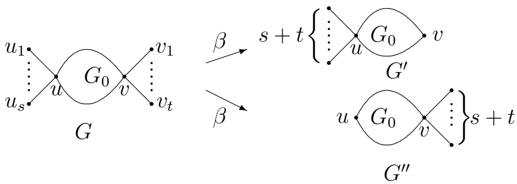

Figure 2.The transformation β

Lemma 2.3. Let G', G'' be the graphs transformed from the graph G, $d(u) \geq 1$ described in Figure 2. Then $RH(G) < RH(G')$ or $RH(G) < RH(G'')$.

Proof. For the convenience, one let $V_1 = \{u_1, u_2, \cdots, u_s\}$, $V_2 = \{v_1, v_2, \cdots, v_t\}$ in G, and $V_3 = \{u_1, u_2, \cdots, u_s, v_1, v_2, \cdots, v_t\}$ in G'. By the definition of Resistance-Harary index, one has

$$RH(G) = \sum_{x,y\in V(G_0)} \frac{1}{r(x,y)} + \sum_{x,y\in V(G_1)} \frac{1}{r(x,y)} + \sum_{x,y\in V(G_2)} \frac{1}{r(x,y)} + \sum_{x\in V(G_0),y\in V(G_1)} \frac{1}{r(x,y)}$$
$$+ \sum_{x\in V(G_0),y\in V(G_2)} \frac{1}{r(x,y)} + \sum_{x\in V(G_1),y\in V(G_2)} \frac{1}{r(x,y)} = RH(G_0) + \frac{1}{2}\binom{s}{2} + \frac{1}{2}\binom{t}{2}$$
$$+ s\sum_{x\in V(G_0)} \frac{1}{r(x,u)+1} + t\sum_{x\in V(G_0)} \frac{1}{r(x,v)+1} + \frac{st}{r(u,v)+2},$$

and

$$RH(G') = RH(G_0) + \frac{1}{2}\binom{s+t}{2} + (s+t)\sum_{x\in V(G_0)} \frac{1}{r(x,u)+1},$$

$$RH(G'') = RH(G_0) + \frac{1}{2}\binom{s+t}{2} + (s+t)\sum_{x\in V(G_0)} \frac{1}{r(x,v)+1} \ .$$

Thus,

$$\begin{aligned}\Delta_1 &= RH(G) - RH(G') \\ &= t\left(\sum_{x\in V(G_0)} \frac{1}{r(x,v)+1} - \sum_{x\in V(G_0)} \frac{1}{r(x,u)+1}\right) + st\left(\frac{1}{l+2} - \frac{1}{2}\right).\end{aligned}$$

and

$$\begin{aligned}\Delta_2 &= RH(G) - RH(G'') \\ &= s\left(\sum_{x\in V(G_0)} \frac{1}{r(x,u)+1} - \sum_{x\in V(G_0)} \frac{1}{r(x,v)+1}\right) + st\left(\frac{1}{l+2} - \frac{1}{2}\right).\end{aligned}$$

If $\Delta_1 > 0$, then $\sum_{x\in V(G_0)} \frac{1}{r(x,u)+1} < \sum_{x\in V(G_0)} \frac{1}{r(x,v)+1} + s\left(\frac{1}{l+2} - \frac{1}{2}\right)$,

thus

$$\begin{aligned}\Delta_2 &< s\left(\sum_{x\in V(G_0)} \frac{1}{r(x,v)+1} + \frac{s}{l+2} - \frac{s}{2}\right) - s\sum_{x\in V(G_0)} \frac{1}{r(x,v)+1} + st\left(\frac{1}{l+2} - \frac{1}{2}\right) \\ &= s(s+t)\left(\frac{1}{l+2} - \frac{1}{2}\right) < 0.\end{aligned}$$

The proof is completed.

3 Main Results

When we study some property of graphs, a tree is generally regarded as the simplest graph to be firstly considered. In this section, we firstly give the lower and upper bound on trees with respect to Resistance-Harary index.

From Ref. [8, 9], it is easy to see that,

Theorem 3.1. Let T be a tree of order n. Then we have

$$RH(P_n) \le RH(T) \le RH(S_n)$$

with left equality holding if and only if $T \cong P_n$, and right equality holding if and only if $T \cong S_n$.

Secondly, we'll investigate the Resistance-Harary index of $\mathscr{U}(n)$.

By Lemma 2.2 and Lemma 2.3, we arrive at,

Theorem 3.2. Let $G \in \mathcal{U}(n;g)$, then $RH(G) \le RH(S_n^g)$.

Nextly, we'll determine the graph in $\mathscr{U}(n)$ with the maximum Resistance-Harary index.

Theorem 3.3. Let $G \in \mathscr{U}(n)$, then we have $RH(G) \leq \frac{1}{20}(n^2+9n+18)$ with equality holding if and only if $G \cong S_n^3$ for $n \geq 9$ and $G \cong C_n$ for $n \leq 8$.

Proof. Let $H = G - C_g$, by the definition of Resistance-Harary index, one has,

$$
\begin{aligned}
RH(S_n^g) &= \sum_{\{u,v\}\subseteq V(G)} \frac{1}{r(u,v)} \\
&= \sum_{\{u,v\}\subseteq V(C_g)} \frac{1}{r(u,v)} + \sum_{\{u,v\}\subseteq V(H)} \frac{1}{r(u,v)} + \sum_{u\in V(C_g),v\in V(H)} \frac{1}{r(u,v)} \\
&= g\left(1+\frac{1}{2}+\frac{1}{3}+\cdots+\frac{1}{g-1}\right)+\frac{1}{4}(n-g)(n+3-g) \\
&+ g(n-g)\left(\frac{1}{2g-1}+\frac{1}{3g-4}+\cdots+\frac{1}{g\cdot g-(g-1)^2}\right)
\end{aligned}
$$

Similarly,

$$
\begin{aligned}
RH(S_n^{g-1}) = (g-1)\left(1+\frac{1}{2}+\frac{1}{3}+\cdots+\frac{1}{g-2}\right)+\frac{1}{4}(n+1-g)(n+4-g)+(g-1) \\
(n+1-g)\left(\frac{1}{2g-3}+\frac{1}{3s-7}+\cdots+\frac{1}{(g-1)\cdot(g-1)-(g-2)^2}\right)
\end{aligned}
$$

Further, by the symmetry of C_g, one has

$$
\begin{aligned}
\Delta &= RH(S_n^{g-1}) - RH(S_n^g) \\
&= (g-1)(n+1-g)\left(\frac{1}{2g-3}+\frac{1}{3g-7}+\cdots+\frac{1}{(g-1)\cdot(g-1)-(g-2)^2}\right) \\
&+ \frac{1}{2}(n-g) - g(n-g)\left(\frac{1}{2g-1}+\frac{1}{3g-4}+\cdots+\frac{1}{g\cdot g-(g-1)^2}\right) \\
&- \left(1+\frac{1}{2}+\frac{1}{3}+\cdots+\frac{1}{g-1}\right) \\
&= (n-g)\left\{\left[\underbrace{\left(\frac{g-1}{2g-3}+\frac{g-1}{3g-7}+\cdots+\frac{g-1}{2g-3}\right)}_{g-2}+\frac{1}{2}\right]\right. \\
&\left. - \left(\underbrace{\frac{g}{2g-1}+\frac{g}{3g-4}+\cdots+\frac{g}{2g-1}}_{g-1}\right)\right\} + (g-1)\left(\frac{1}{2g-3}+\frac{1}{3g-7}+\cdots\right. \\
&\left. + \frac{1}{(g-1)^2-(g-2)^2}\right) - \left(1+\frac{1}{2}+\frac{1}{3}+\cdots+\frac{1}{g-1}\right)
\end{aligned}
$$

Let

$$
\Theta = \left[\left(\frac{g-1}{2g-3}+\frac{g-1}{3g-7}+\cdots+\frac{g-1}{2g-3}\right)+\frac{1}{2}\right] - \left(\frac{g}{2g-1}+\frac{g}{3g-4}+\cdots+\frac{g}{2g-1}\right),
$$

then

$$\Theta = \begin{cases} \left(\frac{g-1}{2g-3} - \frac{g}{2g-1}\right) + \left(\frac{g-1}{3g-7} - \frac{g}{3g-4}\right) + \cdots + \left(\frac{g-1}{2g-3} - \frac{g}{2g-1}\right) \\ +\frac{1}{2} - \frac{4}{g+4}, & \text{If } g \geq 4 \text{ and } g \text{ is even,} \\ \left(\frac{g-1}{2g-3} - \frac{g}{2g-1}\right) + \left(\frac{g-1}{3g-7} - \frac{g}{3g-4}\right) + \cdots + \left(\frac{g-1}{2g-3} - \frac{g}{2g-1}\right) \\ +\frac{1}{2} - \frac{4g}{(g+2)^2-5}, & \text{If } g \geq 5 \text{ and } g \text{ is odd,} \end{cases} > 0 \ .$$

If $n \geq 9$, by gradually reducing the girth number, we have the desired result.

If $n \leq 8$, We can easily check that $RH(C_n) > RH(S_n^3)$.

Lastly, we'll determine the graph in $\mathscr{U}(n)$ with the minimum Resistance-Harary index.

Lemma 3.4([20]). Let G be a unicyclic graph of order $n \geq 5$. Then we have

$$H(P_n^3) \leq H(G) \leq H(S_n^3)$$

where the left equality holds if and only if $G \cong P_n^3$, and the right equality holds if and only if $G \cong S_n^3$ for $n \geq 6$ and $G \cong S_n^3$ or $G \cong C_5$ for $n = 5$.

Theorem 3.4. Let G be a unicyclic graph of order $n \geq 5$. Then we have

$$RH(G) \geq RH(P_n^3),$$

with equality holding if and only if $G \cong P_n^3$.

Proof. Let $G \in \mathscr{U}(n)$, $u, v \in V(G)$, one has $r(u,v) \leq d(u,v)$, then

$$RH(G) = \sum_{\{u,v\} \subseteq V(G)} \frac{1}{r(u,v)} \geq \sum_{\{u,v\} \subseteq V(G)} \frac{1}{d(u,v)} = H(G).$$

By combining Lemma 3.3, we have the desired result.

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