arXiv:2304.02256v1 [math.CO] 5 Apr 2023

关于 p-Sombor 谱半径的极值树、单圈图和双圈图

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摘要

For a graph $G = (V, E)$ and $v_i \in V$, denote by d_{v_i} (or d_i for short) the degree of vertex v_i. The p-Sombor matrix $\mathbf{S_p}(G)$ ($p \neq 0$) of a graph G is a square matrix, where the (i, j)-entry is equal to $(d_i^p + d_j^p)^{\frac{1}{p}}$ if the vertices v_i and v_j are adjacent, and 0 otherwise. The p-Sombor spectral radius of G, denoted by $\rho(\mathbf{S_p}(G))$, is the largest eigenvalue of the p-Sombor matrix $\mathbf{S_p}(G)$. In this paper, we consider the extremal trees, unicyclic and bicyclic graphs with respect to the p-Sombor spectral radii. We characterize completely the extremal graphs with the first three maximum Sombor spectral radii, which answers partially a problem posed by Liu et al. in [MATCH Commun. Math. Comput. Chem. 87 (2022) 59-87].

关键词： p-Sombor谱半径；加权邻接矩阵；树；单环图；双环图

*2020*年数学学科分类： 05C09,05C35, 05C50

1. 引言

Graphs considered in this paper are all connected and simple, i.e., have no loops and parallel edges. Let $G = (V(G)\ E(G))$ be a graph with vertex set $V(G) = \{v_1, v_2, \ldots, v_n\}$ and edge set $E(G)$. An edge $e \in E(G)$ with end vertices v_i and v_j is usually denoted by v_iv_j. For $i = 1, 2, \ldots, n$, we denote by d_{v_i} (or d_i for short) the degree of the vertex v_i in G, $N(v_i)$ the set of neighbours of vertex v_i in G and $N[v_i] = N(v_i) \cup \{v_i\}$. As usual, let P_n, S_n and C_n be the path, star and cycle of order $n \geq 3$. In molecular graph theory, the topological

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indices of molecular graphs are used to reflect chemical properties of chemical molecules. There are many topological indices and among them there is a family of vertex-degree-based indices. The vertex-degree-based index $TI_f(G)$ of G with positive symmetric function $f(x, y)$ is defined as

$$TI_f(G) = \sum_{v_iv_j \in E(G)} f(d_i, d_j),$$

例如，Randi´c 指数 [18], 原子键连接指数 [4] 以及算术几何指数 [20]等。

Gutman [5] 提出了 Sombor 指数，这是化学图论中一种新颖的基于顶点度数的拓扑指数。其定义为

$$SO(G) = \sum_{v_iv_j \in E(G)} \sqrt{d_i^2 + d_j^2}.$$

由于 Sombor 指标的形式对应于一个 2-范数，R´eti 等人 [19]定义了一种更一般的形式，即 p-Sombor 指标（$p \neq 0$），其定义为

$$SO_p(G) = \sum_{v_iv_j \in E(G)} (d_i^p + d_j^p)^{\frac{1}{p}}.$$

Each index maps a molecular graph into a single number. Li [13] proposed that if we use a matrix to represent the structure of a molecular graph with weights separately on its pairs of adjacent vertices, it will completely keep the structural information of the graph. For example, the Randić matrix [16, 17], Atom-Bond Connectivity matrix [3] and Arithmetic-Geometric matrix [23] were considered separately. Based on these examples, Das et al. [2] proposed the weighted adjacency matrix $A_f(G)$, and it is defined as

$$A_f(G)(i, j) = \begin{cases} f(d_i, d_j), & v_iv_j \in E(G); \\ 0, & \text{otherwise.} \end{cases}$$

Since G is a connected graph, the weighted adjacency matrix $A_f(G)$ is an $n \times n$ nonnegative and irreducible symmetric matrix. Thus $\rho(A_f(G))$ is exactly the largest eigenvalue of $A_f(G)$ and it has a positive eigenvector $\mathbf{x} = (x_1, x_2, \ldots, x_n)^\intercal$. As a special case, the adjacency matrix $A(G)$ is $f(x, y) = 1$ and the adjacency spectral radius of G is denoted as $\rho(G)$. If $f'_x(x, y) \geq 0$ and $f''_x(x, y) \geq 0$, then $f(x, y)$ is said to be increasing and convex in variable x. If $f(x, y) > 0$ is increasing and convex in variable x and for any $x_1 + y_1 = x_2 + y_2$ and $\mid x_1 - y_1 \mid > \mid x_2 - y_2 \mid$, $f(x_1, y_1) \geq f(x_2, y_2)$, then $A_f(G)$ is called the weighted adjacency matrix with property P^* of G in [24].

Recently, corresponding to the p-Sombor index, Liu et al. [11] defined the p-Sombor matrix as $\mathbf{S_p}(G) = [s_{ij}^p]_{n\times n}$ $(p \neq 0)$, where

$$s_{ij}^p = \begin{cases} (d_i^p + d_j^p)^{\frac{1}{p}}, & v_iv_j \in E(G); \\ 0, & \text{otherwise.} \end{cases}$$

For $p = 2$, it is the Sombor matrix. Clearly, if $p \geq 1$, then the p-Sombor matrix is a weighted adjacency matrix with property P^*. Throughout this paper, we denote $\rho(\mathbf{S_p}(G))$ the largest eigenvalue of $\mathbf{S_p}(G)$. Choose the positive eigenvector $\mathbf{x}$ such that $\|\mathbf{x}\|_2 = 1$ and x_i corresponds to the vertex v_i and we call the unique unit positive vector $\mathbf{x}$ principal eigenvector of G.

Gutman [6] studied many spectral properties of the Sombor matrix. Gutman and Gowtham [7] obtained some results on the coefficients of the characteristic polynomial and bounds for the energy of Sombor matrix. There is a wealthy literature about Sombor matrix and its related topics, see [8, 15, 21, 22, 14]. Moreover, Liu et al. [11] considered some bounds of p-Sombor spectral radius and p-Sombor spectral spread and the Nordhaus-Gaddum-type results for p-Sombor spectral radius. They obtained that for a tree T of order n and $p \geq 1$,

$$\rho(\mathbf{S_p}(T)) \leq \rho(\mathbf{S_p}(S_n))$$

当且仅当$T \cong S_n$时等号成立。与此同时，他们提出了以下问题。

问题 1.1。 *[11] Sombor* 谱半径最大的前三个和最小的前三个树、单圈图和双圈图分别具有怎样的结构?

In this paper, we consider the extremal trees, unicyclic and bicyclic graphs with respect to the p-Sombor spectral radii. We characterize completely the extremal graphs with the first three maximum Sombor spectral radii, which answers partially Problem 1.1. Our main results can be summarized as follows, where the undefined extremal graphs will be characterized in corresponding sections.

1. Among all trees of order $n \geq 6$, we obtain S_n, $S_{2,n-2}$, $S_{3,n-3}$ are, respectively, the unique trees with the first three maximum spectral radii for the weighted adjacency matrices with property P^*. In addition, we get $\rho(A_f(P_4)) = \rho(A_f(S_{2,2})) < \rho(A_f(S_4))$ and $\rho(A_f(P_5)) < \rho(A_f(S_{2,3})) < \rho(A_f(S_5))$. The result also holds for the p-Sombor matrix with $p \geq 1$;

2. Among all unicyclic graphs of order $n \geq 7$, $S_n + e$, U_1, U_2, U_3 and U_4 are, respectively, the unique unicyclic graphs with the first five maximum p-Sombor spectral radii for $p \geq 2$. For $n = 6$, we get $S_6 + e$, U_1 and U_2 are, respectively, the unique unicyclic graphs with the first three maximum p-Sombor spectral radii and the unicyclic graph with the fourthly largest p-Sombor spectral radius depends on the choice of parameter p. Furthermore, we obtain $\rho(\mathbf{S_p}(C_5)) < \rho(\mathbf{S_p}(U_3)) < \rho(\mathbf{S_p}(U_2)) < \rho(\mathbf{S_p}(U_1)) < \rho(\mathbf{S_p}(S_5 + e))$ for $n = 5$;

3. Among all bicyclic graphs of order $n \geq 6$, we obtain B_1 is the unique bicyclic graph with the largest spectral radius of the weighted adjacency matrix with property P^*. In addition, B_1, B_2 and B_3 are, respectively, the unique bicyclic graphs with the first three maximum p-Sombor spectral radii for $p \geq 2$. For $n = 5$, we have $B_1 \cong B_3$ is the unique bicyclic graph with the largest p-Sombor spectral radius, the bicyclic graphs with the secondly and thirdly largest p-Sombor spectral radii depend on the choice of parameter p and they are B_2 and B_4.

此外，我们在附录 1 中给出了一种算法，用于计算所有阶数为 n、边数为 m 的图中 Sombor 谱半径最小的前三个极值图。

2. 预备结果

本节将介绍非负矩阵的矩阵理论知识、关于图谱的一些结果，以及一个将在后续章节中使用的新引理。

2.1. 既有结果

我们首先回顾矩阵理论中的若干著名结果。

Theorem 2.1. *[9] Let A and B be both $n \times n$ nonnegative symmetric matrices. Then $\rho(A + B) \geq \rho(A)$. Furthermore, if A is irreducible and $B \neq 0$, then $\rho(A + B) > \rho(A)$.*

定理 2.2。 *[1]* 设 A 为一个 $n \times n$ 非负对称矩阵。则 $\rho(A) \geq \boldsymbol{x}^\top A\boldsymbol{x}$ 对任意单位向量$\boldsymbol{x}$均成立，且等号成立当且仅当$A\boldsymbol{x} = \rho(A)\boldsymbol{x}$。

Definition 2.1. Let A be an $n \times n$ real matrix whose rows and columns are indexed by $X = \{1, 2, ..., n\}$. We partition X into $\{X_1, X_2, ..., X_k\}$ in order and rewrite A according to $\{X_1, X_2, ..., X_k\}$ as follows:

$$A = \begin{pmatrix} A_{1,1} & \cdots & A_{1,k} \\ \vdots & \ddots & \vdots \\ A_{k,1} & \cdots & A_{k,k} \end{pmatrix},$$

where $A_{i,j}$ is the block of A formed by rows in X_i and the columns in X_j. Let $b_{i,j}$ denote the average row sum of $A_{i,j}$. Then the matrix $B = [b_{i,j}]$ will be called the **quotient matrix** of the partition of A. In particular, the partition is called an **equitable partition** when the row sum of each block $A_{i,j}$ is constant.

关于图的邻接谱半径的一个结果。

定理 2.3。 *[1]* 设 $A \geq 0$ 为不可约矩阵， B 为 A的一个平衡划分的商矩阵。则 $\rho(A) = \rho(B)$。

Theorem 2.4. *[12] Let $U(n, n_1, n_2)$ be the unicyclic graph of order n as shown in Figure 1. If $max\{n_1, n_2\} + 3 \geq \frac{(1+\sqrt{6n+10})^2}{9}$, then $\rho(U(n, n_1, n_2)) \leq \sqrt{max\{n_1, n_2\} + 3}$.*

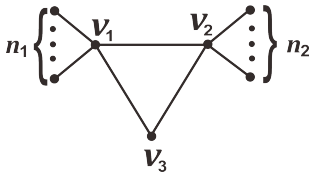


图 1: 单圈图 $U(n, n_1, n_2)$。

2.2. 新结果

在本小节中，我们将列出一些关于边移动与具有性质P^*的加权邻接矩阵谱半径之间关系的结果。这些操作将在后续证明中反复使用。

Kelmans [10] 引入了一种简单的图局部操作，用于描述移边与谱半径之间的关系，如下所示。

Definition 2.2. Let v_1, v_2 be two vertices of the graph G. And we denote: $N_1 = N(v_1) - N[v_2]$, $N_2 = N(v_2) - N[v_1]$. We use the Kelmans operation of G as follows: Replace the edge v_1v_w by a new edge v_2v_w for all vertices $v_w \in N_1$ (as shown in Figure 2). In general, we will denote the obtained graph by G'.

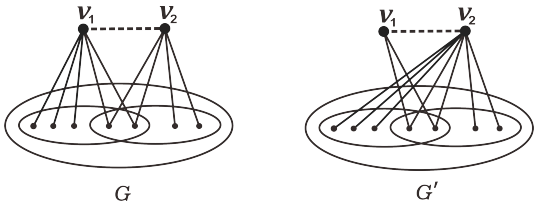


图 2: Kelmans 运算。

Theorem 2.5. *[24] Let G be a connected graph and G' be the graph after a Kelmans operation on any two vertices v_1 and v_2 of G as shown in Figure 2. If $G \ncong G'$, then $\rho(A_f(G)) < \rho(A_f(G'))$.*

以下定理是定理 2.5 的推论。

Theorem 2.6. *[24] Let G be a connected graph which consists of a proper induced subgraph H and a tree T of order $m+1$ ($m \geq 2$) such that H and T has a unique common vertex u and T is not a star with center u. Let $G^* = H + uv_1 + \cdots + uv_m$, where $v_1, v_2, \ldots, v_m \in V(T)$ are distinct pendent vertices of G^*. Then $\rho(A_f(G)) < \rho(A_f(G^*))$.*

对于另一种简单的局部操作（如下所述），文献 [24] 得到了定理 2.7。

The graph F is shown in Figure 3. v_1, v_2 are adjacent vertices of F and the vertices belong to $N(v_1) - N[v_2]$ (resp. $N(v_2) - N[v_1]$) are all pendent vertices and denoted as v_w (resp. v_y). And $v_{z_1}, \ldots, v_{z_m}$ ($m \geq 0$) are the common neighbours of v_1 and v_2. In addition, we denote $|N(v_1) - N[v_2]| = n_1$ and $|N(v_2) - N[v_1]| = n_2$. Without loss of generality, we assume that $1 \leq n_1 \leq n_2$. We replace edge v_1v_w in F by a new edge v_2v_w for one pendent vertex $v_w \in N(v_1) - N[v_2]$ to obtain a new graph F'' as shown in Figure 3. Then we have the following result.

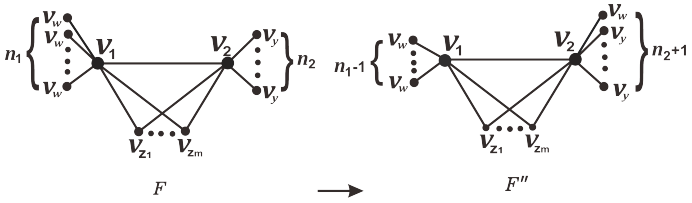


图 3: 图 F 和 F''。

Theorem 2.7. *[24] Let G be a connected graph of order n which consists of F and a proper induced subgraph H such that F and H have common vertices*

$v_{z_1}, \ldots, v_{z_m} (0 \leq m \leq n-4)$. *Replace* F *by* F'' *to obtain a new connected graph* G'' *(as shown in Figure 4). Then* $\rho(A_f(G)) < \rho(A_f(G''))$.

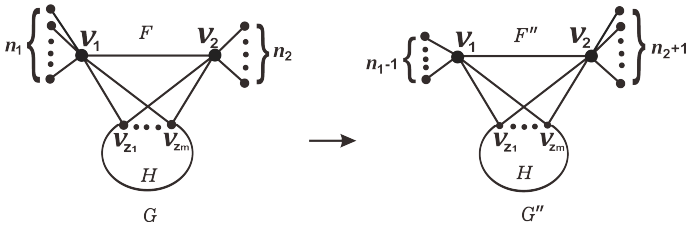


图 4: 图 G 和 G''。

2.3. 一个引理

在本小节中，我们给出一个引理，用于后续各节中极值单圈图和双圈图的研究。

[1]引理 2.8。 $f(x, y, p) = (x^p + y^p)^{\frac{1}{p}}$关于变量 $p \geq 2$单调递减，其中 $x, y \geq 1$。

证明。由于

$$f_p'(x, y, p) = \Big[\frac{x^p \ln x + y^p \ln y}{p(x^p + y^p)} - \frac{\ln(x^p + y^p)}{p^2}\Big] \cdot (x^p + y^p)^{\frac{1}{p}}$$

and

$$p\big[x^p \ln x + y^p \ln y\big] = x^p \ln x^p + y^p \ln y^p < (x^p + y^p) \ln(x^p + y^p)$$

对于 $x, y \geq 1$和 $p \geq 2$，我们有 $f_p'(x, y, p) < 0$。因此 $f(x, y, p)$ 关于变量 $p \geq 2$ 在 $x, y \geq 1$上递减。 □

3. 极值树

本节将探讨具有性质 P^* 的加权邻接矩阵谱半径对应的极值树。

Let $S_{d,n-d}$ be the double star of order $n \geq 4$ with two centers v_1, v_2 such that $d_1 = d$ and $d_2 = n - d$ where $2 \leq d \leq \lfloor \frac{n}{2} \rfloor$ as shown in Figure 5. Then we have the following theorem.

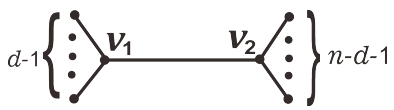


图 5: 阶为 $n \geq 6$ 的双星 $S_{d,\ n-d}$。

定理 3.1. 在所有阶为 $n \geq 6$ 的树中， S_n、 $S_{2,n-2}$、 $S_{3,n-3}$ 分别是具有性质 P^* 的加权邻接矩阵谱半径前三大的唯一树。

证明。 我们考虑以下两种情况来证明该定理。

情形1。 T 是一棵双星， $T \ncong S_n$, $S_{2,\ n-2}$, $S_{3,\ n-3}$。根据定理2.7，我们得到

$$\rho(A_f(T)) < \rho(A_f(S_{3,n-3})) < \rho(A_f(S_{2,n-2})) < \rho(A_f(S_n)).$$

情况 2. T 不是双星。

由于 T 不是双星， T 包含 P_5 作为其子图，如图6所示。不失一般性，我们假设 $d_2 \geq d_4 \geq 2$。

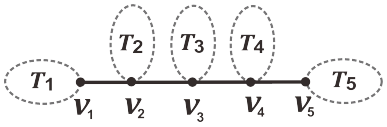


图6：子情形2.2中的树 T 。

子情形 2.1. $d_2 \geq 3$.

我们对相邻顶点 v_3 和 v_4 使用如图 7 所示的 Kelmans 操作。由定理 2.5、2.6 和 2.7，我们得到 $\rho(A_f(T)) < \rho(A_f(S_{3,\ n-3}))$。

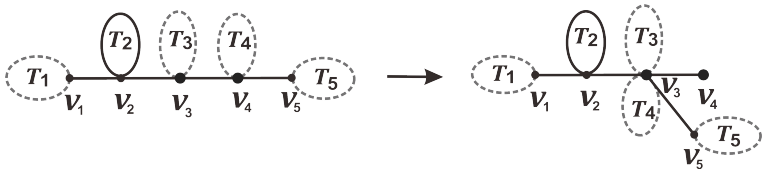


图7：子情形2.1的凯尔曼操作。

子情形 2.2. $d_2 = d_4 = 2$。

Without loss of generality, we assume that $d_1 \geq d_5 \geq 1$. If $d_3 = 2$, then $d_1 \geq 2$. We use Kelmans operation on the adjacent vertices v_3 and v_4 as shown in Figure 8. Analogically, we have $\rho(A_f(T)) < \rho(A_f(S_{3,n-3}))$.



图 8：相邻顶点 v_3 与 v_4 上的 Kelmans 运算。

Otherwise, $d_3 > 2$. We use Kelmans operation on the vertices v_2 and v_4 as shown in Figure 9. We also can obtain $\rho(A_f(T)) < \rho(A_f(S_{3,n-3}))$.

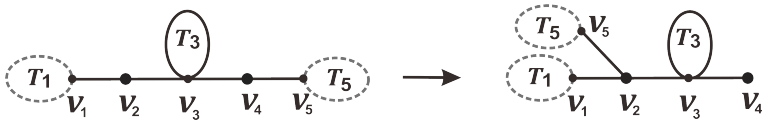


图 9: 对顶点 v_2 和 v_4 进行 Kelmans 操作。

因此，我们有 S_n, $S_{2,n-2}$, $S_{3,n-3}$ 分别是满足性质 P^* 的加权邻接矩阵谱半径最大的前三棵唯一树。

□

该结论对于带有 $p \geq 1$ 的 p-Sombor 矩阵同样成立。因此，我们得到以下定理。

定理3.2。 在所有阶为 $n \geq 6$、 S_n、 $S_{2,\ n-2}$、 $S_{3,\ n-3}$ 的树中，分别是对于 $p \geq 1$具有前三个最大 p-*Sombor*谱半径的唯一树。

注 3.1。 对于具有性质 P^* 和 n =4,5 的加权邻接矩阵，我们有

$$\rho(A_f(P_4)) = \rho(A_f(S_{2,2})) < \rho(A_f(S_4))$$

and

$$\rho(A_f(P_5)) < \rho(A_f(S_{2,3})) < \rho(A_f(S_5)).$$

这是定理 2.5 的直接推论，并且对于带有 $p \geq 1$ 的 p-Sombor 矩阵也成立。

Remark 3.2. Liu et al. [11] has obtained S_n is the unique tree with the largest p-Sombor spectral radius for $p \geq 1$. We consider the trees with the first three maximum p-Sombor spectral radii with $p \geq 1$. For the largest case, we obtain the same result.

4. 极值单环图

From now on, we assume that $f(x, y, p) = (x^p + y^p)^{\frac{1}{p}}$ with $x, y \geq 1$ and $p \geq 2$, then $f(x, y, p) > 0$ is strictly increasing and convex in variable x. And we consider the p-Sombor matrix $\mathbf{S_p}(G) = [f(d_i, d_j, p)]_{n\times n}$ with $p \geq 2$ which is the weighted adjacency matrix with property P^* of G.

In this section, we will think about the extremal unicyclic graphs with respect to the p-Sombor spectral radii.

The unicyclic graph $S_n + e$ with $n \geq 4$ is obtained from S_n by adding an edge as shown in Figure 10 (the first one). The unicyclic graphs U_1, U_2, U_3, U_4 and U_5 that will be considered in this section are also shown in Figure 10.

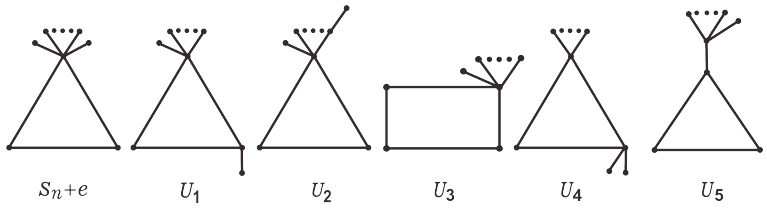


图 10: 阶为 $n \geq 7$ 的单圈图 $S_n + e$、U_1、U_2、U_3、U_4 和 U_5。

我们首先回顾一个关于具有性质 P^* 的单圈图的加权邻接矩阵谱半径的结果。

Theorem 4.1. *[24] If G is a unicyclic graph of order $n \geq 7$ and is not isomorphic to the graphs $S_n + e$, U_1, U_2, U_3, U_4 and U_5 (as shown in Figure 10), then $\rho(A_f(G)) < \rho(A_f(U_4))$. In addition, $\rho(A_f(U_3)) < \rho(A_f(U_2)) < \rho(A_f(U_1)) < \rho(A_f(S_n + e))$.*

接下来，我们考虑具有前五大最大p-Sombor谱半径的唯一单圈图。

引理 4.2。 U_4 和 U_5 是图 *10* 所示的阶为 $n \geq 7$ 的单圈图。则有 $\rho(\boldsymbol{S}_{\boldsymbol{p}}(U_5)) < \rho(\boldsymbol{S}_{\boldsymbol{p}}(U_4))$.

证明。 我们考虑以下两种情况。

情形 1. $n \geq 10$.

Suppose that the vertices of U_5 are denoted as Figure 11 and $\mathbf{x}$ be the principal eigenvector of U_5. We assume that the pendent vertices belonging to $N(v_1)$ are denoted as v_w. As $\mathbf{S_p}(G)\mathbf{x} = \rho(\mathbf{S_p}(G))\mathbf{x}$, the entries corresponding to these pendent vertices in $\mathbf{x}$ are equal.

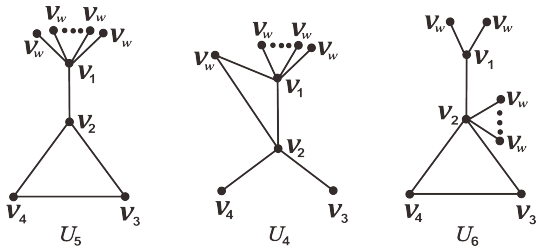


图 11: 阶数为 n 的单圈图 U_4、 U_5 和 U_6。

此外，因为 $\mathbf{S_P}(U_5)\mathbf{x} = \rho(\mathbf{S_P}(U_5))\mathbf{x}$，我们得到

$$\rho(\mathbf{S_p}(U_5))x_1 = (n-4)f(1,n-3,p)x_w + f(3,n-3,p)x_2,$$

and

$$\rho(\mathbf{S_p}(U_5))x_2 = f(3,n-3,p)x_1 + 2f(2,3,p)x_3.$$

因此，若 $x_1 \le x_2$，则 $x_w < x_3$。同时，

$$\rho(\mathbf{S_p}(U_5))x_3 = f(2,3,p)x_2 + f(2,2,p)x_4$$

and

$$\rho(\mathbf{S_p}(U_5))x_w = f(1,n-3,p)x_1.$$

We obtain if $x_1 > x_2$, then $x_2 > x_3$ for $n \ge 10$. Thus we have $x_1 > x_2 > x_3$. According to Lemma 2.8, we obtain $f(1,n-3,p) > f(2,3,p) + f(2,2,p)$ for $n \ge 10$. It is easy to see $x_1 > x_2 > x_w > x_3$. Then we consider the following two cases.

子情形1.1. $x_1 > x_2$.

将 U_5 中的边 v_3v_4 替换为一条新边 v_2v_w，得到图 11 所示的 U_4。于是有

$$\mathbf{x}^\top\mathbf{S_p}(U_4)\mathbf{x} - \mathbf{x}^\top\mathbf{S_p}(U_5)\mathbf{x} =$$
$$2\big[f(4,n-3,p) - f(3,n-3,p)\big]x_1x_2 + 4\big[f(1,4,p) - f(2,3,p)\big]x_2x_3 +$$
$$2\big[f(2,n-3,p) - f(1,n-3,p)\big]x_1x_w + 2\big[f(2,4,p)x_2x_w - f(2,2,p)x_3x_4\big] > 0.$$

Thus by Theorem 2.2, we obtain $\rho(\mathbf{S_p}(U_5)) < \rho(\mathbf{S_p}(U_4))$.

情形1.2. $x_1 \le x_2$.

将边 v_1v_w 在 U_5 中替换为一条新边 v_2v_w，为 $n-6$ 个悬挂顶点$v_w \in N(v_1)$，从而得到如图11所示的新图 U_6。我们得到

$$\mathbf{x}^\top\mathbf{S_p}(U_6)\mathbf{x} - \mathbf{x}^\top\mathbf{S_p}(U_4)\mathbf{x} =$$
$$4\big[f(1,3,p) - f(1,n-3,p)\big]x_1x_w + 4\big[f(2,n-3,p) - f(2,3,p)\big]x_2x_3$$
$$+2(n-6)\big[f(1,n-3,p)x_2x_w - f(1,n-3,p)x_1x_w\big].$$

因为 $x_1 \le x_2$，我们有

$(n-4)f(1,n-3,p)x_w + f(3,n-3,p)x_2 \le f(3,n-3,p)x_1 + 2f(2,3,p)x_3$，由此可得

$$(n-4)f(1,n-3,p)x_w \le 2f(2,3,p)x_3, \text{ i.e. } x_w \le \frac{2f(2,3,p)}{(n-4)f(1,n-3,p)}x_3.$$

Th我们或 $n \ge 10$我们有

$$\begin{aligned}
&\big[f(1,3,p)-f(1,n-3,p)\big]x_1x_w + \big[f(2,n-3,p)-f(2,3,p)\big]x_2x_3\\
>&\Big\{\big[f(1,3,p)-f(1,n-3,p)\big]\frac{2f(2,3,p)}{(n-4)f(1,n-3,p)} + f(2,n-3,p)-f(2,3,p)\Big\}x_2x_3\\
=&\frac{1}{(n-4)f(1,n-3,p)}\Big\{2f(2,3,p)\big[f(1,3,p)-f(1,n-3,p)\big]\\
&+(n-4)f(1,n-3,p)\big[f(2,n-3,p)-f(2,3,p)\big]\Big\}x_2x_3\\
=&\frac{1}{(n-4)f(1,n-3,p)}\Big\{2f(2,3,p)f(1,3,p)+f(1,n-3,p)\big[(n-4)f(2,n-3,p)\\
&-2f(2,3,p)-(n-4)f(2,3,p)\big]\Big\}x_2x_3\\
>&\frac{2f(2,3,p)f(1,3,p)+f(1,n-3,p)\big[n^2-(7+\sqrt{13})n+2\sqrt{13}+12\big]}{(n-4)f(1,n-3,p)}x_2x_3 \text{ (by Lemma 2.8)}\\
>&0.
\end{aligned}$$

Thus we get $\mathbf{x}^\top\mathbf{S_p}(U_6)\mathbf{x}-\mathbf{x}^\top\mathbf{S_p}(U_5)\mathbf{x} > 0$. By Theorem 2.2, we have $\rho(\mathbf{S_p}(U_5)) < \rho(\mathbf{S_p}(U_6))$. According to Theorem 2.5, we obtain $\rho(\mathbf{S_p}(U_6)) < \rho(\mathbf{S_p}(U_4))$. Thus we get $\rho(\mathbf{S_p}(U_5)) < \rho(\mathbf{S_p}(U_4))$ for $n \ge 10$.

子情形 2.。

With the aid of MATLAB, we obtain $\rho(\mathbf{S_{p=2}}(U_5)) < \lim\limits_{p\to\infty}\rho(\mathbf{S_p}(U_4))$ for $7 \le n \le 9$. Then by Lemma 2.8, we obtain $\rho(\mathbf{S_p}(U_5)) < \rho(\mathbf{S_p}(U_4))$ for $7 \le n \le 9$.

至此，证明完成。 □

引理4.3。 U_3 和 U_4 是阶为 $n \ge 7$ 的如图*10*所示的单环图。那么有 $\rho(\boldsymbol{S}^p(U_4)) < \rho(\boldsymbol{S}^p(U_3))$。

证明。 设 U_3 的顶点如图 12 所示。

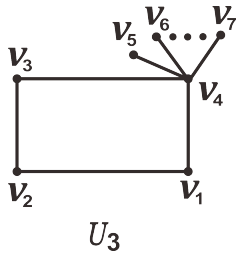


图 12: 阶为 n 的单环图 U_3。

关于 $\mathbf{p}(U_3)$ 的平衡划分 $\{\{v_1, v_3\}, \{v_2\}, \{v_4\}, \{v_5, \ldots, v_n\}\}$ 对应的商矩阵为$\mathbf{S}$

$$\begin{pmatrix} 0 & f(2,2) & f(2,n-2) & 0 \\ 2f(2,2) & 0 & 0 & 0 \\ 2f(2,n-2) & 0 & 0 & (n-4)f(1,n-2) \\ 0 & 0 & f(1,n-2) & 0 \end{pmatrix}.$$

我们假设 $P(x,\ U_3)$ 是商矩阵的特征多项式。经计算，我们得到

$$\begin{aligned} P(x,U_3) = x^4 &- \big[2f^2(2,2,p) + 2f^2(2,n-2,p) + (n-4)f^2(1,n-2,p)\big]x^2 \\ &+ 2(n-4)f^2(2,2,p)f^2(1,n-2,p). \end{aligned}$$

由于对于任意 x，我们有

$$\begin{aligned} P(x,U_3) \ &< \ x^4 - \big[2f^2(2,2,p) + 2f^2(2,n-2,p) + (n-4)f^2(1,n-2,p)\big]x^2 \\ &+ \ 2f^2(2,2,p)\big[2f^2(2,n-2,p) + (n-4)f^2(1,n-2,p)\big], \end{aligned}$$

由此可得

$$2f^2(2,n-2,p) + (n-4)f^2(1,n-2,p) < \rho(\mathbf{S_p}(U_3))^2.$$

我们考虑以下两种情况。

情况 1. $n \geq 17$。

根据定理 2.1 和定理 2.4，可得

$$\rho(\mathbf{S_p}(U_4))^2 < (n-2)f^2(4,n-3,p).$$

那么我们只需证明

$$(n-2)f^2(4,n-3,p) < 2f^2(2,n-2,p) + (n-4)f^2(1,n-2,p).$$

Let

$$\begin{aligned} Q(n,p) &= 2f^2(2,n-2,p)+(n-4)f^2(1,n-2,p)-(n-2)f^2(4,n-3,p) \\ &= 2\big[2^p+(n-2)^p\big]^{\frac{2}{p}}+(n-4)\big[1+(n-2)^p\big]^{\frac{2}{p}}-(n-2)\big[4^p+(n-3)^p\big]^{\frac{2}{p}}. \end{aligned}$$

我们考虑

$$h(x,y)=1+(x-2)^y-\big[4^y+(x-3)^y\big].$$

由于

$$h'_x(x,y)=y(x-2)^{y-1}-y(x-3)^{y-1}>0$$

对于 $y\geq 2$ 和 $x\geq 17$，我们得到

$$h(x,y)\geq h(17,y)=1+15^y-4^y-14^y.$$

As

$$\begin{aligned} h'_y(17,y) &= 15^y\ln 15-4^y\ln 4-14^y\ln 14 \\ &\geq 15^{y-2}\big[15^2\ln 15-4^2\ln 4-14^2\ln 14\big]>0 \end{aligned}$$

对于 $y\geq 2$，我们得到 $h(x,\ y)\geq h(17,\ 2)>0$。容易证明 $Q(n,\ p)>0$。

因此，我们推得对于 $n\geq 17,\ \ \rho(S_P(U_4))<\rho(S_P(U_3))$。

情形 2. $7\leq n\leq 16$.

Similarly, by Lemma 2.8 and with the aid of MATLAB, we obtain $\rho(\mathbf{S_p}(U_4))<\rho(\mathbf{S_p}(U_3))$. The proof of this result is quite similar to that given for Case 2 of Lemma 4.2. It is not difficult but is too long to give here.

引理的证明至此完成。 □

Theorem 4.4. *Among all unicyclic graphs of order $n\geq 7$, S_n+e, U_1, U_2, U_3 and U_4 (see in Figure 10) are, respectively, the unique unicyclic graphs with the first five maximum p-Sombor spectral radii.*

Proof. According to Theorem 4.1 and Lemmas 4.2 and 4.3, we get S_n+e, U_1, U_2, U_3 and U_4 as shown in Figure 10 are, respectively, the unique unicyclic graphs with the first five maximum p-Sombor spectral radii. □

注记 4.1。对于 $n=5$，我们有 $S_5+e\cong U_4$ 和 $U_2\cong U_5$。借助 MATLAB 并根据定理 2.5，我们得到

$$\rho(\mathbf{S_p}(S_5+e))>\rho(\mathbf{S_p}(U_1))>\rho(\mathbf{S_p}(U_2))>\rho(\mathbf{S_p}(U_3))>\rho(\mathbf{S_p}(C_5)).$$

And for $n=6$, we get S_6+e, U_1 and U_2 are, respectively, the unique unicyclic graphs with the first three maximum p-Sombor spectral radii. Moreover, we find the unicyclic graph with the fourthly largest p-Sombor spectral radius depends on the choice of parameter p.

5. 极值双环图

本节将研究关于具有性质 P^* 的加权邻接矩阵的谱半径以及 p-Sombor 谱半径的极值双圈图。

The bicyclic graph obtained from two cycles C_q and C_t $(q \geq t \geq 3)$ with a common path P_l such that $2 \leq l \leq t-l+2$ is denoted by $P(q,l,t)$ as shown in Figure 13 (left). Set $\mathcal{P} = \{P(q,l,t) \mid q \geq t \geq 3, 2 \leq l \leq t-l+2\}$.

In addition, suppose that C_q and C_t are two vertex-disjoint cycles $(q \geq t \geq 3)$, z_1 is a vertex of C_q and z_l is a vertex of C_t. We join z_1 and z_l by a path $z_1 z_2 \ldots z_l$ of length $l-1$, where $l \geq 1$ and $l = 1$ means identifying z_1 with z_l. The resulting graph is denoted by $B(q,l,t)$ as shown in Figure 13 (right). Set $\mathcal{B} = \{B(q,l,t) \mid q \geq t \geq 3, l \geq 1\}$.

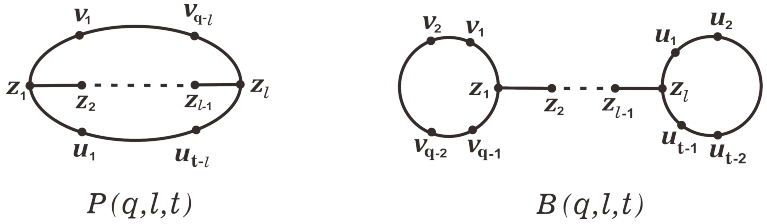


图13: 双环图 $P(q,l,t)$ 和 $B(q,l,t)$。

$\hat{}$ 对于一个双环图 G， G的基，记为 G，是 G的唯一极小双环子图。设 $\mathcal{B}(n)$是所有阶为 n 的双环图的集合。我们可以定义以下两个阶为n的双环图类:

$$\mathcal{B}_1(n) = \{G \in \mathcal{B}(n) \mid \hat{G} \in \mathcal{P}\} \text{ and } \mathcal{B}_2(n) = \{G \in \mathcal{B}(n) \mid \hat{G} \in \mathcal{B}\}.$$

It is easy to see that $\mathcal{B}(n) = \mathcal{B}_1(n) \bigcup \mathcal{B}_2(n)$ and $\mathcal{B}_1(n) \cap \mathcal{B}_2(n) = \emptyset$. In addition, the bicyclic graphs B_1, B_2, B_3 and B_4 that will be considered in this section are shown in Figure 14. And it is obviously that B_1, B_3, $B_4 \in \mathcal{B}_1(n)$ and $B_2 \in \mathcal{B}_2(n)$.

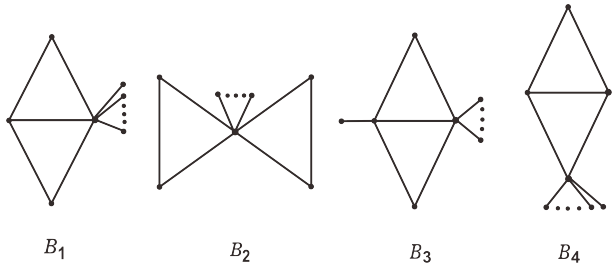


图 14: 阶为 $n \geq 7$ 的双环图 B_1、 B_2、 B_3 和 B_4。

在下文中，我们首先考虑具有性质 P^* 的加权邻接矩阵中谱半径最大的唯一双圈图。

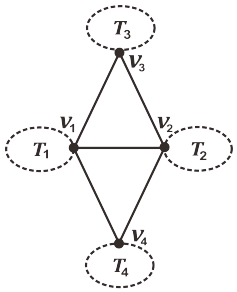
Theorem 5.1. *If G is a bicyclic graph of order $n \geq 6$ and is not isomorphic to the bicyclic graphs B_1, B_2, B_3 and B_4 as shown in Figure 14, then we have $\rho(A_f(G)) < \rho(A_f(B_3))$.*

证明。 我们考虑以下两种情况。

情形1. $G \in \mathcal{B}_1(n)$.

子情形 1.1。 $\hat{G} \in \mathcal{P}$ 使得 $l = 2, q = t = 3$。

B_5 is the bicyclic graph of order $n \geq 6$ as shown in Figure 15, where T_i is a tree and has a unique common vertex v_i with $P(3, 2, 3)$ in B_5 for $1 \leq i \leq 4$. Without loss of generality, let $v(T_i)$ be the order of T_i such that $v(T_1) \geq v(T_2) \geq 1$ and $v(T_3) \geq v(T_4) \geq 1$. If $\hat{G} \in \mathcal{P}$ such that $l = 2, q = t = 3$, then G has the same structure as B_5.



B_5

图 15: 双圈图 B_5。

子情形 1.1.1. $v(T_1) \geq 2$.

如果 T_1中存在与v_1相邻的非悬挂顶点 $w_1, \ldots, w_s (1 \leq s \leq \lfloor \frac{n-4}{2} \rfloor)$，那么我们对顶点 v_2和 $w_1, \ldots, w_s$进行凯尔曼操作，

v_2 and v_3, v_2 and v_4, respectively. Otherwise, we only use Kelmans operations on the vertices v_2 and v_3, v_2 and v_4. We denote the obtained graph by G' (see Figure 16). Because $G \ncong B_1$, we have $v(T_2'') \geq 2$.

若 $G' \cong B_3$，则根据定理 2.5，可得 $\rho(A_f(G)) < \rho(A_f(B_3))$。

否则，由定理 2.5、2.6 和 2.7，得到 $\rho(A_f(G)) < \rho(A_f(B_3))$。

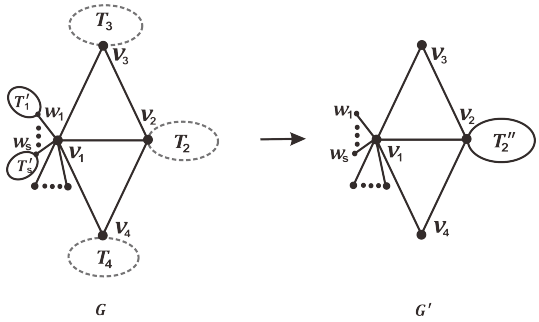


图 16：子情形 1.1.1 的 Kelmans 操作。

子情形 1.1.2. $v(T_1) = 1$.

As $v(T_1) \geq v(T_2)$, we have $v(T_1) = v(T_2) = 1$. If there are non-pendent vertices $w_1, \ldots, w_s$ $(1 \leq s \leq \lfloor \frac{n-4}{2} \rfloor)$ adjacent to v_3 in T_3, then we use Kelmans operations on the vertices v_1 and $w_1, \ldots, w_s$, v_1 and v_4, v_2 and v_3, respectively. Otherwise, we only use Kelmans operations on the vertices v_1 and v_4, v_2 and v_3. We denote the obtained graph by G' (see Figure 17). Since $G \ncong B_4$, then $v(T_1'') \geq 2$.

If $G' \cong B_3$, then by Theorem 2.5, we have $\rho(A_f(G)) < \rho(A_f(B_3))$. Otherwise, according to Theorems 2.5, 2.6 and 2.7, we obtain $\rho(A_f(G)) < \rho(A_f(B_3))$.

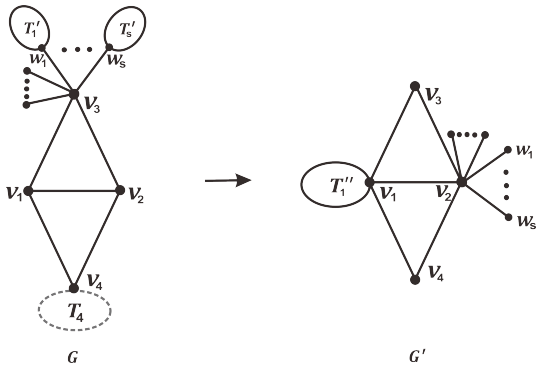


图 17：子情形 1.1.2 的 Kelmans 操作。

ˆ**子情形 1.2**。 $G \in \mathcal{P}$ 使得 $l = 2,\ \ q > 3$。

Let $d_{z_1} + d_{v_1} \leq d_{z_2} + d_{v_{q-2}}$. We firstly use Kelmans operations on the vertices v_1 and z_1, then z_2 and v_{q-2}, ..., v_2, u_{t-2}, ..., u_1 in order to obtain a resulting graph G'. Because $d_{z_1} + d_{v_1} \leq d_{z_2} + d_{v_{q-2}}$, then $G' \ncong B_1$.

If $G' \cong B_3$, according to Theorem 2.5, we have $\rho(A_f(G)) < \rho(A_f(B_3))$. Otherwise, by Theorems 2.5, 2.6 and 2.7, we obtain $\rho(A_f(G)) < \rho(A_f(B_3))$.

ˆ**子情形 1.3.** $G \in \mathcal{P}$ 使得 $\ l \geq 3$。

We firstly use Kelmans operations on the vertices z_l and v_{q-l}, ..., v_2, u_{t-l}, ..., u_2 (the vertices v_{q-l}, ..., v_2, u_{t-l}, ..., u_2 are not necessarily all exist, we use Kelmans operations on the existing vertices) in order. Then we use Kelmans operations on the vertices z_3 and z_3, ..., z_l in order. Suppose the resulting graph is G'. Then G' has the same structure as B_6 (see Figure 18 (left)). Afterward, we use Kelmans operations on the vertices u_1 and z_2, then z_2 and v_1 to obtain a resulting graph that has the same structure as B_7 (see Figure 18 (center)). Without loss of generality, we assume that $v(T_2) \geq v(T_3) \geq 1$. Next, we use Kelmans operation on the vertices z_2 and z_3 to obtain a new graph G'' that has the same structure as B_8 (see Figure 18 (right)). Clearly, G'' is not isomorphic to B_1 and B_4.

If $G'' \cong B_3$, then by Theorem 2.5, we have $\rho(A_f(G)) < \rho(A_f(B_3))$. Otherwise, by Subcase 1.1, we get $\rho(A_f(G)) < \rho(A_f(B_3))$.

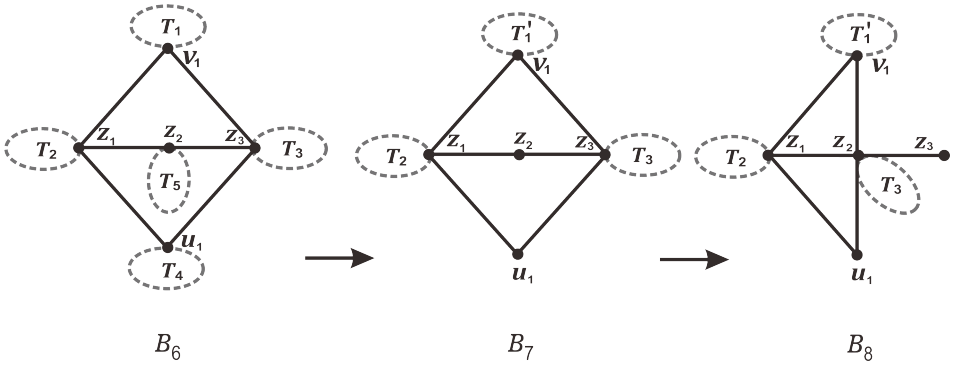


图 18: 双环图 B_6、 B_7 和 B_8。

情况2. $G \in \mathcal{B}_2(n)$.

ˆ**子情形 2.1.** $G \in \mathcal{B}$ 使得 $l = 1$。

Firstly, we use Kelmans operations on the vertices v_1 and v_2, ..., v_{q-1}, u_1 and ..., u_{t-1} in order. Suppose the resulting graph is G'. We obtain G' has the same structure as B_9 (see Figure 19 (left)). Then we use Kelmans operation on the vertices v_1 and u_{t-1} to obtain a new graph G'' as shown in

Figure 19. It is clear that $G'' \ncong B_4$. Because $G \ncong B_2$, we have $G'' \ncong B_1$.

If $G'' \cong B_3$, then by Theorem 2.5, we have $\rho(A_f(G)) < \rho(A_f(B_3))$. Otherwise, according to Subcase 1.1, we get $\rho(A_f(G)) < \rho(A_f(B_3))$.

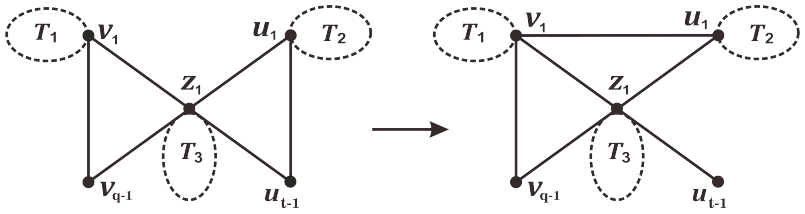


图 19: 双环图 B_9 及 Subcase 2.1 的 Kelmans 操作。

子情形 2.2. $G \in \mathcal{B}$ 使得 $l \geq 2$。

Firstly, we use Kelmans operations on the vertices v_1 and v_2, v_3, ..., v_{q-1}, the vertices u_1 and u_2, u_3, ..., u_{t-1}, the vertices z_2 and z_2, z_3, ..., z_{l-1}, z_l of G in order. Suppose the resulting graph is G'. Then we use Kelmans operation on the vertices v_1 and z_2 to obtain a new graph G'' as shown in Figure 20. We have $G'' \ncong B_2$. Analogously, we get $\rho(A_f(G)) < \rho(A_f(B_3))$.

证明完成。 □

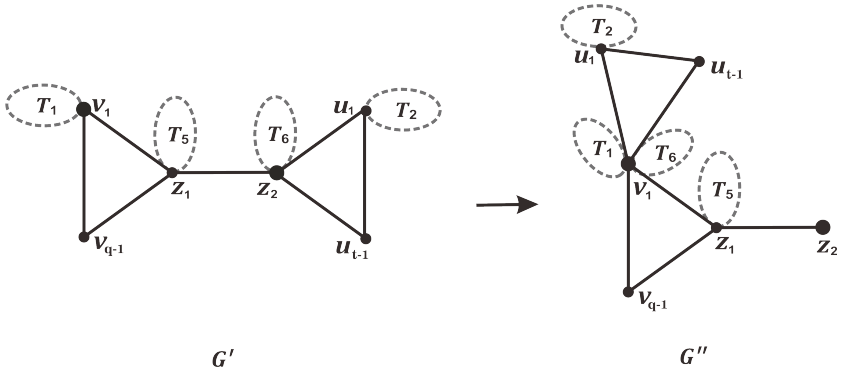


图20: 子情形2.2的凯尔曼操作。

定理 5.2. 在所有阶为 $n \geq 6$ 的双圈图中， B_1 是唯一具有性质 P^* 且其加权邻接矩阵谱半径最大的双圈图。

证明。在双环图 B_1、 B_2、 B_3 和 B_4中，根据定理2.5，我们得到 B_1 具有满足性质 P^*的加权邻接矩阵的最大谱半径。结合定理 5.1，我们由此证明了该定理。

□

接下来，我们将探讨具有前三大 p-Sombor 谱半径的唯一双环图。

引理5.3。 B_3、 B_4 是如图*14*所示的阶为 $n \geq 6$ 的双圈图。则有 $\rho(\boldsymbol{S}_{\boldsymbol{p}}(B_4)) < \rho(\boldsymbol{S}_{\boldsymbol{p}}(B_3))$。

证明。 在证明中，我们考虑以下两种情况。

情况 1. $n \geq 10$.

设 B_4 的顶点如图21（左）所示。

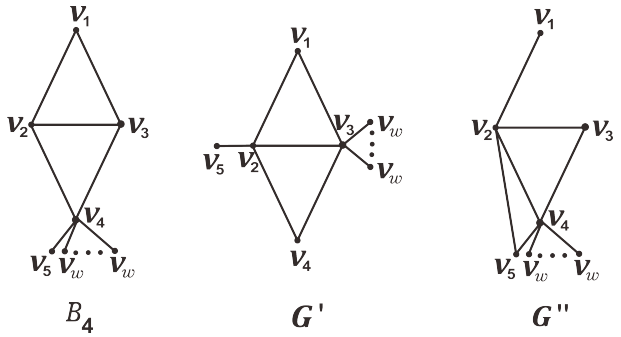


图21：引理5.3中的双环图 B_4、 G' 和 G'' 。

设 $\mathbf{x}$ 是 B_4 的主特征向量。由 $\mathbf{S_p}(B_4)\mathbf{x} = \rho(\mathbf{S_p}(B_4))\mathbf{x}$可知，$\mathbf{x}$ 中与悬挂顶点 v_w 和 v_5 对应的分量相等。我们得到

$$\begin{aligned}
&\rho(\mathbf{S_p}(B_4))x_1 = 2f(2,3,p)x_2,\\
&\rho(\mathbf{S_p}(B_4))x_2 = f(2,3,p)x_1 + f(3,3,p)x_2 + f(3,n-2,p)x_4,\\
&\rho(\mathbf{S_p}(B_4))x_4 = 2f(3,n-2,p)x_2 + (n-4)f(1,n-2,p)x_5,\\
&\rho(\mathbf{S_p}(B_4))x_5 = f(1,n-2,p)x_4.
\end{aligned}$$

我们考虑以下两种情况。

子情形 1.1. $x_1 > x_5$.

Since $f(1,n-2,p) > 2f(2,3,p)$ for $n \geq 10$, we obtain if $x_1 > x_5$, then $x_2 > x_4$. We have $x_2 = x_3 > x_4 > x_1 > x_5$. Replace edge v_4v_5 in B_4 by a new

将 $n-5$ 个悬挂顶点 $v_w \in N(v_4)$ 之间的边 v_2v_5 和 v_4v_w 替换为一条新边 v_3v_w，得到新图 $G' \cong B_3$，如图 21（中）所示。于是我们有

$$\begin{aligned}
&\mathbf{x}^\top \mathbf{S_p}(G')\mathbf{x} - \mathbf{x}^\top \mathbf{S_p}(B_4)\mathbf{x} = \\
&2\big[f(2,4,p) - f(2,3,p)\big]x_1x_2 + 2\big[f(2,n-2,p) - f(2,3,p)\big]x_1x_3 \\
&+2\big[f(1,4,p)x_2x_5 - f(1,n-2,p)x_4x_5\big] \\
&+2\big[f(4,n-2,p) - f(3,3,p)\big]x_2x_3 + 2\big[f(2,4,p) - f(3,n-2,p)\big]x_2x_4 \\
&+2\big[f(2,n-2,p) - f(3,n-2,p)\big]x_3x_4 \\
&+2(n-5)\big[f(1,n-2,p)x_3x_w - f(1,n-2,p)x_4x_w\big] \\
&>2\big[f(2,4,p) - f(2,3,p) + f(2,n-2,p) - f(2,3,p) + f(1,4,p) - f(1,n-2,p)\big]x_2x_5 \\
&+2\big[f(4,n-2,p) - f(3,3,p) + f(2,4,p) - f(3,n-2,p) + f(2,n-2,p) \\
&-f(3,n-2,p)\big]x_2x_3 + 2(n-5)\big[f(1,n-2,p)x_3x_w - f(1,n-2,p)x_4x_w\big] > 0.
\end{aligned}$$

因此我们有 $\rho(\mathbf{S_P}(B_4)) < \rho(\mathbf{S_P}(B_3))$.

子情形1.2. $x_1 \le x_5$.

我们把边 v_1v_3 在 B_4 中替换为一条新边 v_2v_5，从而得到新图$G'' \cong B_3$，如图21（右）所示。于是有

$$\begin{aligned}
&\mathbf{x}^\top \mathbf{S_p}(G'')\mathbf{x} - \mathbf{x}^\top \mathbf{S_p}(B_4)\mathbf{x} = \\
&2\big[f(1,4,p) - f(2,3,p)\big]x_1x_2 + 2\big[f(2,4,p) - f(3,3,p)\big]x_2x_3 \\
&+2\big[f(2,n-2,p) - f(3,n-2,p)\big]x_3x_4 + 2\big[f(4,n-2,p) - f(3,n-2,p)\big]x_2x_4 \\
&+2\big[f(2,n-2,p) - f(1,n-2,p)\big]x_4x_5 + 2\big[f(2,4,p)x_2x_5 - f(2,3,p)x_1x_3\big] > 0.
\end{aligned}$$

因此，对于 $n \ge 10$，我们得到 $\rho(\mathbf{S_P}(B_4)) < \rho(\mathbf{S_P}(B_3))$。

情形 2. $6 \le n \le 9$.

根据引理2.8并借助MATLAB，我们还可以得到 $\rho(\mathbf{S_P}(B_4)) < \rho(\mathbf{S_P}(B_3))$，对于 $6 \le n \le 9$。该结果的证明与引理4.2中情形2的证明非常相似。

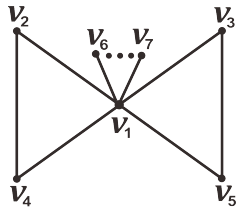
我们由此证明了该引理。 □

引理 5.4. B_3 和 B_2 是如图 *14* 所示的阶为 $n \ge 6$ 的双圈图。于是我们有 $\rho(\boldsymbol{S_P}(B_3)) < \rho(\boldsymbol{S_P}(B_2))$。

证明。该引理的证明分为以下两种情况。

情形 1. $n \ge 18$.

设 B_2 的顶点如图 22 所示。



B_2

图 22：阶为 n 的双环图 B_2。

我们将 $\{\{v_1\},\{v_2,v_3,v_4,v_5\},\{v_6,v_7,\ldots,v_n\}\}$ 的$\mathbf{Sp}(B_2)$的等距划分商矩阵记为

$$Q=\begin{pmatrix} 0 & 4f(2,n-1,p) & (n-5)f(1,n-1,p) \\ f(2,n-1,p) & f(2,2,p) & 0 \\ f(1,n-1,p) & 0 & 0 \end{pmatrix}.$$

设 $P(x,B_2)$ 为商矩阵 Q 的特征多项式。我们可以得到

$$\begin{aligned} P(x,B_2) &= x^3-f(2,2,p)x^2-\big[4f^2(2,n-1,p)+(n-5)f^2(1,n-1,p)\big]x \\ &\quad +(n-5)f(2,2,p)f^2(1,n-1,p). \end{aligned}$$

类似地，设 $P'(x,\ B_3)$ 为邻接矩阵 $A(B_3)$ 的一个均衡划分的商矩阵的特征多项式，我们有

$$P'(x,B_3)=x^4-(n+1)x^2-4x+3n-13.$$

经计算，我们得到 $\rho(B_3)<\sqrt{n}$ 对于 $n\geq 18$。因此 $\rho(\mathbf{Sp}(B_3))<\sqrt{nf}(\mathbf{4},n-2,p)$。这很容易证明

$$\begin{aligned} &P(\sqrt{n}f(4,n-2,p),B_2) \\ =&n\sqrt{n}f^3(4,n-2,p)-nf(2,2,p)f^2(4,n-2,p) \\ &-\sqrt{n}f(4,n-2,p)\big[4f^2(2,n-1,p)+(n-5)f^2(1,n-1,p)\big]+(n-5)f(2,2,p)f^2(1,n-1,p) \\ =&\sqrt{n}f(4,n-2,p)\big[nf^2(4,n-2,p)-4f^2(2,n-1,p)-(n-5)f^2(1,n-1,p)\big] \\ &+f(2,2,p)\big[(n-5)f^2(1,n-1,p)-nf^2(4,n-2,p)\big] \\ \leq&\sqrt{n}f(4,n-2,p)\big\{n[16+(n-2)^2]-4(n-1)^2-(n-5)(n-1)^2\big\} \\ &+f(2,2,p)\big\{(n-5)[1+(n-1)^2]-n(n-2)^2\big\}\ \text{(by Lemma 2.8)} \\ =&\sqrt{n}f(4,n-2,p)(-n^2+17n+1)+f(2,2,p)(-3n^2+8n-10)<0 \end{aligned}$$

对于 $n \geq 18$。

那么，对于 $n \geq 18$， $\rho(\mathbf{Sp}(B_3)) < \rho(\mathbf{Sp}(B_2))$。

情形 2。 $6 \leq n \leq 17$。

类似地，借助 MATLAB 并由引理 2.8，我们有 $\rho(\mathbf{Sp}(B_3)) < \rho(\mathbf{Sp}(B_2))$ 对 $6 \leq n \leq 17$ 成立。该结果的证明与引理 4.2 情形 2 中所给的证明十分相似。

证明至此完成。 □

定理5.5。在所有阶为 $n \geq 6$、 B_1、 B_2 和 B_3的双环图中（见图 *14*），它们分别是具有前三个最大 p-*Sombor*谱半径的唯一双环图。

Proof. By Theorem 2.5, we have $\rho(\mathbf{S_p}(B_2)) < \rho(\mathbf{S_p}(B_1))$. Then according to Theorem 5.1 and Lemmas 5.3 and 5.4, it is easy to see B_1, B_2 and B_3 are, respectively, the unique bicyclic graphs with the first three maximum p-Sombor spectral radii for $n \geq 6$. □

Remark 5.1. For $n = 5$, we have $B_1 \cong B_3$. Under the help of MATLAB and by Theorem 2.5, we get B_1 is the unique bicyclic graph with the largest p-Sombor spectral radius, the bicyclic graphs with the secondly and thirdly largest p-Sombor spectral radii depend on the choice of parameter p and they are B_2 and B_4.

6. 结论

在本文中，在所有阶为 $n \geq 6$ 的树中，我们得到 S_n, $S_{2,n-2}$, $S_{3,n-3}$ 分别是具有性质 P^* 的加权邻接矩阵谱半径最大的前三棵树，且它们均唯一。此外，我们还得到

$$\rho(A_f(P_4)) = \rho(A_f(S_{2,2})) < \rho(A_f(S_4)) \text{ for } n = 4$$

and

$$\rho(A_f(P_5)) < \rho(A_f(S_{2,3})) < \rho(A_f(S_5)) \text{ for } n = 5.$$

该结果对含有 $p \geq 1$ 的 p-Sombor 矩阵同样成立。

Among all unicyclic graphs of order $n \geq 7$, we get $S_n + e$, U_1, U_2, U_3 and U_4 are, respectively, the unique unicyclic graphs with the first five maximum p-Sombor spectral radii for $p \geq 2$. For $n = 6$, we get $S_6 + e$, U_1 and U_2 are, respectively, the unique unicyclic graphs with the first three maximum p-Sombor spectral radii and the unicyclic graph with the fourthly largest p-Sombor spectral radius depends on the choice of parameter p. Furthermore, we obtain

$$\rho(\mathbf{S_p}(C_5)) < \rho(\mathbf{S_p}(U_3)) < \rho(\mathbf{S_p}(U_2)) < \rho(\mathbf{S_p}(U_1)) < \rho(\mathbf{S_p}(S_5 + e))$$

对于 $n = 5$。

Moreover, among all bicyclic graphs of order $n \geq 6$, we obtain B_1 is the unique bicyclic graph with the largest spectral radius of the weighted adjacency matrices with property P^*. In addition, B_1, B_2 and B_3 are, respectively, the unique bicyclic graphs with the first three maximum p-Sombor spectral radii for $p \geq 2$. For $n = 5$, we have $B_1 \cong B_3$ is the unique bicyclic graph with the largest p-Sombor spectral radius, the bicyclic graphs with the secondly and thirdly largest p-Sombor spectral radii depend on the choice of parameter p and they are B_2 and B_4.

In Appendix 1, we give an algorithm to obtain the extremal graphs with the first three minimum Sombor spectral radii among all graphs with order n and size m. For example, we get $B'(n, 1)$, $B'(n, 2)$ and $B'(n, 3)$ (see Figure 23) are, respectively, the bicyclic graphs with the first three minimum Sombor spectral radii for $n = 5, 6, 7$, which dose not show much sign of regularity. We find the problem for the first three minimum Sombor spectral radii of these three classes of graphs in Problem 1.1 is hard for us. The authors have obtained P_n (resp. C_n) is the unique tree (resp. unicyclic graph) with the smallest spectral radius for the weighted adjacency matrix with property P^* in [24]. Thus we are interested in the following problems. Determine the unique bicyclic graph with the smallest spectral radius for the weighted adjacency matrix with property P^* among all bicyclic graphs of order n. Consider the extremal graph with respect to the spectral radius of weighted adjacency matrix with property P^* in the set of graphs with prescribed degree sequence.

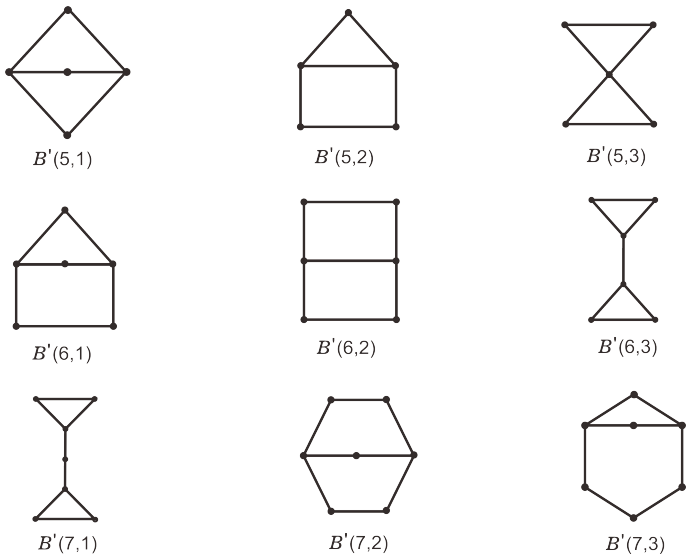


图23： 二环图 $B'(n,\ 1)$、 $B'(n,\ 2)$ 和 $B'(n,\ 3)$ 对于 $n = 5,\ 6,\ 7$。

致谢

本工作得到国家自然科学基金（编号：12171402）的资助。

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附录 1

To find the extremal graphs with the first three minimum Sombor spectral radii among all graphs with order n and size m, we present an algorithm which can be achieved by a computer program written in the MATLAB language. For given n and m, it is not difficult to construct recurrently all the graphs with order n and size m which are non-isomorphic to each other by using graph theory toolbox in MATLAB. In the following algorithm, we assume that all graphs with order n and size m which are non-isomorphic to each other have been produced, and store them as a matrix M, where $(2i-1)$-th row and $2i$-th row of M are edge-information-table (that is, EdgeTable in MATLAB) for $i = 1, 2, \ldots$.

算法 1： 获取具有第一
所有阶数为 n的图中三个最小的索伯谱半径
且大小为 m。

输入： 阶数 n 和大小 m。
输出： 具有前三个最小 Sombor 谱半径的极值图中，位列其中的图是
所有阶数为 n 、边数为 m 的图。
令 $\mathcal{G} = \{G_1, G_2, \ldots, G_t\}$ 为具有 n 且阶为 m 的图的集合。
彼此不同构。令 $S = \emptyset$。
为 *i=1:t* **执行**
  计算 $S_p(G_i)$;
  计算 $\rho(S_p(G_i))$;
  设 $S = S \cup \rho(S_p(G_i))$。
end
for *s=1:3* **do**
  找出 S中的最大元素 s ，即最大的 p-Sombor谱半径
  在所有阶数为 n 、边数为 m 的图中;
  确定在 $\mathcal{G}$中具有最大 p-Sombor谱半径的图 G ;
  集合 $S = S \setminus \{s\}$ 和 $\mathcal{G} = \mathcal{G} \setminus \{G\}$。
end

图的数量=size(M,1); 谱半径=[];

```
for k=1:Numbergraphs/2;
    edgetablerow1=M(2*k-1,:);
    edgetablerow2=M(2*k,:);
    Graph=graph(edgetablerow1,edgetablerow2);
    Degreeofvertexu=degree(Graph,edgetablerow1);
    Degreeofvertexv=degree(Graph,edgetablerow2);
    Weights=[(Degreeofvertexu.^(2)+Degreeofvertexv.^(2)).^(1/2)];
    Weightedgraph=graph(edgetablerow1,edgetablerow2,Weights);
    Weightedadjacency=adjacency(Weightedgraph,'weighted');
    Spectrum=eig(Weightedadjacency);
    Spectralradius(k)=max(abs(Spectrum));
end
for s=1:3;
    [Maxspec,Maxspecpposition]=max(Spectralradius);
    Maxgrow1=M(2*Maxspecpposition-1,:);
    Maxgrow2=M(2*Maxspecpposition,:);
    Maxgraph=graph(Maxgrow1,Maxgrow2);
    Maxgraphdegu=degree(Maxgraph,Maxgrow1);
    Maxgraphdegv=degree(Maxgraph,Maxgrow2);
    Maxgraphweights=[(Maxgraphdegu.^(2)+Maxgraphdegv.^(2)).^(1/2)];
    Maxggraphweighted=graph(Maxgrow1,Maxgrow2,Maxgraphweights);
    Spectralradius(Maxspecpposition)=0;
    figure
    plot(Maxggraphweighted,'EdgeLabel',Maxggraphweighted.Edges.Weight);
    暂缓结束
```