Article

General Randić Index of Unicyclic Graphs and Its Applications to Drugs

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Abstract: In this work, we determine the maximum general Randić index (a general symmetric function of vertex degrees) for $\eta_0 \leq \eta < 0$ among all n-vertex unicyclic graphs with a fixed maximum degree Δ and the maximum and the second maximum general Randić index for $\eta_0 \leq \eta < 0$ among all n-vertex unicyclic graphs, where $\eta_0 \approx -0.21$. We establish sharp inequalities and identify the graphs attaining the inequalities. Thereby, extremal graphs are obtained for the general Randić index, and certain open gaps in the theory of extremal unicyclic graphs are filled (some open problems are provided). We use computational software to calculate the Randić index for the chemical trees up to order 7 and use the statistical (linear regression) analysis to discuss the various applications of the Randić index with the physical properties of drugs on the said chemical trees. We show that the Randić index is better correlated with the heat of vaporization for these alkanes.

Keywords: Randić index; general Randić index; unicyclic graph; extremal graphs; maximum degree

MSC: 05C07; 05C15

1. Introduction

Consider a simple graph $G = (V, E)$ with a set of vertices $V = V(G)$ and a set of edges $E = E(G)$. The degree of a vertex u, denoted by $d(u)$, is the number of edges incident with u. The neighbor set of u, denoted by $N(u)$, is the set of all vertices that are connected to u by an edge, and the maximum degree of vertices in G is denoted by $\delta(G)$. $G + uv$ denotes the graph that is obtained from G by adding an edge $uv \notin E(G)$, and $G - uv$ denotes the subgraph of G that is obtained by deleting an edge $uv \in E(G)$ from G. Consider the path and cycle graphs on $n \geq 3$ vertices, denoted by P_n and C_n, respectively. To attach P_r to a vertex u in G means to add an edge from u and any endpoint of P_r. For $r = 1$, we attach a vertex of degree 1 to u. $N_G(u)$ denotes the neighborhood of u.

In [1], Randić introduced one of the most widely used molecular descriptors (topological index) in structure–activity and structure–property relationship studies, which was called the Randić index $R(G)$ [2–5]. Moreover, the product-connectivity index is another way to refer to this index, and it is defined as follows:

$$R(G) = \sum_{uv \in E(G)} (d(u)d(v))^{-\frac{1}{2}}.$$

The authors in [6] generalized $R(G)$ by introducing the general Randić index as

$$R_\eta(G) = \sum_{uv \in E(G)} (d(u)d(v))^\eta,$$

where η is real.

Determining the upper and lower bounds for the general Randić index and the characterization of the corresponding extremal graphs have received increasing attention. Several results related to extremal graphs have been published for various topological indices among the different classes of graphs, since for general graphs extremal problems are very hard. Most of the time, these extremal problems are studied for classes of graphs so that a deep analysis can be carried out and thereby some extremal families with respect to a topological index can be identified. In this study, we consider the general Randić index for the class of unicyclic graphs with order n and fix their invariants like the maximum degree.

In [7,8], two variants of $R_\eta(G)$ were studied along with lower and upper bounds for connected graphs, trees, and chemical trees. Also, in [9], Li and Yang found the maximum and the minimum general Randić indices of graphs for any value of η. Researchers have recently made progress on several open problems related to the general Randić index. Rada and Cruz [10] studied an unsolved case, while Cavers et al. [11] established a relationship between the general Randić index and the normalized eigenvalues of the Laplacian matrix of a graph. Guji and Vumar [12] determined, for $\eta \geq 1$, the maximum general Randić index of bicyclic graphs, and in [13] the minimum $R_\eta(G)$ was found for chemical trees with a given number of pendent vertices for any η. Hu et al. [14,15] determined the maximum and minimum general Randić indices of trees for certain ranges of η. An extensive survey of the Randi index was carried out by Li and Shi in [16]. Dalfó [17] obtained interesting results related to the Randić of graphs. Recently, some new results related to the Randić index were given in [18]. Zhand and Wu [19] and Liang and Wu [20] obtained results for the Randić index of line graphs. The Randić index and the Randić energy of graphs is a well studied branch of theory (see the recently published [21] and the references cited therein).

For the n-vertex trees with k ($3 \leq k \leq n - 2$) pendent vertices with $-1 \leq \eta < 0$, Liu et al. [22] found bounds for $R_\eta(G)$. Cui and Zhong [23] determined the maximum general Randić indices of n-vertex trees and chemical trees with k pendent vertices for $4 \leq k \leq \left\lfloor \frac{n+2}{3} \right\rfloor$ and $\eta_0 \leq \eta < 0$, where $\eta_0 \approx -0.5122$. Liu et al. [24] characterized the trees with extremal $R_\eta(G)$ for trees with the maximum degree. See [25–32] for more mathematical properties of the general Randić index. There are several other well-known indices and spectral invariants like in [33,34].

In this paper, we start with some lemmas and use them to determine the maximum general Randić index for $\eta_0 \leq \eta < 0$ among all n-vertex unicyclic graphs with a fixed maximum degree Δ and characterize the extremal graphs attaining the bounds (see Theorem 1). Moreover, in Theorem 2, we find the maximum and the second maximum general Randić index for $\eta_0 \leq \eta < 0$ among all n-vertex unicyclic graphs, where $\eta_0 \approx -0.21$ is a solution of the equation $9^\eta + 2^\eta - 2 \times 4^\eta = 0$, and some unique maximal graphs are identified with respect the mentioned invariants. At the end of Section 2, some open problems are given. In Section 3, we carry out QSPR/QSAR analysis of the Randić index and its linear regression analysis, with the help of computational software. We were able to successfully show that the Randić index is better correlated with the heat of vaporization for these chemical tress of orders up to 7 (alkanes).

2. Unicyclic Graphs with Maximum General Randić Index

Next, we give some lemmas, which will be applied in the main results.

Lemma 1. *Consider a connected graph Q of order $n \geq 2$. If G_1 and G_2 are the graphs obtained from Q by attaching P_a and P_b to $u \in V(Q)$ and attaching u to a path P_{a+b}, respectively, where a and b are positive integers, then*

$$R_\eta(G_2) > R_\eta(G_1) \text{ for } \eta_1 < \eta < 0,$$

where $\eta_1 \approx -0.284$ is a solution of the equation $2 \cdot 6^\eta + 2^\eta - 3 \cdot 4^\eta = 0$.

Proof. Let $d_Q(u) = t$ and $N_Q(u) = \{u_1, u_2, \cdots, u_t\}$. We have three cases.

(i) If $a = b = 1$, then

$$R_\eta(G_1) - R_\eta(G_2) = \sum_{i=1}^{t} d(u_i)^\eta \left[(t+2)^\eta - (t+1)^\eta \right]$$
$$+ 2(t+2)^\eta - 2^\eta(t+1)^\eta - 2^\eta$$
$$< 0,$$

since $\eta < 0$, $g'(t) = 2\eta\left((t+2)^{\eta-1} - (2t+2)^{\eta-1}\right) < 0$, for $g(t) = 2(t+2)^\eta - 2^\eta(t+1)^\eta - 2^\eta$ and $g(t) < g(0) = 2 \cdot 2^\eta - 2^\eta - 2^\eta = 0$.

(ii) If $a \geq 2$ and $b = 1$, then

$$R_\eta(G_1) - R_\eta(G_2) = \sum_{i=1}^{t} d(u_i)^\eta \left[(t+2)^\eta - (t+1)^\eta \right] + 2^\eta(t+2)^\eta + (t+2)^\eta$$
$$- 2^\eta(t+1)^\eta - 4^\eta$$
$$< 6^\eta + 3^\eta - 2 \cdot 4^\eta < 0.$$

In fact, let $g(t) = 2^\eta(t+2)^\eta + (t+2)^\eta - 2^\eta(t+1)^\eta - 4^\eta$; then,

$$g'(t) = \eta\left((2^\eta + 1)(t+2)^{\eta-1} - 2^\eta(t+1)^{\eta-1}\right),$$

and

$$(2^\eta + 1)(t+2)^{\eta-1} - 2^\eta(t+1)^{\eta-1} > 0$$

if and only if $(\frac{t+2}{t+1})^{1-\eta} < 1 + 2^{-\eta}$. We note that $t \geq 1$, $\eta < 0$, $(\frac{t+2}{t+1})^{1-\eta} \leq (\frac{3}{2})^{1-\eta}$, and $(\frac{3}{2})^{1-\eta} < 1 + 2^{-\eta}$. So, $g'(t) < 0$, $g(t) \leq g(1) = 6^\eta + 3^\eta - 2 \cdot 4^\eta < 0$ and $R_\eta(G_1) - R_\eta(G_2) < 0$, which implies the result.

(iii) If $a, b \geq 2$, then

$$R_\eta(G_1) - R_\eta(G_2) = \sum_{i=1}^{t} d(u_i)^\eta \left[(t+2)^\eta - (t+1)^\eta \right] + 2 \cdot 2^\eta(t+2)^\eta + 2^\eta$$
$$- 2^\eta(t+1)^\eta - 2 \cdot 4^\eta.$$

Clearly, the function $f(t) = 2 \cdot 2^\eta(t+2)^\eta + 2^\eta - 2^\eta(t+1)^\eta - 2 \cdot 4^\eta$ is decreasing, since $f'(t) = 2^\eta\eta(2(t+2)^{\eta-1} - (t+1)^{\eta-1})$, and $2(t+2)^{\eta-1} - (t+1)^{\eta-1} > 0$ if and only if $2 > (\frac{t+2}{t+1})^{1-\eta}$, and $(\frac{t+2}{t+1})^{1-\eta} \leq (\frac{3}{2})^{1-\eta} < 2$, for $t \geq 1$ and $-0.7 < \eta < 0$. Thus,

$$2 \cdot 2^\eta(t+2)^\eta + 2^\eta - 2^\eta(t+1)^\eta - 2 \cdot 4^\eta \leq 2 \cdot 6^\eta + 2^\eta - 3 \cdot 4^\eta < 0$$

provided $\eta_1 < \eta < 0$. So, we have

$$R_\eta(G_1) - R_\eta(G_2) < 0$$

for $\eta_1 < \eta < 0$.

The proof is complete. $\square$

Lemma 2. *Consider a connected graph M such that $|V(M)| \geq 3$. Let $u \in V(M)$ be a degree 2 vertex with its two neighbors u_1 and u_2. If $d(u_2) \leq 3$, $H = M \cup P_a + uv_1$ is the graph obtained from M by attaching a path $P_a = v_1v_2 \cdots v_a$ to u and $H' = H - \{uu_2\} + \{v_au_2\}$, then*

$$R_\eta(H') > R_\eta(H) \text{ for } \eta_0 \leq \eta < 0,$$

where $\eta_0 \approx -0.21$ is a solution of the equation $9^\eta + 2^\eta - 2 \times 4^\eta = 0$.

Proof. Note that $f(x) = (2x)^\eta - (3x)^\eta$ is decreasing for $x \geq 1$ and $\eta < 0$.

If $d_H(u, v_a) = 1$, i.e., $a = 1$, then, for $\eta_0 \leq \eta < 0$, we have

$$
\begin{aligned}
R_\eta(H) - R_\eta(H') &= 3^\eta (d(u_1))^\eta + 3^\eta + 3^\eta (d(u_2))^\eta - 2^\eta (d(u_1))^\eta - 4^\eta - 2^\eta (d(u_2))^\eta \\
&= (3^\eta - 2^\eta)((d(u_1))^\eta + (d(u_2))^\eta) + 3^\eta - 4^\eta \\
&< (3^\eta - 2^\eta) d(u_2)^\eta + 3^\eta - 4^\eta \\
&< 9^\eta - 6^\eta + 3^\eta - 4^\eta < 0.
\end{aligned}
$$

If $d_H(u, u') \geq 2$, i.e., $a > 1$, then, for $\eta_0 \leq \eta < 0$, we have

$$
\begin{aligned}
R_\eta(H) - R_\eta(H') &= 3^\eta (d(u_1))^\eta + 3^\eta (d(u_2))^\eta + 6^\eta + 2^\eta - 2^\eta (d(u_1))^\eta \\
&\quad - 2 \cdot 4^\eta - 2^\eta (d(u_2))^\eta \\
&= (3^\eta - 2^\eta)((d(u_1))^\eta + (d(u_2))^\eta) + 6^\eta + 2^\eta - 2 \cdot 4^\eta \\
&< (3^\eta - 2^\eta)(d(u_2))^\eta + 6^\eta + 2^\eta - 2 \cdot 4^\eta \\
&< 9^\eta + 2^\eta - 2 \cdot 4^\eta < 0,
\end{aligned}
$$

as $9^\eta + 2^\eta - 2 \cdot 4^\eta < 0$, for $\eta_0 \leq \eta < 0$. $\quad\square$

Next, we consider the maximum $R_\eta(G)$ of unicyclic graphs with a given maximum degree.

For $n \geq 3$, let $\mathcal{U}(n, \Delta)$ be a class of simple unicyclic graphs with n vertices and a maximum degree of Δ ($2 \leq \Delta \leq n - 1$). Specifically, $\mathcal{U}(n, \Delta) = \{C_n\}$ for $\Delta = 2$.

For $\frac{n+2}{2} \leq \Delta \leq n - 1$, $U_{n,\Delta}$ denotes the unicyclic graph obtained by attaching $n - \Delta - 1$ paths of a length of at least one to a vertex of K_3 and $2\Delta - n - 1$ pendant vertices.

In the following, we will determine the maximum value of $R_\eta(G)$ of graphs in $\mathcal{U}(n, \Delta)$ along with identifying corresponding extremal graphs. Consequently, for $\eta_0 \leq \eta < 0$, we find the unicyclic graph with the first and the second maximum $R_\eta(G)$.

Theorem 1. *Let $G \in \mathcal{U}(n, \Delta)$ be a unicyclic graph and $\eta_0 \leq \eta < 0$. Then,*

$$
R_\eta(G) \leq
\begin{cases}
(n - \Delta - 1)2^\eta + (n - \Delta + 1)(2\Delta)^\eta + (2\Delta - n - 1)(\Delta)^\eta + 4^\eta, \\
\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\quad if \ \frac{n+2}{2} \leq \Delta \leq n - 1 \\
\\
(\Delta - 2)2^\eta + \Delta(2\Delta)^\eta + (n - 2\Delta + 2)4^\eta, \quad if \ 2 \leq \Delta \leq \frac{n+1}{2}.
\end{cases}
$$

with equality if and only if $G = U_{n,\Delta}$ for $\frac{n+2}{2} \leq \Delta \leq n - 1$, and G is a unicyclic graph obtained from a cycle by attaching $\Delta - 2$ paths of a length of at least one to a vertex for $2 \leq \Delta \leq \frac{n+1}{2}$.

Proof. Let G be a graph that belongs to $\mathcal{U}(n, \Delta)$ with a maximum general Randić index, v be a vertex in G with degree Δ, and C be the unique cycle of G.

The case $\Delta = 2$ is trivial since in this case $G = C_n$. In the following, we assume that $\Delta \geq 3$.

If $\Delta = 3$ and there exists a vertex of degree 3 outside the cycle C, then Lemma 1 implies that we can obtain a graph that belongs to $\mathcal{U}(n, 3)$ with a greater general Randić index, and this gives a contradiction. If C has at least two vertices of degree 3, then, using Lemma 2, the same conclusion is obtained. Thus, the unique vertex of degree 3 in G is $v \in V(C)$.

Now, if v has a neighbor of degree 1, then

$$
R_\eta(G) = (n - 3)4^\eta + 2 \times 6^\eta + 3^\eta \ \text{for} \ n \geq 4.
$$

But if v has no neighbors of degree 1, then

$$
R_\eta(G) = (n - 4)4^\eta + 3 \times 6^\eta + 2^\eta \ \text{for} \ n \geq 5.
$$

By subtracting the two values, we obtain

$$[(n-3)4^\eta + 2 \times 6^\eta + 3^\eta] - [(n-4)4^\eta + 3 \times 6^\eta + 2^\eta]$$
$$= 4^\eta - 6^\eta + 3^\eta - 2^\eta < 0 \text{ for } \eta < 0.$$

Hence, $G = U_{4,3}$ is a graph obtained by adding a vertex, which is a pendant to K_3 (triangle) for $n = 4$, and G is a graph that is obtained by attaching a cycle for $n \geq 5$ to a path of a length of at least 2.

Let $\Delta \geq 4$. Similar to the case where $\Delta = 3$, it can be concluded that v is the unique vertex with the maximum degree in G. We will show that $v \in V(C)$. Otherwise, consider a vertex w on the cycle C where $d_G(v, w)$ is equal to $\min\{d_G(v, y) : y \in V(C)\}$. If there is a vertex different from v of a degree greater than 2 outside C, or if there is a vertex different from w of a degree greater than 2 on C, then, using Lemmas 1 and 2, we can obtain a graph in $\mathcal{U}(n, \Delta)$ with a greater $R_\eta(G)$, and this leads to a contradiction. Therefore, w and v are vertices of a degree higher than 2 in G. Moreover, $d_G(v) = \Delta$ and $d_G(w) = 3$. Now, consider the path connecting v and w, say Q, and let $v_1, v_2, \cdots, v_{\Delta-1}$ be the neighbors of v outside Q and $d_i = d_G(v_i)$ for $i = 1, \cdots, \Delta - 1$. Then, $d_1, \cdots, d_{\Delta-1} \in \{1, 2\}$. Otherwise, we can obtain a graph in $\mathcal{U}(n, \Delta)$ with a higher $R_\eta(G)$ using Lemma 1. Now, let

$$G_1 = G - \{vv_3, \cdots, vv_{\Delta-1}\} + \{wv_3, \cdots, wv_{\Delta-1}\}.$$

Then, $G_1 \in \mathcal{U}(n, \Delta)$, $d_{G_1}(w) = \Delta$, $d_{G_1}(v) = 3$, and

$$R_\eta(G_1) - R_\eta(G) = (3d_1)^\eta - (d_1\Delta)^\eta + (3d_2)^\eta - (d_2\Delta)^\eta + 2(2\Delta)^\eta - 2 \times 6^\eta$$
$$> 6^\eta - (2\Delta)^\eta + 6^\eta - (2\Delta)^\eta + 2(2\Delta)^\eta - 2 \times 6^\eta = 0,$$

since the function $(3x)^\eta - (x\Delta)^\eta$ is strictly decreasing for $x \geq 1$ for $\Delta \geq 4$.

Note that $d_{G_1}(v) = 3$. Using Lemma 1 again, we can obtain a graph $G' \in \mathcal{U}(n, \Delta)$ with $d_{G'}(w) = \Delta$ and $d_{G'}(v) = 2$ such that $R_\eta(G') > R_\eta(G_1) \geq R_\eta(G)$, a contradiction. Hence, v is on C.

If a vertex of a degree higher than 2 exists outside cycle C or a vertex different from v of a degree greater than 2 exists on C, then, using the same proof as before, we can obtain a graph that belongs to $\mathcal{U}(n, \Delta)$ with a greater general Randić index, and this is a contradiction. Therefore, G is obtained from C by attaching v to $\Delta - 2$ paths. Now, suppose that v has k neighbors of degree 2. Thus, $k \leq \min\{n - \Delta - 1, \Delta - 2\}$. When $n - \Delta - 1 \geq \Delta - 2$, i.e., $\Delta \leq \frac{n+1}{2}$, we have $0 \leq k \leq \Delta - 2$. When $n - \Delta - 1 < \Delta - 2$, that is, $\Delta \geq \frac{n+2}{2}$, we have $0 \leq k \leq n - \Delta - 1$. From the definition of the general Randić index,

$$R_\eta(G) = k2^\eta + (k+2)(2\Delta)^\eta + (\Delta - k - 2)\Delta^\eta + (n - \Delta - k)4^\eta$$
$$= (2^\eta + (2\Delta)^\eta - \Delta^\eta - 4^\eta)k + (\Delta - 2)\Delta^\eta + 2(2\Delta)^\eta + 4^\eta(n - \Delta).$$

As the function $f(x) = (2x)^\eta - x^\eta$ is strictly increasing for $x \geq 1$ with $\eta < 0$, we have $f(\Delta) \geq f(4) > f(2)$ and

$$2^\eta + (2\Delta)^\eta - \Delta^\eta - 4^\eta = f(\Delta) - f(2) > 0.$$

It follows that

$$R_\eta(G) \leq \begin{cases} (2^\eta + (2\Delta)^\eta - \Delta^\eta - 4^\eta)(n - \Delta - 1) + (\Delta - 2)\Delta^\eta + 2(2\Delta)^\eta + 4^\eta(n - \Delta), \\ \qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad if \ \frac{n+2}{2} \leq \Delta \leq n - 1 \\ \\ (2^\eta + (2\Delta)^\eta - \Delta^\eta - 4^\eta)(\Delta - 2) + (\Delta - 2)\Delta^\eta + 2(2\Delta)^\eta + 4^\eta(n - \Delta), \\ \qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad if \ 2 \leq \Delta \leq \frac{n+1}{2} \end{cases}$$

$$= \begin{cases} (n - \Delta - 1)2^\eta + (n - \Delta + 1)(2\Delta)^\eta + (2\Delta - n - 1)\Delta^\eta + 4^\eta, \\ \qquad\qquad\qquad\qquad\qquad\qquad if \ \frac{n+2}{2} \leq \Delta \leq n - 1 \\ \\ (\Delta - 2)2^\eta + \Delta(2\Delta)^\eta + (n - 2\Delta + 2)4^\eta, \quad if \ 2 \leq \Delta \leq \frac{n+1}{2}, \end{cases}$$

with equality if and only if $k = n - \Delta - 1$; that is, $G = U_{n,\Delta}$ for $\frac{n+2}{2} \leq \Delta \leq n - 1$, and $k = \Delta - 2$. G is unicyclic and obtained by adding $\Delta - 2$ paths of a length of at least one to a common vertex on C for $2 \leq \Delta \leq \frac{n+1}{2}$. $\square$

The following result characterizes the extremal graphs with the first and the second maximum general Randić index for $\eta_0 \leq \eta < 0$ among all n-vertex unicyclic graphs.

Theorem 2. *Let $\eta_0 \leq \eta < 0$. Then, for all unicyclic graphs with at least four vertices, we have the following:*

(i) C_n is a unique graph attaining the maximum $R_\eta(G)$, and $R_\eta(C_n) = n \times 4^\eta$;

(ii) In the case where $n = 4$, then $U_{4,3}$ is a unique graph with the second largest $R_\eta(G)$, and $R_\eta(U_{4,3}) = 2 \times 6^\eta + 4^\eta + 3^\eta$;

(iii) For $n \geq 5$, the graphs with the second maximum $R_\eta(G)$ are the graphs that are obtained by attaching a vertex on a cycle to a path of a length of at least one, and their general Randić indices are equal to $(n - 4)4^\eta + 3 \times 6^\eta + 2^\eta$.

Proof. For $n = 4$, there are only two unicyclic graphs C_4 and $U_{4,3}$ such that

$$R_\eta(U_{4,3}) - R_\eta(C_4) = (2 \times 6^\eta + 4^\eta + 3^\eta) - 4 \times 4^\eta$$
$$= 2 \times 6^\eta - 3 \times 4^\eta + 3^\eta < 0.$$

The result is true.

Now, let $n \geq 5$ and G be an n-vertex unicyclic graph with the maximum degree Δ, where $2 \leq \Delta \leq n - 1$.

Let $f(x) = (x - 2)2^\eta + x(2x)^\eta + (n - 2x + 2)4^\eta$.

If $\frac{n+2}{2} \leq \Delta \leq n - 1$, then using Theorem 3,

$$R_\eta(G) \leq (n - \Delta - 1)2^\eta + (n - \Delta + 1)(2\Delta)^\eta + (2\Delta - n - 1)\Delta^\eta + 4^\eta$$
$$= f(\Delta) + (n - 2\Delta + 1)(2^\eta - 4^\eta + (2\Delta)^\eta - \Delta^\eta)$$
$$< f(\Delta),$$

since $n - 2\Delta + 1 < 0$, and the function $x^\eta - (2x)^\eta$ is strictly decreasing for $x \geq 1$ and $\Delta \geq 4$.

If $2 \leq \Delta \leq \frac{n+1}{2}$, then, using Theorem 3, we have $R_\eta \leq f(\Delta)$ with equality if G is a unicyclic graph that is obtained by attaching a unique vertex of a cycle to $\Delta - 2$ paths of a length of at least one.

In what follows, we shall prove that $f(x)$ is strictly decreasing for $x \geq 2$ by showing that $f'(x) < 0$. Therefore, we calculate

$$f'(x) = 2^\eta + (2x)^\eta + 2\eta x(2x)^{\eta-1} - 2 \times 4^\eta.$$

Let

$$g(x) = (2x)^\eta + 2\eta x (2x)^{\eta-1} = 2^\eta (1+\eta) x^\eta.$$

Then,

$$g'(x) = 2^\eta (1+\eta) \eta x^{\eta-1} < 0,$$

i.e., $g(x)$ is strictly decreasing for $x \geq 2$, and this implies that $g(x) \leq 4^\eta + \eta \times 4^\eta$.

So,

$$f'(x) \leq 4^\eta \left(\left(\frac{1}{2}\right)^\eta + \eta - 1 \right).$$

Consider $h(\eta) = \eta + \left(\frac{1}{2}\right)^\eta$. We have $h''(\eta) = (ln2)^2 \left(\frac{1}{2}\right)^\eta > 0$, and $h(\eta)$ is strictly convex. Since $h(-1) = h(0) = 1$, we have $h(\eta) < 1$ for $-1 < \eta < 0$, and $f'(x) < 0$ for every $-\frac{1}{2} \leq \eta < 0$. Hence, $f(x)$ is strictly decreasing for $x \geq 2$.

It follows that

$$R_\eta(G) < f(\Delta) < f(3) < f(2) \quad \text{for} \quad 3 < \frac{n+2}{2} \leq \Delta \leq n-1,$$

and

$$R_\eta(G) \leq f(\Delta) \leq f(3) < f(2) \quad \text{for} \quad 3 \leq \Delta \leq \frac{n+1}{2}.$$

Thus, among all n-vertex simple unicylic graphs, the maximum general Randić index is $f(2)$ and the corresponding extremal graph is C_n. Moreover, the second maximum general Randić index is $f(3)$, and the corresponding extremal graphs are these graphs with the maximum $R_\eta(G)$ among all n-vertex unicyclic graphs with $\Delta = 3$, i.e., n-vertex graphs that are obtained by attaching a vertex on a cycle to a path of a length of at least one. $\square$

We know that Li et al. [29] found, for $\eta > 0$, the graphs with the maximum $R_\eta(G)$ among all n-vertex unicyclic graphs, and Liu et al. [24] characterized the trees with maximal and minimal $R_\eta(G)$, respectively, among all trees with Δ. In connection with these results, the following problems are still open:

Problem 1. *For $\eta < 0$, determine the graphs with the maximum $R_\eta(G)$ among all unicyclic graphs with n vertices.*

Problem 2. *Characterize the graphs with minimal and maximal $R_\eta(G)$, respectively, among all unicyclic graphs with a given Δ.*

Problem 3. *Characterize the graphs with minimal and maximal $R_\eta(G)$, respectively, among all bicyclic graphs with a given Δ, more generally, for c-cyclic graphs.*

3. QSPR/QSAR of Randić Index

Topological indices are used for translating the chemical properties into numbers that can be applied for statistical analysis like correlation with physical properties in QSPR/QSAR (quantitative structure–property/activity relationship) studies. In recent years, the topological indices have become one of the major research topics in QSPR and QSAR analysis. For some applications of topological indices, see [33,35–39]. The use of graph entities in QSPR/QSAR analysis has attracted attacted many researchers in recent years. Topological indices have a wide range of application in non-empirical quantitative structure–property relationships (QSPRs) and quantitative structure–activity relationships (QSARs) like in [35,38,40–42]. These chemical properties are studied since they have a direct impact on drug transits and bioactivity in the human body. Thus, with the help of topological indices, we can design better drugs.

We will use the Randić index for modeling physical properties of 67 alkanes (n-butanes to nonanes). The well-known physical properties are molar volumes (mv's) at 20 °C, heats

of vaporization (hv's) at 25 °C, molar refractions (mr's) at 20 °C, the boiling point (bp), and surface tensions (st's) at 20 °C. The data are taken from [39] (see also [43]). The values of RA were calculated using the AutoGraphiX III system [44].

We consider the following linear regression model:

$$\beta = a + b(TI), \tag{1}$$

where β is a physical property and TI is a topological index. Using (1), we carry out the analysis for the Randić index $R_{-1}(G)$ with the bp, mv's, mr's, hv's, and st's.

The following table gives the correlation of the Randić index $R_{-1}(G)$ with the boiling point (bp), the molar volumes (mv's) at 20 °C, the molar refractions (mr's) at 20 °C, the heats of vaporization (hv's) at 25 °C, and the surface tensions (st's) 20 °C for chemical graphs up to order 7.

From Table 1, we see that all the physical properties are very well correlated with the Randić index $R_{-1}(G)$. Heats of vaporization (hv's) at 25 °C give the best correlation with $R_{-1}(G)$. This gives us a good sign for modeling physical properties of alkanes with the Randić index.

Table 1. Correlation of $R_{-1}(G)$ with bp, mv, mr, hv, and st for chemical graphs up to order 7.

$R_{-1}(G)$ vs. bp	$R_{-1}(G)$ vs. mv	$R_{-1}(G)$ vs. mr	$R_{-1}(G)$ vs. hv	$R_{-1}(G)$ vs. st
0.976893697	0.947992593	0.952529194	0.987125973	0.893037379

The Table 2 gives the R^2 (coefficient of determination) of $R_{-1}(G)$ with the bp, mv, mr, hv, and st for chemical graphs up to order 7.
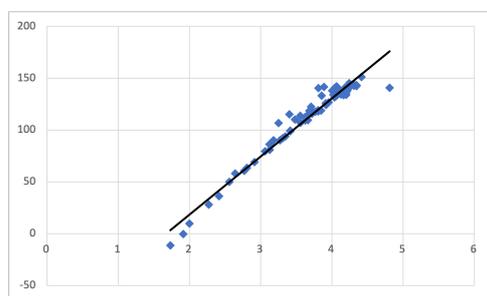
Table 2. Correlation of $R_{-1}(G)$ with bp, mv, mr, hv, and st for chemical graphs up to order 7.

$R_{-1}(G)$ vs. bp	$R_{-1}(G)$ vs. mv	$R_{-1}(G)$ vs. mr	$R_{-1}(G)$ vs. hv	$R_{-1}(G)$ vs. st
0.9543	0.8987	0.9073	0.9744	0.8307

The best coefficient of determination for $R_{-1}(G)$ is achieved by heats of vaporization (hv's).

Figure 1 shows the linear regression between $R_{-1}(G)$ and the boiling point (bp), with the rounded equation

$$bp = 56.07 \cdot R_{-1}(G) - 93.727.$$
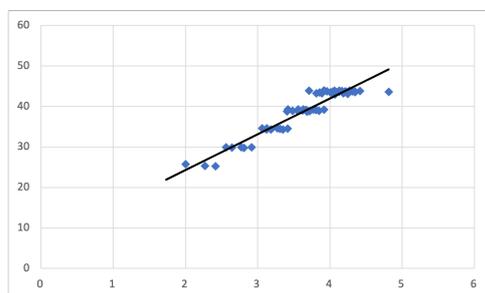

$$bp = 56.07 \cdot R_{-1}(G) - 93.727$$
$$R^2 = 0.9543$$

Figure 1. Linear regression for bp vs. $R_{-1}(G)$.

Figure 2 shows the linear regression between $R_{-1}(G)$ and the molar volumes (mv's), with the rounded equation

$$mv = 29.575 \cdot R_{-1}(G) + 52.61.$$

The linear regression illustrates that the correlation of the boiling point is better with $R_{-1}(G)$, where $R^2 = 0.9543$, than with molar volumes, where $R^2 = 0.8987$.
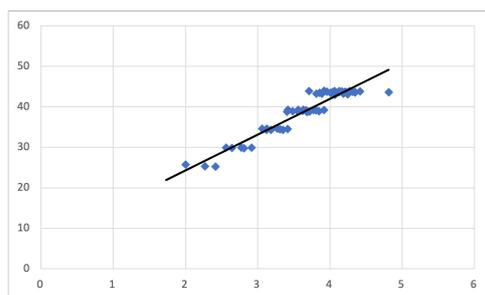

$$\text{mv} = 29.575 \cdot R_{-1}(G) + 52.61$$
$$R^2 = 0.8987$$

Figure 2. Linear regression for mv vs. $R_{-1}(G)$.

Figure 3 shows the linear regression between $R_{-1}(G)$ and the molar refractions (mr's), with the rounded equation

$$\text{mr} = 8.8376 \cdot R_{-1}(G) + 6.6387.$$
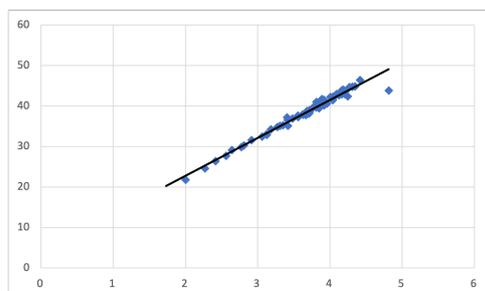

$$\text{mr} = 8.8376 \cdot R_{-1}(G) + 6.6387$$
$$R^2 = 0.9073$$

Figure 3. Linear regression for mr vs. $R_{-1}(G)$.

Figure 4 shows the linear regression between $R_{-1}(G)$ and the heats of vaporization (hv's), with the rounded equation

$$\text{hv} = 9.3676 \cdot R_{-1}(G) + 4.033.$$

The linear regression illustrates that the correlation of the heats of vaporization is better with $R_{-1}(G)$, where $R^2 = 0.9744$, than with molar refractions, where $R^2 = 0.9073$.
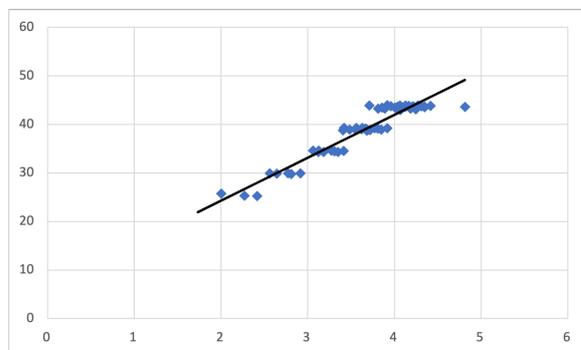

$$\text{hv} = 9.3676 \cdot R_{-1}(G) + 4.033.$$
$$R^2 = 0.9744$$

Figure 4. Linear regression for hv vs. $R_{-1}(G)$.

Figure 5 shows the linear regression between $R_{-1}(G)$ and the surface tension (st), with the rounded equation

$$st = 3.2906 \cdot R_{-1}(G) + 8.6697$$

and $R^2 = 0.7975$.

$$st = 3.2906 \cdot R_{-1}(G) + 8.6697$$
$$R^2 = 0.7975$$

Figure 5. Linear regression for st vs. $R_{-1}(G)$.

The overall significant observation is that the Randić index $R_{-1}(G)$ gives a very high correlation with the heats of vaporization of alkanes, and thereby it will help in designing better models for the applicability of $R_{-1}(G)$ with such physical properties.

4. Conclusions

In this paper, some extremal results are presented that are related to the general Randić index among classes of unicyclic graphs in terms of different parameters, like the maximum degree and order n of the graph. In addition, we find the maximum and the second maximum general Randić index for $\eta_0 \leq \eta < 0$ for classes of unicyclic graphs with $\eta_0 = -0.21$. Furthermore, we carried out statistical analysis of the Randić index with physical properties of chemical graphs of alkanes up to order 7. We observed that the Randić index is highly correlated with the heats of vaporization of alkanes. A similar type of analysis can be studied for the general Randić index for the class of bicyclic graphs and for c-cyclic graphs in general, though we need some more advanced tools and techniques for handling extremal problems related to the general Randić index.

Author Contributions: Conceptualization, A.A. and M.I.; software, M.I.; writing—original draft preparation, A.A. and M.I.; writing—review and editing, A.A. and M.I.; formal analysis, A.A. and M.I.; validation, A.A. and M.I.; methodology, A.A. and M.I.; investigation, A.A. and M.I.; resources, A.A. and M.I.; project administration, A.A. and M.I.; funding acquisition, A.A. All authors have read and agreed to the published version of this manuscript.

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