Extremal polyomino chains with respect to general sum-connectivity index

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Abstract: For a (molecular) graph G, the general sum-connectivity index $\chi_\alpha(G)$ is defined as the sum of the weights $[d_u + d_v]^\alpha$ of all edges uv of G, where d_u (or d_v) denotes the degree of a vertex u (or v) in G and α is an arbitrary real number. In this paper, we give an efficient formula for computing the general sum-connectivity index of polyomino chains and characterize the extremal polyomino chains with respect to this index, which generalizes one of the main results in [Z. Yarahmadi, A. Ashrafi, S. Moradi, Extremal polyomino chains with respect to Zagreb indices, Appl. Math. Lett. 25 (2012): 166-171].

Keywords: General sum-connectivity index; Polyomino chain.

1. Introduction

All graphs considered in this paper are simple and connected. Let $G = (V, E)$ be a graph, with vertex set V and edge set E. The **degree** of a vertex $u \in V$ is the number of edges incident to u, denoted by $d_G(u)$, or d_u when no confusion is possible. For other undefined terminology and notations from graph theory, the readers are referred to [1].

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A topological index is a numerical descriptor of the molecular structure derived from the corresponding molecular graph. There are numerous topological descriptors that have found some applications in theoretical chemistry, especially in quantitative structure-activity relationship (QSAR) and quantitative structure-property relationship (QSPR) researches [8]. Among these useful topological descriptors, we will present several ones that are relevant for our work.

The first indices presented here are the **Zagreb indices**, which have been introduced more than thirty years ago by Gutman and Trinajstić, [2]. They are originally defined as follows:

$$M_1(G) = \sum_{u \in V(G)} d_u^2,$$

$$M_2(G) = \sum_{e=uv \in E(G)} d_u d_v.$$

Here $M_1(G)$ and $M_2(G)$ denote the first and the second Zagreb indices, respectively. These two topological indices reflect the extent of branching of the molecular carbon-atom skeleton [8]. The first Zagreb index can be also expressed as a sum over edges of G,

$$M_1(G) = \sum_{e=uv \in E(G)} [d_u + d_v].$$

For the proof of this fact and more information on Zagreb indices we encourage the interested reader to [6].

Later, in 1975, Randić proposed a molecular structure descriptor in studying the properties of alkane [7] which he called the branching index, and is now called the **Randić index**. It is defined as the sum over all edges of the (molecular) graph of the terms $[d_u d_v]^{-\frac{1}{2}}$, i.e.,

$$R(G) = \sum_{e=uv \in E(G)} [d_u d_v]^{-\frac{1}{2}}.$$

This index is also called as the product-connectivity index of G.

Recently, a closely related variant of the Randić index called the **sum-connectivity index** was introduced by Zhou and Trinajstić [14] in 2009, which is denoted by $\chi = \chi(G)$ and originally defined as:

$$\chi(G) = \sum_{e=uv\in E(G)} [d_u + d_v]^{-\frac{1}{2}}.$$

These two molecular descriptors are highly intercorrelated quantities; for example, the value of the correlation coefficient is 0.99088 for 136 trees representing the lower alkanes taken from Ivanciuc et al. [3].

The ordinary Randić index has been extended to the **general Randić index** by Li and Gutman, which is defined as [5]:

$$R_\alpha(G) = \sum_{e=uv\in E(G)} [d_u d_v]^\alpha,$$

where α is an arbitrary real number. The properties of the general Randić index can be found in [e.g., 5, 13].

Motivated by the above definition, Zhou and Trinajstić proposed the **general sum-connectivity index** [15], which is defined as:

$$\chi_\alpha(G) = \sum_{e=uv\in E(G)} [d_u + d_v]^\alpha,$$

where α is an arbitrary real number. They obtained some properties, especially lower and upper bounds in terms of other graph invariants, of this index.

Evidently, $\chi_{-\frac{1}{2}}$ is the ordinary sum-connectivity index and χ_1 is the first Zagreb index. Thus, the general sum-connectivity index generalizes both the ordinary sum-connectivity index and the first Zagreb index.

Zeng et al. [16] distinguished the extremal polyomino chains on k-matchings and k-independent sets. Xu et al. studied the PI index of polyomino chains, [9]. Later, Yang et al. continued this problem to the Randić index and sum-connectivity index, respectively, see [10, 11]. Recently, Yarahmadi et al. [12] studied this item to the Zagreb indices. In this work, we continue this program to calculate the general sum-connectivity index of polyomino chains, and determine the extremal polyomino chains with respect to this index, which generalizes one of the main results in [12].

2. Preliminaries

A polyomino system is a finite 2-connected plane graph such that each interior face (or say a cell) is surrounded by a regular square of length one. In other words, it is an edge-connected union of cells in the planar square lattice. This figure divides the plane into one infinite external region and a number of finite internal, all internal region must be squares. Polyominoes have a long and rich history, we convey for the origin polyominoes, [4]. A polyomino chain is a polyomino system, in which the joining of the centers of its adjacent regular forms a path $c_1c_2\cdots c_n$, where c_i is the center of the i-th square.

Let $\mathbf{B}_n$ be the set of polyomino chains with n squares. For $B_n \in \mathbf{B}_n$, it is easy to see that $|V(B_n)| = 2n+2$ and $|E(B_n)| = 3n+1$. If the subgraph of B_n induced by the vertices with degree 3 is a graph with exactly $n-2$ squares, then B_n is called a linear chain and denoted by L_n. If the subgraph of B_n induced by the vertices with a degree bigger than two is a path with $n-1$ edges, then B_n is called a zig-zag chain and denoted by Z_n. Fig. 1(a) and (b) illustrate L_5 and Z_7, respectively.

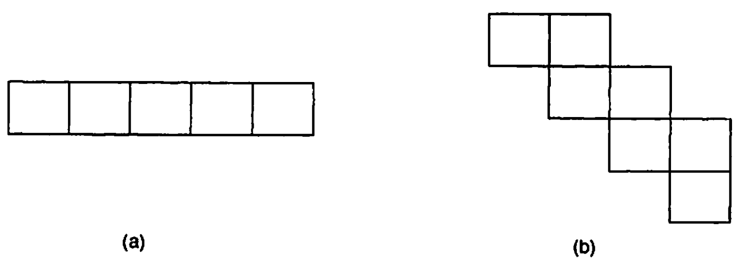

Fig. 1. (a) The graph L_5; (b) The graph Z_7.

For calculating the general sum-connectivity index of a polyomino chains, we introduce some conceptions in a polyomino chain. A **kink** of a polyomino chain is the branched or angularly connected squares. A **segment** of a polyomino chain is a maximal linear chain in the polyomino chain, including the kinks and/or terminal squares at its end, the segments of Z_7 are shown in Fig. 2. The number of squares in a segment S is called its length and is denoted by $l(S)$. For any segment S of a polyomino chain with $n \geq 2$ squares, $2 \leq l(S) \leq n$. Particularly, a polyomino chain is a linear chain if and only if it contains only one segment; a polyomino chain is a zig-zag chain if and only if the length of each segment is 2.

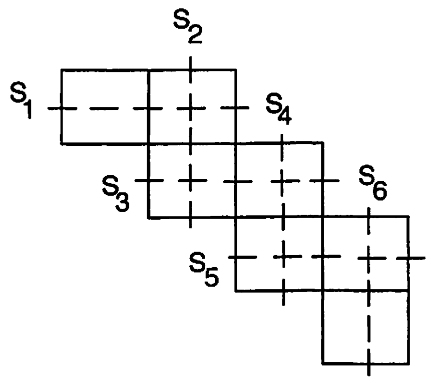

Fig. 2. The segments of Z_7.

A polyomino chain with n squares consists of a sequence of segments $S_1, S_2, \cdots, S_r, r \geq 1$, with lengths $l(S_i) = l_i, i = 1, 2, \cdots, r$, where $l_1 + l_2 + \cdots + l_r = n + r - 1$.

3. The general sum-connectivity index of polyomino chains

In this section, we give an explicit formula for computing the general sum-connectivity index of polyomino chains. We first define two parameters $\alpha(S_i), 1 \leq i \leq r$, and $\phi(\alpha, r)$ as follows:

$$\alpha(S_i) = \begin{cases} 1 & l_i = 2 \\ 0 & l_i > 2, \end{cases}$$

$$\phi(\alpha, r) = \begin{cases} 0 & \alpha = 1 \\ 1 & \alpha > 1 \text{ and } r = 1 \\ 0 & \alpha > 1 \text{ and } r > 1, \end{cases}$$

where $\alpha \geq 1$ is an arbitrary real number.

For example, the simple polyomino chain with three segments S_1, S_2 and S_3 illustrated in Fig. 3 satisfies that $\alpha(S_1) = \alpha(S_3) = 0, \alpha(S_2) = 1$ and $\phi(\alpha, 3) = 0$, for arbitrary real number $\alpha \geq 1$.

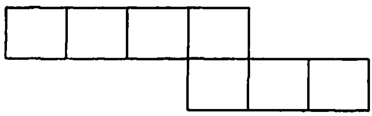

Fig. 3. A simple polyomino chain with three segments S_1, S_2 and S_3.

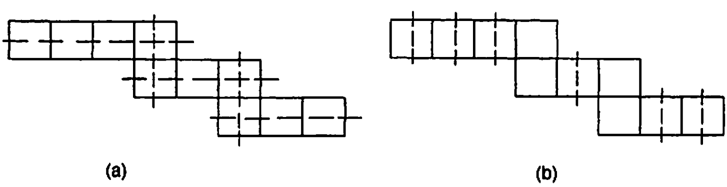

Fig. 4. (a) The edges of E_1; (b) The edges of E_2.

Theorem 3.1. Let B_n be a polyomino chain with n squares, $n \geq 3$, and consisting of r segments $S_1, S_2, \cdots, S_r, r \geq 1$, with lengths $l_1, l_2, \cdots, l_r$, respectively. Let $\alpha \geq 1$ be an arbitrary real number. Then

$$\begin{aligned} \chi_\alpha(B_n) =& 4(r-1) \cdot 7^\alpha + (3n - 6r + 1) \cdot 6^\alpha + 2[3 - \phi(\alpha, r)] \cdot 5^\alpha \\ & + 2\sum_{i=2}^{r-1}[5 + \alpha(S_i)]^\alpha - (4 \cdot 7^\alpha - 8^\alpha - 3 \cdot 6^\alpha) \sum_{i=2}^{r-1} \alpha(S_i) \\ & - (7^\alpha - 2 \cdot 6^\alpha + 5^\alpha) [\alpha(S_1) + \alpha(S_r)] + 2 \cdot 4^\alpha. \end{aligned}$$

Proof. We partition the edge set of B_n into two subsets. The subset E_1

contains, all edge $e = uv$ which is cut across by straight dashed line passed through the centers of squares S_i for $1 \leq i \leq r$, Fig. 4(a).

Suppose $E_2 = E(B_n) \setminus E_1$, the elements of E_2 are shown in Fig. 4(b), by straight dashed lines. Then if $r = 1$, by direct calculation,

$$\chi_\alpha(B_n) = (3n-5)\cdot 6^\alpha + 4\cdot 5^\alpha + 2\cdot 4^\alpha.$$

If $r > 1$, by definition

$$\begin{aligned}\chi_\alpha(B_n) &= \sum_{e=uv\in E(G)} [d_u + d_v]^\alpha \\ &= \sum_{e=uv\in E_1} [d_u + d_v]^\alpha + \sum_{e=uv\in E_2} [d_u + d_v]^\alpha.\end{aligned}$$

For the first summation, one can see that:

$$\sum_{e=uv\in E_1} [d_u + d_v]^\alpha = \sum_{i=1}^{r} \sum_{e=uv\in E_1\cap E(S_i)} [d_u + d_v]^\alpha.$$

In what follows, each summation is evaluated, separately. For $1 < i < r$, we have:

$$\begin{aligned}\sum_{e=uv\in E_1\cap E(S_i)} [d_u + d_v]^\alpha =& (l_i - 3)\cdot 6^\alpha + 2\cdot 7^\alpha [5 + \alpha(S_{i-1})]^\alpha \\ &+ [5 + \alpha(S_{i+1})]^\alpha - (2\cdot 7^\alpha - 8^\alpha - 6^\alpha)\cdot \alpha(S_i),\end{aligned}$$

$$\sum_{e=uv\in E_1\cap E(S_1)} [d_u + d_v]^\alpha = (l_1 - 2)\cdot 6^\alpha + 7^\alpha + [5 + \alpha(S_2)]^\alpha + 4^\alpha,$$

$$\sum_{e=uv\in E_1\cap E(S_r)} [d_u + d_v]^\alpha = (l_r - 2)\cdot 6^\alpha + 7^\alpha + [5 + \alpha(S_{r-1})]^\alpha + 4^\alpha.$$

Therefore,

$$\begin{aligned}\sum_{e=uv\in E_1} [d_u + d_v]^\alpha =& 6^\alpha \sum_{i=1}^{r} l_i + 2\sum_{i=2}^{r-1} [5 + \alpha(S_i)]^\alpha + 2(r-1)\cdot 7^\alpha + 2\cdot 5^\alpha \\ &- (2\cdot 7^\alpha - 8^\alpha - 6^\alpha)\sum_{i=2}^{r-1} \alpha(S_i) - (3r-2)\cdot 6^\alpha \\ &+ 2\cdot 4^\alpha.\end{aligned}$$

On the other hand, we have

$$\sum_{e=uv\in E_2}[d_u+d_v]^\alpha=\sum_{i=1}^{r}\sum_{e=uv\in E_2\cap E(S_i)}[d_u+d_v]^\alpha.$$

For $1<i<r$,

$$\sum_{e=uv\in E_2\cap E(S_i)}[d_u+d_v]^\alpha=(2l_i-6)\cdot 6^\alpha+2\cdot 7^\alpha-2(7^\alpha-6^\alpha)\cdot\alpha(S_i),$$

$$\begin{aligned}\sum_{e=uv\in E_2\cap E(S_1)}[d_u+d_v]^\alpha=&(2l_1-6)\cdot 6^\alpha+7^\alpha+6^\alpha+2\cdot 5^\alpha\\&-(7^\alpha-2\cdot 6^\alpha+5^\alpha)\cdot\alpha(S_1),\\ \sum_{e=uv\in E_2\cap E(S_r)}[d_u+d_v]^\alpha=&(2l_r-6)\cdot 6^\alpha+7^\alpha+6^\alpha+2\cdot 5^\alpha\\&-(7^\alpha-2\cdot 6^\alpha+5^\alpha)\cdot\alpha(S_r).\end{aligned}$$

Thus,

$$\begin{aligned}\sum_{e=uv\in E_2}[d_u+d_v]^\alpha=&2\cdot 6^\alpha\sum_{i=1}^{r}l_i-2(7^\alpha-6^\alpha)\sum_{i=2}^{r-1}\alpha(S_i)+2(r-1)\cdot 7^\alpha\\&-(7^\alpha-2\cdot 6^\alpha+5^\alpha)[\alpha(S_1)+\alpha(S_r)]\\&-2(3r-1)\cdot 6^\alpha+4\cdot 5^\alpha.\end{aligned}$$

By the above demonstration one can see that:

$$\begin{aligned}\chi_\alpha(B_n)=&4(r-1)\cdot 7^\alpha+(3n-6r+1)\cdot 6^\alpha+6\cdot 5^\alpha+2\cdot 4^\alpha\\&+2\sum_{i=2}^{r-1}[5+\alpha(S_i)]^\alpha-(4\cdot 7^\alpha-8^\alpha-3\cdot 6^\alpha)\sum_{i=2}^{r-1}\alpha(S_i)\\&-(7^\alpha-2\cdot 6^\alpha+5^\alpha)\left[\alpha(S_1)+\alpha(S_r)\right].\end{aligned}$$

Hence for all $r\geq 1$ and $\alpha\geq 1$,

$$\begin{aligned}\chi_\alpha(B_n)=&4(r-1)\cdot 7^\alpha+(3n-6r+1)\cdot 6^\alpha+2[3-\phi(\alpha,r)]\cdot 5^\alpha\\&+2\sum_{i=2}^{r-1}[5+\alpha(S_i)]^\alpha-(4\cdot 7^\alpha-8^\alpha-3\cdot 6^\alpha)\sum_{i=2}^{r-1}\alpha(S_i)\\&-(7^\alpha-2\cdot 6^\alpha+5^\alpha)\left[\alpha(S_1)+\alpha(S_r)\right]+2\cdot 4^\alpha.\ \blacksquare\end{aligned}$$

Note that $\chi_1=M_1$, the following corollary is obtained straightforwardly from Theorem 3.1.

Corollary 3.2. (Theorem 2.1, [12]) Let B_n be a polyomino chain with n squares, $n \geq 3$, and consisting of r segments $S_1, S_2, \cdots, S_r, r \geq 1$, with lengths $l_1, l_2, \cdots, l_r$, respectively. Then

$$M_1(B_n) = 18n + 2r - 4.$$

As an immediate consequence of Corollary 3.2, we obtain the following result.

Corollary 3.3. The first Zagreb indices of linear and zig-zag chains are computed as follows:

(i) $M_1(L_n) = 18n - 2$,

(ii) $M_1(Z_n) = 20n - 6$.

We also get the following:

Corollary 3.4. The general sum-connectivity indices of linear and zig-zag chains with $n \geq 3$ squares are computed as follows:

(i) $\chi_\alpha(L_n) = (3n-5) \cdot 6^\alpha + 4 \cdot 5^\alpha + 2 \cdot 4^\alpha$,

(ii) $\chi_\alpha(Z_n) = (n-3) \cdot 8^\alpha + 2 \cdot 7^\alpha + 2(n-2) \cdot 6^\alpha + 4 \cdot 5^\alpha + 2 \cdot 4^\alpha$.

Proof. If $\alpha = 1$, then the desired result holds by Corollary 3.3; If $\alpha > 1$, then the desired result follows directly from Theorem 3.1. ■

4. Extremal polyomino chains with respect to general sum-connectivity index

In this section, we will characterize the extremal polyomino chains with respect to general sum-connectivity index. We first give two lemmas which will be used repeatedly in our proof.

Lemma 4.1. If $\alpha > 1$, then $4 \cdot 7^{\alpha} - 6^{\alpha+1} + 2 \cdot 5^{\alpha} > 0$.

Proof. Let $g(\alpha) = 4 \cdot 7^{\alpha} - 6^{\alpha+1} + 2 \cdot 5^{\alpha}$. Then,

$$\begin{aligned} g(\alpha) =& 4[7^{\alpha} - 6^{\alpha}] - 2[6^{\alpha} - 5^{\alpha}] \\ =& 4\alpha\xi^{\alpha-1} - 2\alpha\eta^{\alpha-1} \\ =& 2\alpha\xi^{\alpha-1} + 2\alpha[\xi^{\alpha-1} - \eta^{\alpha-1}] > 0, \end{aligned}$$

where $5 < \eta < 6 < \xi < 7$. ■

By the similar method used in the above proof we get the following.

Lemma 4.2. If $\alpha > 1$, then $8^{\alpha} - 2 \cdot 7^{\alpha} + 2 \cdot 6^{\alpha} - 5^{\alpha} > 0$.

We also need the following result.

Lemma 4.3. (Corollary 2.3, [12]) For any $B_n \in \mathbf{B}_n$, we have

$$M_1(L_n) \leq M_1(B_n) \leq M_1(Z_n),$$

with left (right, respectively) equality if and only if $B_n \cong L_n (B_n \cong Z_n$, respectively).

Now we present our main result.

Theorem 4.4. For any $B_n \in \mathbf{B}_n$, if $n \geq 3$ and $\alpha \geq 1$, then we have

$$\chi_{\alpha}(L_n) \leq \chi_{\alpha}(B_n) \leq \chi_{\alpha}(Z_n),$$

with left (right, respectively) equality if and only if $B_n \cong L_n (B_n \cong Z_n$, respectively).

Proof. If $\alpha = 1$, then the desired result follows by Lemma 4.3. Hence we assume $\alpha > 1$ in the following. For convenience, we let $f_i(r)_{max}$ and $f_i(r)_{min}$ denote the maximum and minimum values of the function $f_i(r)$ of parameter r, $i = 1, 2, 3, 4$, respectively. Let $A = (3n+1)\cdot 6^\alpha - 4\cdot 7^\alpha + 6\cdot 5^\alpha + 2\cdot 4^\alpha$. Then by Theorem 3.1,

$$\begin{aligned} f(r) := \chi_\alpha(B_n) =& A + (4\cdot 7^\alpha - 6^{\alpha+1})r + 2\sum_{i=2}^{r-1}[5+\alpha(S_i)]^\alpha \\ & - (4\cdot 7^\alpha - 8^\alpha - 3\cdot 6^\alpha)\sum_{i=2}^{r-1}\alpha(S_i) - 2\phi(\alpha, r)\cdot 5^\alpha \\ & - (7^\alpha - 2\cdot 6^\alpha + 5^\alpha)\left[\alpha(S_1) + \alpha(S_r)\right]. \end{aligned}$$

We distinguish the following two cases to discuss.

Case 1. Each $l_i > 2$, for $i = 1, 2, \cdots, r$. Note that in this case, $1 \le r \le \frac{n-1}{2}$, since $n + r - 1 \ge 3r$. Then if $r > 1$,

$$\begin{aligned} f_1(r) :=& A + (4\cdot 7^\alpha - 6^{\alpha+1})r + 2(r-2)\cdot 5^\alpha \\ =& A + (4\cdot 7^\alpha - 6^{\alpha+1} + 2\cdot 5^\alpha)r - 4\cdot 5^\alpha. \end{aligned}$$

If $r = 1$,

$$\begin{aligned} f_1(r) :=& A + (4\cdot 7^\alpha - 6^{\alpha+1})\cdot 1 - 2\cdot 5^\alpha \\ =& (3n-5)\cdot 6^\alpha + 4\cdot 5^\alpha + 2\cdot 4^\alpha. \end{aligned}$$

By Lemma 4.1,

$$\begin{aligned} f_1(r)_{max} =& A + (4\cdot 7^\alpha - 6^{\alpha+1} + 2\cdot 5^\alpha)\cdot \frac{n-1}{2} - 4\cdot 5^\alpha \\ =& (2n-6)\cdot 7^\alpha + 4\cdot 6^\alpha + (n+1)\cdot 5^\alpha + 2\cdot 4^\alpha, \end{aligned}$$

$$f_1(r)_{min} = (3n-5)\cdot 6^\alpha + 4\cdot 5^\alpha + 2\cdot 4^\alpha.$$

Case 2. There is at least one segment with length at most 2. Without loss of generality, we assume that there exist k segments $S_{i_1}, S_{i_2}, \cdots, S_{i_k}$, such that $l_{i_1}, l_{i_2}, \cdots, l_{i_k} \le 2$. Clearly, $1 \le k \le r$ and $2 \le r \le \frac{n-1+k}{2}$, since $n + r - 1 \ge 3(r-k) + 2k$. Then we consider the following three cases.

Subcase 2.1. $\{S_1, S_r\} \subseteq \{S_{i_1}, S_{i_2}, \cdots, S_{i_k}\}$. In this case, $3 \le r \le \frac{n-1+k}{2}$ and $2 \le k \le r$.

$$\begin{aligned} f_2(r) :=& A + (4\cdot 7^\alpha - 6^{\alpha+1})r + 2(k-2)\cdot 6^\alpha + 2(r-k)\cdot 5^\alpha \\ & - (k-2)(4\cdot 7^\alpha - 8^\alpha - 3\cdot 6^\alpha) - 2(7^\alpha - 2\cdot 6^\alpha + 5^\alpha) \\ =& A + (4\cdot 7^\alpha - 6^{\alpha+1} + 2\cdot 5^\alpha)r + (k-2)\cdot 8^\alpha - (4k-6)\cdot 7^\alpha \\ & + (5k-6)\cdot 6^\alpha - (2k+2)\cdot 5^\alpha. \end{aligned}$$

By Lemma 4.1,

$$\begin{aligned} f_2(r)_{max} =& A + (4\cdot 7^\alpha - 6^{\alpha+1} + 2\cdot 5^\alpha)\cdot \frac{n-1+k}{2} + (k-2)\cdot 8^\alpha \\ & - (4k-6)\cdot 7^\alpha + (5k-6)\cdot 6^\alpha - (2k+2)\cdot 5^\alpha \\ =& (k-2)\cdot 8^\alpha + (2n-2k)\cdot 7^\alpha + (2k-2)\cdot 6^\alpha \\ & + (n-k+3)\cdot 5^\alpha + 2\cdot 4^\alpha, \end{aligned} \tag{1}$$

$$\begin{aligned} f_2(r)_{min} =& A + (4\cdot 7^\alpha - 6^{\alpha+1} + 2\cdot 5^\alpha)\cdot 3 + (k-2)\cdot 8^\alpha \\ & - (4k-6)\cdot 7^\alpha + (5k-6)\cdot 6^\alpha - (2k+2)\cdot 5^\alpha \\ =& (k-2)\cdot 8^\alpha + (14-4k)\cdot 7^\alpha + (3n+5k-23)\cdot 6^\alpha \\ & + (10-2k)\cdot 5^\alpha + 2\cdot 4^\alpha. \end{aligned}$$

The equality (1) is easily transformed into $f_2(r)_{max} = (8^\alpha - 2\cdot 7^\alpha + 2\cdot 6^\alpha - 5^\alpha)k - 2\cdot 8^\alpha + 2n\cdot 7^\alpha - 2\cdot 6^\alpha + (n+3)\cdot 5^\alpha + 2\cdot 4^\alpha$, which is an increasing function of k on the interval $[2, r]$ by Lemma 4.2. Thus $f_2(r)_{max}$ attains the maximum value when $k = r$. Combining this with $r = \frac{n-1+k}{2}$ we obtain $k = r = n-1$. So

$$f_2(r)_{max} = (n-3)\cdot 8^\alpha + 2\cdot 7^\alpha + 2(n-2)\cdot 6^\alpha + 4\cdot 5^\alpha + 2\cdot 4^\alpha.$$

Note that $f_2(r)$ attains the minimum value when $r = 3$, this implies $k = 2$ since n is generally larger than 4. Thus

$$f_2(r)_{min} = 6\cdot 7^\alpha + (3n-13)\cdot 6^\alpha + 6\cdot 5^\alpha + 2\cdot 4^\alpha.$$

Subcase 2.2. $\{S_1, S_r\} \cap \{S_{i_1}, S_{i_2}, \cdots, S_{i_k}\} = \emptyset$. Evidently, in this case

$3 \le r \le \frac{n-1+k}{2}, 1 \le k \le r-2$ and $n > 5$. Then

$$\begin{aligned} f_3(r) :=& A + (4 \cdot 7^\alpha - 6^{\alpha+1})r + 2k \cdot 6^\alpha + 2(r-k-2) \cdot 5^\alpha \\ & - k(4 \cdot 7^\alpha - 8^\alpha - 3 \cdot 6^\alpha) \\ =& A + (4 \cdot 7^\alpha - 6^{\alpha+1} + 2 \cdot 5^\alpha)r + k \cdot 8^\alpha - 4k \cdot 7^\alpha + 5k \cdot 6^\alpha \\ & - (4+2k) \cdot 5^\alpha. \end{aligned}$$

By Lemma 4.1,

$$\begin{aligned} f_3(r)_{max} =& A + (4 \cdot 7^\alpha - 6^{\alpha+1} + 2 \cdot 5^\alpha) \cdot \frac{n-1+k}{2} + k \cdot 8^\alpha - 4k \cdot 7^\alpha \\ & + 5k \cdot 6^\alpha - (4+2k) \cdot 5^\alpha \\ =& k \cdot 8^\alpha + (2n-2k-6) \cdot 7^\alpha + (4+2k) \cdot 6^\alpha \\ & + (n-k+1) \cdot 5^\alpha + 2 \cdot 4^\alpha, \end{aligned} \tag{2}$$

$$\begin{aligned} f_3(r)_{min} =& A + (4 \cdot 7^\alpha - 6^{\alpha+1} + 2 \cdot 5^\alpha) \cdot 3 + k \cdot 8^\alpha - 4k \cdot 7^\alpha \\ & + 5k \cdot 6^\alpha - (4+2k) \cdot 5^\alpha \\ =& k \cdot 8^\alpha + (8-4k) \cdot 7^\alpha + (3n+5k-17) \cdot 6^\alpha \\ & + (8-2k) \cdot 5^\alpha + 2 \cdot 4^\alpha. \end{aligned}$$

The equality (2) is easily transformed into $f_3(r)_{max} = (8^\alpha - 2 \cdot 7^\alpha + 2 \cdot 6^\alpha - 5^\alpha)k + (2n-6) \cdot 7^\alpha + 4 \cdot 6^\alpha + (n+1) \cdot 5^\alpha + 2 \cdot 4^\alpha$, which is an increasing function of k on the interval $[1, r-2]$ by Lemma 4.2. Thus $f_2(r)_{max}$ attains the maximum value when $k = r-2$. Combining this with $r = \frac{n-1+k}{2}$ we obtain $r = n-3$ and $k = n-5$. So

$$f_3(r)_{max} = (n-5) \cdot 8^\alpha + 4 \cdot 7^\alpha + 2(n-3) \cdot 6^\alpha + 6 \cdot 5^\alpha + 2 \cdot 4^\alpha.$$

Note that $f_3(r)$ attains the minimum value when $r = 3$, then $k = 1$ by the hypothesis. Thus

$$f_3(r)_{min} = 8^\alpha + 4 \cdot 7^\alpha + 3(n-4) \cdot 6^\alpha + 6 \cdot 5^\alpha + 2 \cdot 4^\alpha.$$

Subcase 2.3. $|\{S_1, S_r\} \cap \{S_{i_1}, S_{i_2}, \cdots, S_{i_k}\}| = 1$.

Say $S_1 \in \{S_{i_1}, S_{i_2}, \cdots, S_{i_k}\}$. Obviously, in this case $2 \leq r \leq \frac{n-1+k}{2}$ and $1 \leq k \leq r-1$. Then

$$\begin{aligned}
f_4(r) :=& A + (4\cdot 7^\alpha - 6^{\alpha+1})r + 2(k-1)\cdot 6^\alpha + 2(r-k-1)\cdot 5^\alpha \\
&- (k-1)\cdot(4\cdot 7^\alpha - 8^\alpha - 3\cdot 6^\alpha) - (7^\alpha - 2\cdot 6^\alpha + 5^\alpha) \\
=& A + (4\cdot 7^\alpha - 6^{\alpha+1} + 2\cdot 5^\alpha)r + (k-1)\cdot 8^\alpha + (3-4k)\cdot 7^\alpha \\
&+ (5k-3)\cdot 6^\alpha - (2k+3)\cdot 5^\alpha.
\end{aligned}$$

By Lemma 4.1,

$$\begin{aligned}
f_4(r)_{max} =& A + (4\cdot 7^\alpha - 6^{\alpha+1} + 2\cdot 5^\alpha)\cdot\frac{n-1+k}{2} + (k-1)\cdot 8^\alpha \\
&+ (3-4k)\cdot 7^\alpha + (5k-3)\cdot 6^\alpha - (2k+3)\cdot 5^\alpha \\
=& (k-1)\cdot 8^\alpha + (2n-2k-3)\cdot 7^\alpha + (2k+1)\cdot 6^\alpha \\
&+ (n-k+2)\cdot 5^\alpha + 2\cdot 4^\alpha, \qquad (3)
\end{aligned}$$

$$\begin{aligned}
f_4(r)_{min} =& A + (4\cdot 7^\alpha - 6^{\alpha+1} + 2\cdot 5^\alpha)\cdot 2 + (k-1)\cdot 8^\alpha \\
&+ (3-4k)\cdot 7^\alpha + (5k-3)\cdot 6^\alpha - (2k+3)\cdot 5^\alpha \\
=& (k-1)\cdot 8^\alpha + (7-4k)\cdot 7^\alpha + (3n+5k-14)\cdot 6^\alpha \\
&+ (7-2k)\cdot 5^\alpha + 2\cdot 4^\alpha.
\end{aligned}$$

The equality (3) is easily transformed into $f_4(r)_{max} = (8^\alpha - 2\cdot 7^\alpha + 2\cdot 6^\alpha - 5^\alpha)k - 8^\alpha + (2n-3)\cdot 7^\alpha + 6^\alpha + (n+2)\cdot 5^\alpha + 2\cdot 4^\alpha$, which is an increasing function of k on the interval $[1, r-1]$ by Lemma 4.2. Thus $f_2(r)_{max}$ attains the maximum value when $k = r-1$. Combining this with $r = \frac{n-1+k}{2}$ we obtain $r = n-2$ and $k = n-3$. So

$$f_4(r)_{max} = (n-4)\cdot 8^\alpha + 3\cdot 7^\alpha + (2n-5)\cdot 6^\alpha + 5\cdot 5^\alpha + 2\cdot 4^\alpha.$$

Note that $f_4(r)$ attains the minimum value when $r = 2$, then $k = 1$ by the hypothesis. Thus

$$f_4(r)_{min} = 3\cdot 7^\alpha + 3(n-3)\cdot 6^\alpha + 5\cdot 5^\alpha + 2\cdot 4^\alpha.$$

In order to find out the maximum and minimum values of the function $f(r)$, we need to compare these values $f_i(r)_{max}$ and $f_i(r)_{min}$, $i = 1, 2, 3, 4$, respectively. First, we determine the maximum value.

$$
\begin{aligned}
f_2(r)_{max} - f_3(r)_{max} =&2 \cdot 8^{\alpha} - 2 \cdot 7^{\alpha} + 2 \cdot 6^{\alpha} - 2 \cdot 5^{\alpha} \\
=&2[8^{\alpha} - 7^{\alpha}] + 2[6^{\alpha} - 5^{\alpha}] \\
=&2\alpha\xi^{\alpha-1} + 2\alpha\eta^{\alpha-1} > 0,
\end{aligned} \tag{4}
$$

where $5 < \eta < 6$ and $7 < \xi < 8$.
Therefore, $f_2(r)_{max} > f_3(r)_{max}$.

$$
\begin{aligned}
f_3(r)_{max} - f_1(r)_{max} =&(n-5) \cdot 8^{\alpha} + (10-2n) \cdot 7^{\alpha} + (2n-10) \cdot 6^{\alpha} \\
&+ (5-n) \cdot 5^{\alpha} \\
=&(n-5)[8^{\alpha} - 2 \cdot 7^{\alpha} + 2 \cdot 6^{\alpha} - 5^{\alpha}] > 0,
\end{aligned}
$$

since $n > 5$ in Subcase 2.2 and by Lemma 4.2.
Therefore, $f_3(r)_{max} > f_1(r)_{max}$.
Hence, $f_2(r)_{max} > f_3(r)_{max} > f_1(r)_{max}$.
On the other hand,

$$
f_2(r)_{max} - f_4(r)_{max} = 8^{\alpha} - 7^{\alpha} + 6^{\alpha} - 5^{\alpha} > 0,
$$

the reason is the same as Eq. (4). Therefore, $f_2(r)_{max} > f_4(r)_{max}$.

Hence, $f_2(r)_{max}$ attains the maximum value among all values of $f(r)$ of the parameter r. Note that $r = n-1$ in this case, so $B_n \cong Z_n$.

Next, we determine the minimum value.

$$
\begin{aligned}
f_4(r)_{min} - f_1(r)_{min} =&3 \cdot 7^{\alpha} - 4 \cdot 6^{\alpha} + 5^{\alpha} \\
=&3[7^{\alpha} - 6^{\alpha}] - [6^{\alpha} - 5^{\alpha}] \\
=&2\alpha\xi^{\alpha-1} + \alpha[\xi^{\alpha-1} - \eta^{\alpha-1}] > 0,
\end{aligned} \tag{5}
$$

where $5 < \eta < 6 < \xi < 7$.
Therefore, $f_4(r)_{min} > f_1(r)_{min}$.

$$
\begin{aligned}
f_3(r)_{min} - f_4(r)_{min} =&8^{\alpha} + 7^{\alpha} - 3 \cdot 6^{\alpha} + 5^{\alpha} \\
=&[8^{\alpha} - 6^{\alpha}] + [7^{\alpha} - 6^{\alpha}] - [6^{\alpha} - 5^{\alpha}] \\
=&2\alpha\xi^{\alpha-1} + \alpha[\eta^{\alpha-1} - \zeta^{\alpha-1}] > 0,
\end{aligned}
$$

where $5 < \zeta < 6 < \eta < 7$ and $6 < \xi < 8$.
Therefore, $f_3(r)_{min} > f_4(r)_{min}$.
Hence, $f_3(r)_{min} > f_4(r)_{min} > f_1(r)_{min}$.
On the other hand,

$$
\begin{aligned}
f_2(r)_{min} - f_1(r)_{min} =& 6 \cdot 7^\alpha - 8 \cdot 6^\alpha + 2 \cdot 5^\alpha \\
=& 2[3 \cdot 7^\alpha - 4 \cdot 6^\alpha + 5^\alpha] > 0,
\end{aligned}
$$

the reason is the same as Eq. (5). Thus $f_2(r)_{min} > f_1(r)_{min}$.

Hence, $f_1(r)_{min}$ attains the minimum value among all values of $f(r)$ of the parameter r. Note that in this case $r = 1$, so $B_n \cong L_n$.
This completes the proof of Theorem 4.4. ■

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