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On the Ordering of Trees with the General Randić Index of the Nordhaus-Gaddum Type *

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Abstract

The general Randić index of an organic molecule whose molecular graph is G is defined as the sum of $(d(u)d(v))^\alpha$ over all pairs of adjacent vertices of G, where $d(u)$ is the degree of the vertex u in G and α is a real number with $\alpha \neq 0$. In the paper, we obtained sharp bounds on the general Randić index of the Nordhaus-Gaddum type for trees. Also we show that the general Randić index of the Nordhaus-Gaddum type for double stars $S_{p,q}$ is monotonously increasing in p, where $1 < p \leq q$.

1. Introduction

Let $G = (V, E)$ be a simple undirected graph with n vertices and m edges. The complement of the graph G, denoted by G^c, is the graph with the same vertex set as G, where any two distinct vertices are adjacent if and only if they are non-adjacent in G. For a vertex u of G, we denote the neighborhood and the degree of u by $N(u)$ and $d(u)$, respectively.

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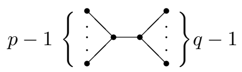
The general Randić index of a (molecular) graph G, denoted by $w_\alpha(G)$, is defined as the sum of $(d(u)d(v))^\alpha$ over all pairs of adjacent vertices of G, where $d(u)$ is the degree of the vertex u in G and α is a real number with $\alpha \neq 0$. Finding the graphs having maximum and minimum general Randić indices and related problem of finding lower and upper bounds for the general Randić index, attracted recently the attention of many researchs, and many results have been achieved (see[1]-[5], [8]-[14], [16]-[19]). It is well known that the Randić index $w_{-\frac{1}{2}}(G)$ was proposed by Randić [17] in 1975 and Bollobás and Erdős [1] generalized the index by replacing $-\frac{1}{2}$ with any real number α in 1998. The research background of Randić index together with its generalization appears in chemical field and can be found in the literature (see [6, 7, 17]).

In 1956, Nordhaus and Daddum [15] first considered the sum of the chromatic number of graph G and its complement G^c. In [19], Zhang and Wu obtained some Nordhaus-Gaddum-type inequalities for some chemical indices. Here, the *(general Randić) index of the Nordhaus-Gaddum type* for a (molecular) graph G is the sum of the general Randić index of G and G^c.

Let S_n be a star. A tree is called a *double star* $S_{p,q}$ (see Fig. 1), if it is obtained from S_{p+1} and S_q by identifying a leaf of S_{p+1} with the center of S_q, where $1 < p \leq q$. Then for a double star $S_{p,q}$ with n vertices, we have $p + q = n$ and $p \leq \lfloor \frac{n}{2} \rfloor$. We call a double star $S_{p,q}$ *balanced*, if $p = \lfloor \frac{n}{2} \rfloor$ and $q = \lceil \frac{n}{2} \rceil$.



$S_{p,q}$

Fig. 1

In this paper, we first obtained a sharp bound on the general Randić index of the Nordaus-Gaddum type for trees. Also we show that the general Randić index of the Nordaus-Gaddum type for double stars $S_{p,q}$ is monotonously increasing in p.

2. Trees with Extremal Index of the Nordaus-Gaddum Type

In the following, we first present two results that will be used in the proof of our first result.

Theorem 2.1 [4, 5]. *Let $G = (V, E)$ be a tree of order n. Then*

$$w_\alpha(T) \geq (n-1)^{\alpha+1} \tag{1}$$

for $-1 \leq \alpha < 0$, and

$$w_\alpha(T) \leq (n-1)^{\alpha+1} \tag{2}$$

for $0 < \alpha \le 1$. *Furthermore, in (1) or (2) equality holds for a particular value of* α *if and only if* $T \cong S_n$, *in which case we have equality in (1) and (2) for every* α, $-1 \le \alpha \le 1$, $\alpha \ne 0$.

Theorem 2.2 [1]. *Let* $G = (V, E)$ *be a graph with* m *edges. Then*

$$w_\alpha(G) \ge m \left(\frac{\sqrt{8m+1} - 1}{2} \right)^{2\alpha} \tag{3}$$

for $-1 \le \alpha < 0$, *and*

$$w_\alpha(G) \le m \left(\frac{\sqrt{8m+1} - 1}{2} \right)^{2\alpha} \tag{4}$$

for $0 < \alpha \le 1$. *Furthermore, in (3) or (4) equality holds for a particular value of* α *if and only if* G *consists of a complete graph and isolated vertices, in which case we have equality in (3) and (4) for every* α, $-1 \le \alpha \le 1$, $\alpha \ne 0$.

Our first main result follows from Theorems 2.1 and 2.2.

Theorem 2.3. *Let* $T = (V, E)$ *be a tree with* n *vertices and* m *edges. Then*

$$w_\alpha(T) + w_\alpha(T^c) \ge \frac{n-1}{2} \left[2(n-1)^\alpha + (n-2)^{2\alpha+1} \right] \tag{5}$$

for $-1 \le \alpha < 0$, *and*

$$w_\alpha(T) + w_\alpha(T^c) \le \frac{n-1}{2} \left[2(n-1)^\alpha + (n-2)^{2\alpha+1} \right] \tag{6}$$

for $0 < \alpha \le 1$. *Furthermore, in (5) or (6) equality holds for a particular value of* α *if and only if* $T \cong S_n$, *in which case we have equality in (5) and (6) for every* α, $-1 \le \alpha \le 1$, $\alpha \ne 0$.

Proof. Clearly, $m = m(T) = n - 1$ and $m^c = m(T^c) = n(n-1)/2 - (n-1) = (n-1)(n-2)/2$. By Theorem 2.2, we have

$$w_\alpha(T^c) \ge m^c \left(\frac{\sqrt{8m^c+1} - 1}{2} \right)^{2\alpha} = \frac{(n-1)(n-2)^{2\alpha+1}}{2} \tag{7}$$

for $-1 \le \alpha < 0$, and

$$w_\alpha(T^c) \le m^c \left(\frac{\sqrt{8m^c+1} - 1}{2} \right)^{2\alpha} = \frac{(n-1)(n-2)^{2\alpha+1}}{2} \tag{8}$$

for $0 < \alpha \le 1$. Furthermore, in (7) or (8) equality holds for a particular value of α if and only if $T^c \cong (K_{n-l} \cup lK_1)$ $(1 \le l \le n-1)$, in which case we have equality in (7) and (8) for every α, $-1 \le \alpha \le 1$, $\alpha \ne 0$. By Theorem 2.1, we have

$$w_\alpha(T) \ge (n-1)^{\alpha+1} \tag{9}$$

for $-1 \leq \alpha < 0$, and

$$w_\alpha(T) \leq (n-1)^{\alpha+1} \tag{10}$$

for $0 < \alpha \leq 1$. Furthermore, in (9) or (10) equality holds for a particular value of α if and only if $T \cong S_n$, in which case we have equality in (9) and (10) for every α, $-1 \leq \alpha \leq 1$, $\alpha \neq 0$. Therefore

$$w_\alpha(T) + w_\alpha(T^c) \geq \frac{n-1}{2}\left[2(n-1)^\alpha + (n-2)^{2\alpha+1}\right]$$

for $-1 \leq \alpha < 0$, and

$$w_\alpha(T) + w_\alpha(T^c) \leq \frac{n-1}{2}\left[2(n-1)^\alpha + (n-2)^{2\alpha+1}\right]$$

for $0 < \alpha \leq 1$.

If $T \cong S_n$, then $S_n^c = K_{1,n-1}^c = K_{n-1} \cup K_1$, a complete graph of order $n-1$ and an isolated vertex. Hence $w_\alpha(S_n^c) = \frac{(n-1)(n-2)^{2\alpha+1}}{2}$. Thus

$$w_\alpha(T) + w_\alpha(T^c) = \frac{n-1}{2}\left[2(n-1)^\alpha + (n-2)^{2\alpha+1}\right].$$

Conversely, if $w_\alpha(T) + w_\alpha(T^c) = \frac{n-1}{2}[2(n-1)^\alpha + (n-2)^{2\alpha+1}]$, then

$$w_\alpha(T) = (n-1)^{\alpha+1} \text{ and } w_\alpha(T^c) = \tfrac{(n-1)(n-2)^{2\alpha+1}}{2}.$$

Thus, by Theorem 2.1, we have $T \cong S_n$.

Hence the proof of the theorem is complete. ■

3. On the Ordering of Double Stars

Note that the extremal graph in (5) or (6) is the unique star graph. In the following, we consider a tree with order n and diameter 3, i.e., a double star $S_{p,q}$, and obtain some bounds on the general Randić index of the Nordhaus-Gaddum type for a double star $S_{p,q}$. The proof of this result is based on the following lemma.

Lemma 3.1. *If* $0 < \alpha \leq 1$, *then* $\alpha 5^\alpha - (\alpha+1)4^\alpha + \alpha + 1 < 0$.

Proof. First we show that

$$\alpha 2^\alpha + 1 - 4^\alpha < 0.$$

Denote $f(x) := x2^x + 1 - 4^x$, where $0 < x \leq 1$. Then $f'(x) = (1 + x\ln 2)2^x - (\ln 4)4^x$ and $f''(x) = (2 + x\ln 2)(\ln 2)2^x - (\ln 4)^2 4^x$. Note that

$$\begin{aligned} f''(x) &= (2 + x\ln 2)(\ln 2)2^x - (\ln 4)^2 4^x \\ &\leq (2 + \ln 2)(\ln 2)2^x - (\ln 4)^2 4^x \\ &< [(2 + \ln 2)(\ln 2) - (\ln 4)^2]2^x \\ &< 0. \end{aligned}$$

Thus, by $f'(0) = 1 - \ln 4 < 0$, we get $f'(x) < 0$. Then, by $f(0) = 0$, we get $f(\alpha) = \alpha 2^\alpha + 1 - 4^\alpha < 0$ for $0 < \alpha \leq 1$.

Next, we have

$$\begin{aligned} \alpha 5^\alpha - (\alpha+1)4^\alpha + \alpha + 1 &= \alpha(5^\alpha - 4^\alpha) + \alpha + 1 - 4^\alpha \\ &\leq \alpha(2^\alpha - 1^\alpha) + \alpha + 1 - 4^\alpha \\ &= \alpha 2^\alpha + 1 - 4^\alpha < 0. \end{aligned}$$

Hence the proof of Lemma 3.1 is complete. ■

The next result follows from Lemma 3.1.

Theorem 3.2. *(i) The general Randić index of a double star $S_{p,q}$ is monotonously increasing for $-1 \leq \alpha < 0$ in p;*

(ii) The general Randić index of a double star $S_{p,q}$ is monotonously decreasing for $0 < \alpha \leq 1$ in p.

Proof. Note that

$$\begin{aligned} w_\alpha(S_{p,q}) &= (p-1)p^\alpha + (q-1)q^\alpha + (pq)^\alpha \\ &= (p-1)p^\alpha + (n-p-1)(n-p)^\alpha + p^\alpha(n-p)^\alpha. \end{aligned}$$

Let $f(p) = (p-1)p^\alpha + (n-p-1)(n-p)^\alpha + p^\alpha(n-p)^\alpha$, $1 < p \leq \lfloor \frac{n}{2} \rfloor$. Then

$$f'(p) = (\alpha+1)p^\alpha - \alpha p^{\alpha-1}[1-(n-p)^\alpha] - [(\alpha+1)(n-p)^\alpha - \alpha(n-p)^{\alpha-1}(1-p^\alpha)]. \quad (*)$$

(i) By $(*)$, we have

$$f'(p) = (\alpha+1)[p^\alpha - (n-p)^\alpha] - \alpha[p^{\alpha-1}(1-(n-p)^\alpha) - (n-p)^{\alpha-1}(1-p^\alpha)].$$

Since $-1 \leq \alpha < 0$, and $n-p \geq p$, we have that $p^\alpha \geq (n-p)^\alpha \geq 0$ and $p^{\alpha-1} \geq (n-p)^{\alpha-1} \geq 0$. Thus $p^{\alpha-1}(1-(n-p)^\alpha) - (n-p)^{\alpha-1}(1-p^\alpha) \geq 0$. This implies $f'(p) \geq 0$ and then $w_\alpha(S_{p,q})$ is monotonously increasing for $-1 \leq \alpha < 0$ in p.

(ii) Let $g(x) = (\alpha+1)x^\alpha - \alpha x^{\alpha-1}[1-(n-x)^\alpha]$, $1 < x < n-1$. Then $f'(p) = g(p) - g(n-p)$ by $(*)$. Note that

$$g'(x) = \alpha x^{\alpha-2} \cdot \left\{(\alpha+1)x - (\alpha-1)[1-(n-x)^\alpha] - \alpha x(n-x)^{\alpha-1}\right\}.$$

To complete the proof of (ii), it suffices to show that $f'(p) \leq 0$, $1 < p \leq \lfloor \frac{n}{2} \rfloor$ for $0 < \alpha \leq 1$.

If $\frac{n}{5} \leq x < n-1$, then

$$g'(x) \;=\; \alpha x^{\alpha-2} \cdot \left\{(\alpha+1)x - (\alpha-1)[1-(n-x)^\alpha] - \alpha x(n-x)^{\alpha-1}\right\}$$

$$
\begin{aligned}
&\geq \alpha x^{\alpha-2}\cdot\{(\alpha+1)x-(\alpha-1)[1-(n-x)^{\alpha}]-\alpha x\}\\
&= \alpha x^{\alpha-2}\cdot\left[x-(1-\alpha)\alpha\xi^{\alpha-1}(n-1-x)\right]\\
&\geq \alpha x^{\alpha-2}\cdot[x-(1-\alpha)\alpha(n-1-x)]\\
&\geq \alpha x^{\alpha-2}\cdot\left[x-\frac{1}{4}(n-1-x)\right]\\
&> 0,
\end{aligned}
$$

where $\xi \in [1, n-x]$. Thus $f'(p) \leq 0$ if $\frac{n}{5} \leq p \leq \frac{n}{2}$.

So in the following proof, we can assume $1 < p < \frac{n}{5}$. Obviously,

$$
\begin{aligned}
f'(p) &= (\alpha+1)p^{\alpha}-(\alpha+1)(n-p)^{\alpha}+\alpha p^{\alpha-1}[(n-p)^{\alpha}-1]\\
&\quad +\alpha(n-p)^{\alpha-1}(1-p^{\alpha})\\
&\leq (\alpha+1)\left(\frac{n}{5}\right)^{\alpha}-(\alpha+1)\left(\frac{4n}{5}\right)^{\alpha}+\alpha p^{\alpha-1}[(n-p)^{\alpha}-1]\\
&\leq (\alpha+1)\left(\frac{n}{5}\right)^{\alpha}-(\alpha+1)\left(\frac{4n}{5}\right)^{\alpha}+\alpha[(n-1)^{\alpha}-1]\\
&= (\alpha+1)\left[\left(\frac{n}{5}\right)^{\alpha}-\left(\frac{4n}{5}\right)^{\alpha}\right]+\alpha\left[(n-1)^{\alpha}-1\right]\\
&< (\alpha+1)\left[\left(\frac{n}{5}\right)^{\alpha}-\left(\frac{4n}{5}\right)^{\alpha}\right]+\alpha n^{\alpha}\\
&= 5^{-\alpha}\cdot n^{\alpha}\left[\alpha\cdot 5^{\alpha}-(\alpha+1)4^{\alpha}+\alpha+1\right]\\
&< 0,
\end{aligned}
$$

where the last inequality follows by Lemma 3.1.

Hence the proof of the theorem is complete. ■

Theorem 3.3. *(i) The general Randić index of $S^c_{p,q}$ is increasing for $-1 \leq \alpha < 0$ in p;*

(ii) The general Randić index of $S^c_{p,q}$ is decreasing for $0 < \alpha \leq 1$ in p.

Proof. Note that

$$
\begin{aligned}
w_{\alpha}(S^c_{p,q}) &= (n-2)^{\alpha}\left[(p-1)^{\alpha+1}+(q-1)^{\alpha+1}+\frac{(n-2)^{\alpha+1}(n-3)}{2}\right]\\
&= (n-2)^{\alpha}\left[(p-1)^{\alpha+1}+(n-p-1)^{\alpha+1}+\frac{(n-2)^{\alpha+1}(n-3)}{2}\right].
\end{aligned}
$$

Let $h(p) = (p-1)^{\alpha+1} + (n-p-1)^{\alpha+1} + \frac{(n-2)^{\alpha+1}(n-3)}{2}$, $1 \leq p \leq \lfloor \frac{n}{2} \rfloor$. Then

$$h'(p) = (\alpha+1)[(p-1)^{\alpha} - (n-p-1)^{\alpha}].$$

If $-1 \leq \alpha < 0$, then $h'(p) \geq 0$; and if $0 < \alpha \leq 1$, then $h'(p) \leq 0$.

Hence the proof of the theorem is complete. ■

By Theorems 3.2 and 3.3, we have the following result.

Theorem 3.4. *(i) The general Randić index of the Nordhaus-Gaddum type for a double star* $S_{p,q}$ *is monotonously decreasing for* $-1 \leq \alpha < 0$ *in* p*;*

(ii) The general Randić index of the Nordhaus-Gaddum type for a double star $S_{p,q}$ *is monotonously increasing for* $0 < \alpha \leq 1$ *in* p*.*

Note 3.5. *(i) For* $-1 \leq \alpha < 0$*, the balanced double star* $S_{\lfloor \frac{n}{2} \rfloor, \lceil \frac{n}{2} \rceil}$ *has the maximum value of the general Randić index among all the double stars* $S_{p,q}$ *with* n *vertices;*

(ii) For $0 < \alpha \leq 1$*, the balanced double star* $S_{\lfloor \frac{n}{2} \rfloor, \lceil \frac{n}{2} \rceil}$ *has the minimum value of the general Randić index among all the double stars* $S_{p,q}$ *with* n *vertices.*

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