Recent results on the majorization theory of graph spectrum and topological index theory

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RECENT RESULTS ON THE MAJORIZATION THEORY OF GRAPH SPECTRUM AND TOPOLOGICAL INDEX THEORY - A SURVEY

MUHUO LIU†, BOLIAN LIU‡, AND KINKAR CH. DAS§

Abstract. Suppose \( \pi = (d_1, d_2, \ldots, d_n) \) and \( \pi' = (d'_1, d'_2, \ldots, d'_n) \) are two positive non-increasing degree sequences, write \( \pi \triangleright \pi' \) if and only if \( \pi \neq \pi', \sum_{i=1}^{n} d_i = \sum_{i=1}^{n} d'_i \), and \( \sum_{i=1}^{j} d_i \leq \sum_{i=1}^{j} d'_i \) for all \( j = 1, 2, \ldots, n \). Let \( \rho(G) \) and \( \mu(G) \) be the spectral radius and signless Laplacian spectral radius of \( G \), respectively. Also let \( G \) and \( G' \) be the extremal graphs with the maximal (signless Laplacian) spectral radii in the class of connected graphs with \( \pi \) and \( \pi' \) as their degree sequences, respectively. If \( \pi \triangleright \pi' \) can deduce that \( \rho(G) < \rho(G') \) (respectively, \( \mu(G) < \mu(G') \)), then it is said that the spectral radii (respectively, signless Laplacian spectral radii) of \( G \) and \( G' \) satisfy the majorization theorem. This paper presents a survey to the recent results on the theory and application of the majorization theorem in graph spectrum and topological index theory.

Key words. (Signless Laplacian) Spectral radius, Degree sequence, Majorization.

AMS subject classifications. 05C35, 05C75, 05C05.

1. Introduction. Throughout the paper, \( G = (V, E) \) is a connected undirected (not necessarily simple) graph with \( V = \{v_1, v_2, \ldots, v_n\} \) and \( E = \{e_1, e_2, \ldots, e_m\} \). The degree of vertex \( v \) of \( G \), denoted \( d(v) \), is the number of edges of \( G \) incident with \( v \), each loop counting as two edges. The degree sequence \( (d_1, d_2, \ldots, d_n) \) of \( G \) is enumerated in a non-increasing ordering, i.e., \( d_1 \geq d_2 \geq \cdots \geq d_n \geq 1 \) (hereafter, we assume that \( d(v_i) = d_i \) for \( 1 \leq i \leq n \)). We use \( \Gamma(\pi) \) to denote the class of connected graphs with degree sequence \( \pi \), and we use \( S(\pi) \) to denote the class of connected simple graphs with degree sequence \( \pi \).

Denote the neighbor set of vertex \( v \) in \( G \) as \( N(v) \). Let \( \Upsilon_{uv} \) be the number of edges joining vertices \( u \) and \( v \) in \( G \). In particular, \( \Upsilon_{uu} \) indicates the number of loops incident with vertex \( u \) in \( G \). The adjacency matrix of \( G \) is an \( n \times n \) matrix \( A(G) = (a_{ij}) \),

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where $a_{ij}$ is the number of edges joining vertices $v_i$ and $v_j$, each loop counting as two edges.

Suppose $f = (f(v_1), f(v_2), \ldots, f(v_n))^T \neq 0$ is a column vector defined on $V(G)$. If there exists a real number $q$ such that for each $u \in V(G)$,

$$qf(u) = (A(G)f)(u) = \sum_{v \in N(u) \setminus \{u\}} \Upsilon_{uv}f(v) + 2\Upsilon_{uu}f(u),$$

then $q$ is called an eigenvalue of $A(G)$. The spectral radius of $G$, denoted $\rho(G)$, is the largest eigenvalue of $A(G)$.

The signless Laplacian matrix of $G$ is $Q(G) = D(G) + A(G)$, where $D(G)$ is the diagonal matrix of vertex degrees of $G$. If there exists a real number $p$ such that for each $u \in V(G)$,

$$pf(u) = (Q(G)f)(u) = \sum_{v \in N(u) \setminus \{u\}} \Upsilon_{uv}(f(u) + f(v)) + 4\Upsilon_{uu}f(u),$$

then $p$ is called an eigenvalue of $Q(G)$. It is easy to see that $Q(G)$ is positive semi-definite \([14]\), and hence, we use $\mu_1(G) \geq \mu_2(G) \geq \cdots \geq \mu_n(G)$ to denote the eigenvalues of $Q(G)$ and use $\mu(G)$ to define the largest eigenvalue of $Q(G)$. That means $\mu(G) = \mu_1(G)$. The signless Laplacian spectral radius of $G$ is $\mu(G)$.

Hereafter, unless specially indicated, we only concern with connected simple graph. In this case, $A(G) = (a_{ij})$ is an $(0,1)$-matrix, where $a_{ij} = 1$ if and only if $v_i$ is adjacent with $v_j$. Furthermore, there is a unique positive unit eigenvector corresponding to $\rho(G)$ (respectively, $\mu(G)$), we use $f$ to denote such a unit eigenvector corresponding to $\rho(G)$ or $\mu(G)$, and we call $f$ the Perron vector of $G$.

The Laplacian matrix of $G$ is defined as $L(G) = D(G) - A(G)$. When $G$ is a connected simple graph, it is well known that $L(G)$ is positive semidefinite \([15]\) so that we can use $\lambda_1(G) \geq \lambda_2(G) \geq \cdots \geq \lambda_n(G)$ to denote the eigenvalues of $L(G)$ and we use $\lambda(G)$ to denote the largest eigenvalue of $L(G)$. From the definition, $\lambda(G) = \lambda_1(G)$, and we will call $\lambda(G)$ the Laplacian spectral radius of $G$.

As usual, if $m = n + c - 1$, then $G$ is called a $c$-cyclic graph. When $c = 0, 1, 2,$ or $3,$ $G$ is always called a tree, unicyclic graph, bicyclic graph and tricyclic graph, respectively.

When $G$ is a tree, let $\partial V$ be the set of pendant vertices (vertices of degrees one) of $G$, and let $V_0 = V \setminus \partial V$. In \([18]\), $\partial V$ is called the boundary vertices of $G$, while $V_0$ is called the interior vertices of $G$. A discrete Dirichlet operator $L_0(G)$ (see \([18]\)) is the Laplacian matrix restricted to interior vertices, i.e., $L_0(G) = D_0(G) - A_0(G)$, where $A_0(G)$ is the adjacency matrix of the graph induced by $V_0$, and where $D_0$ is the degree matrix $D$ restricted to $V_0$. From the definition of $L_0(G)$ and $L(G)$, $L_0(G)$ is obtained
from \(L(G)\) by deleting all rows and columns that correspond to boundary vertices. The first Dirichlet eigenvalue of \(G\), denote by \(\lambda_0(G)\), is the smallest eigenvalue of \(L_0(G)\) (see [13]).

Suppose \(G \in \Gamma(\pi)\). If \(\rho(G) \geq \rho(G')\) (respectively, \(\mu(G) \geq \mu(G')\)) for any other \(G' \in \Gamma(\pi)\), then we say \(G\) has maximal (respectively, signless Laplacian) spectral radius in \(\Gamma(\pi)\). Furthermore, we call \(G\) a maximal extremal graph of \(\Gamma(\pi)\) if \(G\) has the maximal spectral radius or signless Laplacian spectral radius in \(\Gamma(\pi)\).

Suppose \(\pi = (d_1, d_2, \ldots, d_n)\) and \(\pi' = (d'_1, d'_2, \ldots, d'_n)\) are two non-increasing sequences of real numbers, we write \(\pi \prec \pi'\) if and only if \(\pi \neq \pi', \sum_{i=1}^n d_i = \sum_{i=1}^n d'_i\), and \(\sum_{i=1}^j d_i \leq \sum_{i=1}^j d'_i\) for all \(j = 1, 2, \ldots, n\). Such an ordering is sometimes called majorization (see [23]).

This notion was introduced because of the following well-known theorem.

**Theorem 1.1.** [44, p. 218] The spectrum of a positive semidefinite Hermitian matrix majorizes its main diagonal (when both are rearranged in non-increasing order).

From Theorem 1.1 it easily follows:

**Proposition 1.2.** [33] Let \(G\) be a graph with \(n\) vertices. Then, \((d_1, d_2, \ldots, d_n) \prec (\mu_1, \mu_2, \ldots, \mu_n)\) and \((d_1, d_2, \ldots, d_n) \prec (\lambda_1, \lambda_2, \ldots, \lambda_n)\).

From Proposition 1.2, \(\lambda_1 \geq d_1\). Indeed, when \(G\) has at least one edge, Grone and Merris proved that \(\lambda_1 \geq d_1 + 1\) [19] and they also put forward the following conjecture.

**Conjecture 1.3.** [19] Let \(G\) be a connected graph on \(n \geq 2\) vertices. Then, \((d_1 + 1, d_2, \ldots, d_n - 1) \prec (\lambda_1, \lambda_2, \ldots, \lambda_n)\).

For a non-negative integral sequence \(d = (d_1, d_2, \ldots, d_n)\), we define its conjugate degree sequence as the sequence \(d^* = (d^*_1, d^*_2, \ldots, d^*_n)\), where

\[
d^*_k = \# \{i : d_i \geq k\}.
\]

In [19], Grone and Merris raised another question on the Laplacian spectrum sequence and the conjugate degree sequence, and they conjectured that

**Conjecture 1.4.** [19] For any graph \(G\) with \(n\) vertices,

\[
(\lambda_1, \lambda_2, \ldots, \lambda_n) \prec (d^*_1, d^*_2, \ldots, d^*_n).
\]

It is surprised that Conjecture 1.3 was proved in 1995 by Grone [20], while the complete proof of Conjecture 1.4 was given in 2011 by Bai [4]. Furthermore, Liu and
Liu [33] pointed out that the relation \((d_1 + 1, d_2, \ldots, d_n - 1) \prec (\mu_1, \mu_2, \ldots, \mu_n)\) does not hold.

Motivated by the above results on the relation between the Laplacian spectrum and the degree sequence of a graph, Bıyıkoğlu and Leydold [8] considered the relation between the minimal first Dirichlet eigenvalues in two classes of trees with given degree sequences, they proved:

**Theorem 1.5.** [8] Let \(\pi\) and \(\pi'\) be two different non-increasing degree sequences of trees with \(\pi \prec \pi'\). Suppose \(T\) and \(T'\) are the trees with the minimal first Dirichlet eigenvalues in \(S(\pi)\) and \(S(\pi')\), respectively. Then, \(\lambda_0(T) < \lambda_0(T')\).

By Theorem 1.5 we can deduce the size of the relationship between the minimal first Dirichlet eigenvalues of \(S(\pi)\) and \(S(\pi')\) from the majorization relationship of two given degree sequences \(\pi\) and \(\pi'\). Thus, such relation is called the majorization theorem by Jiang et al. [26] and Liu and Liu [37]. This method (i.e., the majorization theorem method) was discovered a long time ago, and was widely applied in different branches of Mathematics. For instance, the following famous “majorization theorem” of strictly Schur-convex function [23] was proved by Schur in 1923, and also discovered by Hardy, Littlewood and Pólya in 1929. Recall that a strictly convex function \(\varphi\) is a real valued function \(\varphi : B \rightarrow \mathbb{R}\), defined on a convex set \(B\) such that

\[
\varphi(px + (1 - p)y) < p\varphi(x) + (1 - p)\varphi(y)
\]

for all \(0 < p < 1\) and all \(x, y \in B\). A symmetric function \(\phi: D \rightarrow \mathbb{R}, D \subseteq \mathbb{R}^n\), is said to be strictly Schur-convex on \(D\) if \(a \prec b\) implies that \(\phi(a) < \phi(b)\), where \((a) = (a_1, a_2, \ldots, a_n)\) and \((b) = (b_1, b_2, \ldots, b_n)\) are two non-increasing sequences of real numbers.

**Theorem 1.6.** [23] Given an interval \(I \subseteq \mathbb{R}\), and a strictly convex function \(\varphi : I \rightarrow \mathbb{R}\), the function \(\phi(b) = \sum_{i=1}^{n} \varphi(b_i)\) is strictly Schur convex on \(I^n\).

The next result follows immediately from Theorem 1.6.

**Corollary 1.7.** [23] If \((a) \prec (b)\) and \(\varphi\) is a strictly convex function, then \(\sum_{i=1}^{n} \varphi(a_i) < \sum_{i=1}^{n} \varphi(b_i)\).

Therefore, it seems impossible to give a survey of all the majorization theorems appear in Mathematics, and hence, this survey mainly focuses on some recent results of the theory and application to the majorization theorem in graph spectrum and topological index theory.
2. The majorization theorem of graph spectrum.

2.1. Some known majorization theorems of graph spectrum. Motivated by Theorem 1.5, Bıyıkoğlu and Leydold [9] also considered the similar relation between the spectral radii of the maximal extremal graphs in two classes of trees with given degree sequences, and Zhang [54] considered the similar problem for the Laplacian spectral radii (i.e., the signless Laplacian spectral radii since \(L(G)\) and \(Q(G)\) share the same spectra [45] when \(G\) is a simple bipartite graph), and they showed that

**Theorem 2.1.** Let \(\pi\) and \(\pi'\) be two different non-increasing degree sequences of trees with \(\pi \prec \pi'\). Suppose \(T\) and \(T'\) are the maximal extremal trees in \(S(\pi)\) and \(S(\pi')\), respectively. Then, \(\rho(T) < \rho(T')\) and \(\lambda(T) < \lambda(T')\).

Furthermore, the majorization theorems for unicyclic and bicyclic graphs were also proved.

**Theorem 2.2.** Let \(\pi\) and \(\pi'\) be two different non-increasing degree sequences of unicyclic (respectively, bicyclic) graphs with \(\pi \prec \pi'\).

(1) Suppose \(U\) and \(U'\) are the maximal extremal unicyclic graphs in \(S(\pi)\) and \(S(\pi')\), respectively. Then, \(\rho(U) < \rho(U')\) and \(\mu(U) < \mu(U')\).

(2) Suppose \(B\) and \(B'\) are the maximal extremal bicyclic graphs in \(S(\pi)\) and \(S(\pi')\), respectively. Then, \(\rho(B) < \rho(B')\) and \(\mu(B) < \mu(B')\).

As usual, \(\rho_1(G) \geq \rho_2(G) \geq \cdots \geq \rho_n(G)\) denote the eigenvalues of \(A(G)\). Let \(I_1,\)
$I_2$ and $I_3$ be the unicyclic graphs as shown in Fig. 2.1, and also let $G_1$, $G_2$, $H_1$, $H_2$, $F_1$, and $F_2$ be the graphs as shown in Fig. 2.2.

In view of Theorems 1.5, 2.1 and 2.2 it is natural for us to consider the following problems:

**Problem 2.3.** Whether Theorem 1.5 also holds for $\rho_n(G)$ and/or $\rho_n(G)$?

**Problem 2.4.** Whether Theorems 2.1 and 2.2 also hold for any connected simple $c$-cyclic graphs?

The answer to Problem 2.3 is negative, since $\lambda_n(G) = 0$ holds for any graph and we have the following example.

**Example 2.5.** Let $\pi_1 = (3,3,2,1,1)$, $\pi_2 = (3,2,2,2,1)$ and $\pi_3 = (2,2,2,2,2)$. By an elementary computation, $I_1$, $I_2$ and $I_3$ are the graphs with minimal smallest adjacency eigenvalues (respectively, minimal smallest signless Laplacian eigenvalues) in $S(\pi_1)$, $S(\pi_2)$ and $S(\pi_3)$, respectively. Clearly, $\pi_3 \prec \pi_2 \prec \pi_1$, but $\rho_n(I_1) = \rho_n(I_3) > \rho_n(I_2)$ and $\mu_n(I_1) = \mu_n(I_3) > \mu_n(I_2)$.

**Remark 2.6.** Since the “symmetrical property” of the eigenvalues of $A(G)$ for a bipartite graph [12], Theorem 2.1 implies that “Let $\pi$ and $\pi'$ be two different non-increasing degree sequences of trees with $\pi \prec \pi'$. Suppose $T$ and $T'$ are the extremal trees with minimal smallest adjacency eigenvalues in $S(\pi)$ and $S(\pi')$, respectively. Then, $\rho_n(T) > \rho_n(T')$”.

The answer to Problem 2.4 is also negative, since we have the following three examples.

**Example 2.7.** [11] Let $\pi = (4,3,3,3,2,2,1)$ and $\pi' = (4,4,3,3,2,2,1)$. By the data of the spectra of connected graphs with seven vertices [12], $G_1$ and $G_2$ are the graphs with maximal spectral radii in $S(\pi)$ and $S(\pi')$, respectively. Clearly, $\pi \prec \pi'$, but $\rho(G_1) > \rho(G_2)$.

**Example 2.8.** [28] Let $\pi = (5,4,3,3,2,2,1)$ and $\pi' = (5,4,4,2,2,2,1)$. By the table of the connected graphs with seven vertices [12], $H_1$ and $H_2$ are the graphs with maximal signless Laplacian spectral radii in $S(\pi)$ and $S(\pi')$, respectively. Clearly, $\pi \prec \pi'$, but $\mu(H_1) > \mu(H_2)$.

**Example 2.9.** [28] Let $\pi = (4,2,2,2,1,1)$ and $\pi' = (4,3,2,1,1,1)$. By the table of the connected graphs with six vertices [13], $F_1$ and $F_2$ are the graphs with maximal Laplacian spectral radii in $S(\pi)$ and $S(\pi')$, respectively. Clearly, $\pi \prec \pi'$, but $\lambda(F_1) > \lambda(F_2)$.

Though the answers to Problems 2.3 and 2.4 are negative, the majorization theorem also holds for the maximal (signless Laplacian) spectral radii between two degree
sequences with special restriction, as we will see below. To this aim we introduce another important concept.

If \( \pi \triangleleft \pi' \) are two degree sequences of simple \( c \)-cyclic graphs, and there exists some \( t \) (\( 1 \leq t \leq n \)) such that \( d'_i \geq c + 1 \) and \( d_i = d'_i \) holds for all \( t + 1 \leq i \leq n \), then the majorization \( \pi \triangleleft \pi' \) is called a normal majorization [37].

Clearly, a normal majorization must also be a majorization, but not the Vice-Versa. For example, we have

**Example 2.10.** [37] Let \( \pi_1 = (4, 4, 3, 2, 1, 1, 1) \), \( \pi_2 = (5, 4, 2, 1, 1, 1, 1) \), and \( \pi_3 = (5, 3, 3, 2, 1, 1, 1) \). Then, \( \pi_1 \), \( \pi_2 \) and \( \pi_3 \) are three bicyclic degree sequences. One can easily see that \( \pi_1 \triangleleft \pi_2 \) is a majorization, but not a normal majorization, while \( \pi_1 \triangleleft \pi_3 \) is a normal majorization.

Actually, when \( \pi \triangleleft \pi' \) are two degree sequences of trees, then \( \pi \triangleleft \pi' \) must be also a normal majorization. Thus, Theorem 2.1 can be improved to

**Theorem 2.11.** Let \( \pi \) and \( \pi' \) be two different non-increasing \( c \)-cyclic (\( c \geq 0 \)) degree sequences, and let \( G \) and \( G' \) be the maximal extremal graphs in \( S(\pi) \) and \( S(\pi') \), respectively. If \( \pi \triangleleft \pi' \) and it is a normal majorization, then [37] \( \rho(G) < \rho(G') \), and [28] \( \mu(G) < \mu(G') \).

Furthermore, some other majorization theorems between two special degree sequences were given in Liu [30]. For instance, the following is one of them.

**Theorem 2.12.** [30] Let \( \pi = (d_1, d_2, \ldots, d_n) \) and \( \pi' = (d'_1, d'_2, \ldots, d'_n) \) be two different \( c \)-cyclic degree sequences, and let \( G \) and \( G' \) be the maximal extremal \( c \)-cyclic graphs of \( S(\pi) \) and \( S(\pi') \), respectively. Suppose \( \pi \triangleleft \pi' \), \( d_1 = d'_1 \) and \( c \geq 4 \). If there exists some \( t \) such that \( d'_i \geq c + 1 \) and \( d_i = d'_i \) holds for all \( 1 + t \leq i \leq n \), then \( \rho(G) < \rho(G') \) and \( \mu(G) < \mu(G') \).

Astoundingly, when we relax the condition “simple connected graphs” to “general connected graphs”, the result becomes more appealing. In Liu and Liu [30], the following result was proved.

**Theorem 2.13.** [30] Let \( \pi \) and \( \pi' \) be two different non-increasing degree sequences, and let \( G \) and \( G' \) be the maximal extremal graphs in \( \Gamma(\pi) \) and \( \Gamma(\pi') \), respectively. If \( \pi \triangleleft \pi' \), then \( \rho(G) < \rho(G') \), and \( \mu(G) < \mu(G') \).

As claimed in [30], if \( \pi \) is a degree sequence of trees, then \( S(\pi) = \Gamma(\pi) \). So, Theorem 2.13 is another extension to Theorem 2.11.

Given a connected simple graph \( G = (V, E) \), the discrete \( p \)-Laplacian \( L_p(G) \) of a column vector \( g = (g(v_1), g(v_2), \ldots, g(v_n))^T \) defined on \( V(G) \) (\( 1 < p < \infty \)) is given
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by

$$L_p(G)g(v) = \sum_{u \in V, uv \in E} (g(v) - g(u))^{[p-1]},$$

where the symbol \(t^{[q]}\) denotes a “power” function that preserves the sign of \(t\), i.e., \(t^{[q]} = \text{sign}(t)|t|^q\). In Bıyıkoglu et al. [10], it is shown that \(L_2(G) = L(G)\) and \(L_2(G)\) is a non-linear operator. If there exists a column vector \(g(\neq 0)\) defined on \(V(G)\) such that \(L_p(G)g(v) = \lambda g(v)^{[p-1]}\), then the real number \(\lambda\) is called an eigenvalue of \(L_p(G)\). Denote by \(\lambda_p(G)\) the maximal eigenvalue of \(L_p(G)\).

As another extension to Theorem 2.1, Bıyıkoglu et al. [10] showed that

**Theorem 2.14.** [10] Let \(\pi\) and \(\pi'\) be two different non-increasing degree sequences of trees with \(\pi \prec \pi'\). Let \(T\) and \(T'\) be the maximal extremal trees in \(S(\pi)\) and \(S(\pi')\), respectively. Then, \(\lambda_p(T) < \lambda_p(T')\).

Furthermore, Zhang and Zhang [53] extended Theorem 2.14 to \(p\)-Laplacian spectral radii of weighted trees with a positive weight set.

For any \(k \geq 0\), the \(k\)-th spectral moment of \(G\) is defined by \(Z_k(G) = \sum_{i=1}^{n} \rho_k^i(G)\).

Very recently, Andriantiana and Wagner [1] showed that

**Theorem 2.15.** [1] Let \(\pi\) and \(\pi'\) be two different non-increasing degree sequences of trees with \(\pi \prec \pi'\). Let \(T\) and \(T'\) be the trees with maximal \(k\)-th spectral moments in \(S(\pi)\) and \(S(\pi')\), respectively. Then, \(Z_k(T) \leq Z_k(T')\). Furthermore, if \(k \geq 4\) is even, then the inequality is strict.

### 2.2. How to prove the majorization theorem of graph spectrum.

The fundamental tool to prove Proposition 1.2, Conjecture 1.3 and Conjecture 1.4 depends on Theorem 1.1. Different from this, the proofs to majorization theorems of (signless Laplacian) spectral radii are based on the structure of maximal extremal graphs of \(S(\pi)\). Thus, the investigation of majorization theorem is closely related with the maximal extremal graphs of \(S(\pi)\). In this section, we shall introduce some results on the maximal extremal graphs of \(S(\pi)\), and we first need the important concepts of BFS-ordering and BFS-graphs. The BFS-ordering was firstly introduced by Pruss in [16] and called the spiral like ordering. Bıyıkoglu and Leydold [9] found that the extremal graphs with maximal spectral radii of \(S(\pi)\) are BFS-graphs, and Zhang [55] discovered that the extremal graphs with maximal signless Laplacian spectral radii of \(S(\pi)\) are also BFS-graphs. The following concept proposed by Liu [30] is originally from [9, 55].

**Definition 2.16.** [9, 30, 55] Let \(G\) be a connected graph and \(f\) be the Perron vector of \(G\). A well-ordering \(v_1 \prec v_2 \prec \cdots \prec v_n\) of \(V(G)\) is called a BFS-ordering if the following hold for all vertices \(u, v \in V(G)\):
(i) $d(v_1) \geq d(v_2) \geq \cdots \geq d(v_n)$, $f(v_1) \geq f(v_2) \geq \cdots \geq f(v_n)$ and $h(v_1) \leq h(v_2) \leq \cdots \leq h(v_n)$, where $h(v_i)$ is the distance between $v_i$ and $v_1$.
(ii) If $v \in N(u) \setminus N(x)$, $y \in N(x) \setminus N(u)$ such that $h(u) = h(x) = h(v) - 1 = h(y) - 1$, then $f(u) > f(x)$ if and only if $f(v) > f(y)$, and $f(u) = f(x)$ if and only if $f(v) = f(y)$.

Furthermore, if $V(G)$ has a BFS-ordering, then $G$ is called a BFS-graph.

A BFS-tree is also called a greedy tree in [47, 48]. For example, for a given tree degree sequence $\pi^* = (4, 4, 3, 3, 3, 2, 2, 2, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1)$, $T^*_\pi$ is the BFS-tree of order 19 (see Fig. 2.3). Bıyıkoğlu and Leydold [9] and Zhang [55], independently, showed the following theorem.

**Theorem 2.17.** [9, 55] Let $\pi$ be a tree degree sequence. Then, there is a unique BFS-tree, which is the maximal extremal tree of $S(\pi)$.

Let $U^*_\pi$ be the unique unicyclic graph in $S(\pi)$, where $v_1, v_2$ and $v_3$ are mutually adjacent to form $C$, the unique cycle of $U^*_\pi$, and the remaining vertices appear in BFS-ordering with respect to $C$ starting from $v_4$ which is adjacent to $v_1$ [9, 55].

**Theorem 2.18.** [9, 55] Let $\pi$ be a unicyclic degree sequence. Then, $U^*_\pi$ is the unique maximal extremal unicyclic graph of $S(\pi)$.

Denote by $R(G)$ the reduced graph obtained from $G$ by recursively deleting pendant vertices of the resultant graph until no pendant vertices remain. If $G$ is a connected $c$-cyclic graph, it is easy to see that $R(G)$ is unique and $R(G)$ is also a connected $c$-cyclic graph.

Let $\theta(p_1, p_2, \ldots, p_r)$ denote the graph, which is obtained from $r$ vertex-disjoint paths (of orders $p_1 + 1$, $p_2 + 1$, $\ldots$, $p_r + 1$, respectively) by identifying the $r$ initial (respectively, terminal) vertices of them. Specially, let $B_2 = \theta(2, 1, 2)$ be the bicyclic graph such that $V(B_2) = \{v_1, v_2, v_3, v_4\}$ and $E(B_2) = \{v_1v_2, v_1v_3, v_1v_4, v_2v_3, v_2v_4\}$.

Let $C(q_1, q_2, \ldots, q_r)$ denote the graph obtained from $r$ cycles $C_{q_1}, C_{q_2}, \ldots, C_{q_r}$ by identifying a vertex of them. If $\pi = (d_1, d_2, \ldots, d_n)$ is a bicyclic degree sequence, $\pi$ should be one of the following four cases since $\sum_{i=1}^{n} d_i = 2n + 2$ [recently, Bianchi et al. 4] presented the characterization of integers $n - 1 \geq d_1 \geq d_2 \geq \cdots \geq d_n$ to be the
degree sequence of a c-cyclic graph for $0 \leq c \leq 6$). Moreover, we construct a special bicyclic graph $B_n^*$ with degree sequence $\pi$ as follows (For more detail, see [25, 42]).

1. $\pi = (4,2,\ldots,2)$. Let $B_n^* = C(3,n-2)$.
2. $\pi = (3,3,2,\ldots,2)$. Let $B_n^* = \theta(1,2,n-2)$.
3. $d_n = 1$ and $d_2 = 2$. Then we have $d_1 > 4$, $d_i = 2$ $(i = 3,4,5)$, and $d_j \leq 2$ $(6 \leq j \leq n-1)$. Denote by $B_n^*$ the bicyclic graph of order $n$ obtained from $C(3,3)$ by attaching $d_i - 4$ paths of almost equal lengths (i.e., their lengths differ by at most one) to $v_i$ of $C(3,3)$.
4. $d_n = 1$ and $d_1 \geq d_2 \geq 3$. Let $B_n^*$ be the bicyclic graph with $R(B_n^*) = B_D$, and the remaining vertices appear in $BFS$-ordering with respect to $B_D$ starting from $v_6$ that is adjacent to $v_1$.

**Theorem 2.19.** [25, 42] Let $\pi$ be a bicyclic degree sequence. Then, $B_n^*$ is the unique maximal bicyclic graph of $S(\pi)$.

For the case of tricyclic graphs, the maximal extremal graphs become much more complicated.

**Theorem 2.20.** [30] Let $\pi$ be a tricyclic degree sequence, and let $J_n^*$ be a maximal extremal tricyclic graph of $S(\pi)$. Suppose $P_{n-4} = w_1w_2\ldots w_{n-4}$.

1. If $d_1 = 6$ and $d_2 = \cdots = d_n = 2$, then $J_n^* = C(3,3,n-6)$;
2. If $d_1 = 5$, $d_2 = 3$ and $d_3 = \cdots = d_n = 2$, then $J_n^*$ is obtained from $B_D$ and $P_{n-4}$ by adding two edges $v_1w_1$ and $v_1w_{n-4}$;
3. If $d_1 = d_2 = 4$ and $d_3 = \cdots = d_n = 2$, then $J_n^* = \theta(2,1,2,n-3)$;
4. If $d_1 = 4$, $d_2 = d_3 = 3$ and $d_4 = \cdots = d_n = 2$, then $J_n^*$ is obtained from $B_D$ and $P_{n-4}$ by adding two edges $v_1w_1$ and $v_3w_{n-4}$;
5. If $d_1 = d_2 = d_3 = d_4 = 3$ and $d_5 = \cdots = d_n = 2$, then $J_n^*$ is obtained from $B_D$ and $P_{n-4}$ by adding two edges $v_3w_1$ and $v_4w_{n-4}$.

In the following, let $J_1$, $J_2$, $\ldots$, $J_6$ be the tricyclic graphs as shown in Fig. 2.4. Let $W_1$ (respectively, $W_2$, $W_5$, $W_6$) be the unique tricyclic graph with $R(W_1) = J_1$ (respectively, $R(W_2) = J_2$, $R(W_3) = J_3$, $R(W_6) = J_6$), and the remaining vertices appear in $BFS$-ordering with respect to $J_1$ (respectively, $J_2$, $J_3$, $J_6$) starting from $v_6$ (respectively, $v_6$, $v_7$, $v_6$) that is adjacent to $v_1$. Denote $W_3$ the unique tricyclic graph with $R(W_3) = J_3$ so that the remaining vertices appear in $BFS$-ordering with respect to $J_3$ starting from $v_6$ that is adjacent to $v_5$. Let $W_4$ be the unique tricyclic graph obtained from $J_4$ by attaching $k$ paths of almost equal lengths to $v_1$ of $J_4$.

**Theorem 2.21.** [30] Let $\pi$ be a tricyclic degree sequence and let $J_n^*$ be a maximal extremal tricyclic graph of $S(\pi)$ with $d_n = 1$. 
Fig. 2.4. The tricyclic graphs $J_1$, $J_2$, ..., $J_6$.

(1) If $d_1 \geq 4$ and $d_4 \geq 3$, then $J_1^\pi = W_1$ or $J_2^\pi = W_2$;
(2) If $d_1 = 3$ and $d_4 = 3$, then $J_2^\pi = W_3$;
(3) If $d_2 = d_3 = d_4 = 2$, then $J_4^\pi = W_4$;
(4) If $d_2 = 3$ and $d_3 = d_4 = 2$, then $J_3^\pi = W_5$;
(5) If $d_2 = d_3 = 3$ and $d_4 = 2$, then $J_5^\pi = W_6$;
(6) If $d_2 \geq 4$ and $d_4 = 2$, then $J_6^\pi = W_2$.

For the general case, some properties were given to the maximal extremal graphs of $S(\pi)$ \cite{9, 30, 55}, and the main property of maximal extremal graphs of $S(\pi)$ is

**Theorem 2.22.** \cite{9, 30, 55} Suppose $\pi$ is a non-increasing degree sequence. If $G$ is a maximal extremal graph of $S(\pi)$, then it is a BFS-graph.

Recently, more extra properties of maximal extremal graphs of $S(\pi)$ were added by Liu in \cite{30}. Furthermore, for the maximal extremal graphs of $\Gamma(\pi)$, similar results as those in Theorem 2.22 were obtained in Liu and Liu \cite{40}.

Theorem 2.22 shows that the maximal extremal graphs of $S(\pi)$ are BFS-graphs, but the BFS-graphs of $S(\pi)$ are not unique. Thus, from Theorems 2.17, 2.20, it is natural for us to consider the following question: Whether the maximal extremal graph of $S(\pi)$ is unique for any $c$-cyclic degree sequence $\pi$? Actually, Belardo et al. \cite{3} conjectured that the answer is positive.

**Conjecture 2.23.** \cite{3} Let $\pi$ be a $c$-cyclic degree sequence. Then, the extremal graph with the maximal spectral radius of $S(\pi)$ is unique.

It is rather interesting that the structure of maximal extremal graphs of $S(\pi)$ is not unique, as the size of the relationship between $W_1$ and $W_2$ in Theorem 2.24 is uncertain \cite{30}. Actually, Belardo et al. \cite{3} gave a routine to build the maximal extremal graph, but a counterexample to the routine was given by Liu \cite{30} (see Example 24 of...
At the end of this section, let us come back to deal with the proof of majorization theorems of (signless Laplacian) spectral radii. In addition to the maximal extremal graphs theorems, the following results hold.

**Proposition 2.24.** Let $u, v$ be two vertices of the connected graph $G$, and $w_1, w_2, \ldots, w_k$ $(1 \leq k \leq d(v))$ be some vertices of $N(v) \setminus (N(u) \cup \{u\})$. Let $G'$ be a new graph obtained from $G$ by deleting the edges $w_1v, \ldots, w_kv$, and then adding the edges $w_1u, \ldots, w_ku$. Suppose $f$ is the Perron vector of $G$. If $f(u) \geq f(v)$, then $\rho(G') > \rho(G)$ and $\mu(G') > \mu(G)$.

If $d = (d_1, d_2, \ldots, d_n)$ is a non-increasing integer sequence and $d_i \geq d_j + 2$, then the following operation is called a unit transformation from $i$ to $j$ on $d$: subtract 1 from $d_i$ and add 1 to $d_j$. The following famous majorization of integer sequences, is due to Muirhead (see [44]).

**Proposition 2.25.** (Muirhead’s Lemma) If $d$ and $d'$ are two non-increasing integer sequences and $d \preceq d'$, then $d$ can be obtained from $d'$ by a finite sequence of unit transformations.

Suppose $\pi \prec \pi'$, $G$ and $G'$ are the maximal extremal graphs of $\Gamma(\pi)$ and $\Gamma(\pi')$ (or $S(\pi)$ and $S(\pi')$), respectively. In order to prove the majorization theorems of (signless Laplacian) spectral radii, by Proposition 2.24 we may always suppose that $\pi$ and $\pi'$ differ only in two positions where the difference is 1, that is, $d_i = d'_i, i \neq p, q$, $1 \leq p < q \leq n$, and $d'_p = d_p + 1, d'_q = d_q - 1$. In this case, $\pi \prec \pi'$ is also called a star majorization and written as $\pi \prec^* \pi'$ [26]. Let $P_{v_pv_q}$ be a shortest path from $v_p$ to $v_q$. By the choice of $G$ and $p < q$, $f(v_p) \geq f(v_q)$ follows from Theorem 2.22 and Definition 2.10. In the following, if $w$ is a vertex of $G$ such that $w \in N(v_q) \setminus (N(v_p) \cup \{v_p\})$ and $w \not\in V(P_{v_pv_q})$, then we call $w$ a surprising vertex of $G$. If $G$ contains some surprising vertex, say $w$, let $G^* = G + v pw - vqw$. Then, $G^* \in \Gamma(\pi')$. Since $f(v_p) \geq f(v_q)$, by Proposition 2.22, $\rho(G) < \rho(G^*) \leq \rho(G')$ and $\mu(G) < \mu(G^*) \leq \mu(G')$. Therefore, if $G$ contains a surprising vertex, then $\rho(G) < \rho(G')$ and $\mu(G) < \mu(G')$.

Generally speaking, a surprising vertex cannot always exist for $G \in S(\pi)$, as the case $N(v_q) = N(v_p)$ may occur. That is the reason “why majorization theorems cannot hold for any $c$-cyclic graphs”. But from the structure of maximal extremal graph $G$ as described in Theorems 2.17–2.19, we can deduce that $G$ must contain a surprising vertex if $G$ is a maximal extremal graph of $S(\pi)$ when $c \in \{0, 1, 2\}$. In the following, as an illustrated example, we will provide the proof of Theorem 2.22. Actually, the main idea of the proofs of Theorems 2.17–2.19 is similar.

**Proof of Theorem 2.2.** By Proposition 2.25 we may suppose that $\pi \prec^* \pi'$. Theorem 2.18 implies that $U = U^*_p$. If $2 \leq q \leq 3$, then $d_q \geq 3$ and $v_q \in C_3$ since $U' \in S(\pi')$. 


If \( q \geq 4 \), then \( d_q \geq 2 \) and \( v_q \) does not lie on any cycle. In both cases, there exists a vertex \( v_k \) \((k > q)\) such that \( v_k \in N(v_q) \setminus (N(v_p) \cup \{v_p\}) \) and \( v_k \notin V(P_{v_qv_k}) \), namely, \( v_k \) is a surprising vertex. Let \( U'' \) be the graph obtained from \( U \) by deleting the edge \( v_qv_k \), and then adding the edge \( v_pv_k \). Note that \( U'' \) is connected and \( U'' \in S(\pi') \). By Proposition 2.24, \( \rho(U) < \rho(U'') \leq \rho(U) \).

2.3. The application of majorization theorem to graph spectrum. In 1981, Cvetković [11] indicated 12 directions for further investigations of graph spectra, one of which is classifying and ordering graphs. Hence, ordering graphs with various properties by their spectra, especially by their (Laplacian) spectral radii, became an attractive topic (see [24, 35, 43]). Up to now, more than 50 papers were published on this item, but a simple and general method has not yet been obtained. Not long before, we found that the majorization theorem is a good tool to deal with the above Cvetkovic’s problem on the ordering of graphs according to their largest (signless Laplacian) spectral radii [35].

Next we will use an examples to illustrate the application of the majorization theorem to solve Cvetkovic’s problem. Let \( U_n \) be the class of unicyclic graphs on \( n \) vertices, and \( U_{n,k} \) be the class of unicyclic graphs with \( n \) vertices and \( k \) pendant vertices.

**Example 2.26.** Let \( U_1, U_2, \ldots, U_5 \) be the unicyclic graphs on \( n \) vertices as shown in Fig. 2.5. Clearly, \( U_1 \) is the unique unicyclic graph with \( d_1 = n - 1 \), \( U_2, U_3, U_4 \) are all the unicyclic graphs with \( d_1 = n - 2 \).

If \( U \in U_n \setminus \{U_1, U_2, \ldots, U_5\} \), then \( d_1(U) \leq n - 3 \). Let \( (b) = (n - 3, 4, 2, 1, \ldots, 1) \). It is easily checked that \( U_5 \) is the unique unicyclic graph with \( (b) \) as its degree sequence. Suppose the degree sequence of \( U \) is \( (a) = (d_1, d_2, d_3, \ldots, d_n) \). Then, \( (a) \prec (b) \), and hence, \( \rho(U) < \rho(U_5) \) follows from Theorem 2.22.

Clearly, \( U_1 \) is the unique unicyclic graph with \( (c) = (n - 1, 2, 2, 1, \ldots, 1) \) as its degree sequence, \( U_2 \) is the unique unicyclic graph with \( (d) = (n - 2, 3, 2, 1, \ldots, 1) \) as its degree sequence and \( S(e) = \{U_3, U_4\} \), where \( (e) = (n - 2, 2, 2, 2, 1, \ldots, 1) \). Since \( (e) \prec (d) \prec (c) \), \( \rho(U_4) < \rho(U_2) < \rho(U_1) \) according to Theorem 2.22. From Theorem 2.18, \( \rho(U_4) \prec \rho(U_3) \).
Let $\Phi(G, x)$ denote the characteristic polynomial of $A(G)$. By an elementary computation, it easily follows that

$$\Phi(U_4, x) = x^{n-4} (x^4 - nx^2 + 2n - 8),$$

$$\Phi(U_5, x) = x^{n-4} (x^4 - nx^2 - 2x + 3n - 13).$$

From Equation (2.1), it is easy to see that $\rho(U_4) = \sqrt{n + \sqrt{n^2 - 8n + 12}} < \sqrt{n}$ when $n \geq 12$. When $x \geq \sqrt{n}$ and $n \geq 12$, by Equations (2.1) and (2.2), we have

$$\Phi(U_5, x) - \Phi(U_4, x) = x^{n-4}(n - 5 - 2x) \geq \frac{n-4}{n - 5 - 2\sqrt{n}} > 0.$$ 

Thus, $\rho(U_5) < \rho(U_4)$, and hence $\rho(U) < \rho(U_5) < \rho(U_4) < \rho(U_3) < \rho(U_2) < \rho(U_1)$ when $n \geq 12$. Now, the five unicyclic graphs with the first five largest spectral radii in $U_n$ are determined for $n \geq 12$.

As mentioned before, the majorization theorem holds for the maximal (signless Laplacian) spectral radii of the extremal graphs between two classes of trees, unicyclic and bicyclic graphs with given degree sequences. Thus, as claimed in Liu and Liu [35], it is not a difficult problem to order trees, unicyclic graphs and bicyclic graphs via their largest (signless Laplacian) spectral radii by applying the corresponding majorization theorem. But unfortunately, the majorization theorem can not hold for general $c$-cyclic graphs, and hence, this method cannot be applied to deal with Cvetković’s problem in the general case.

The majorization theorem is also effective when we deal with the other extremal problems in some special graph categories. For instance,

**Example 2.27.** Suppose $U \in U_{n,k}$, and suppose the degree sequence of $U$ is $(a) = (d_1, d_2, \ldots, d_{n-k}, 1, \ldots, 1)$, where the multiplicity of 1 is $k$. Let $(b) = (k + 2, 2, 2, \ldots, 2, 1, \ldots, 1)$, where the multiplicity of 1 is $k$. If $(a) \neq (b)$, then $(a) < (b)$. By Theorems 2.14 and 2.18, $\rho(U) < \rho(U^*)$, where $U^*$ is obtained from a triangle by attaching $k$ paths of almost equal lengths to a vertex of the triangle.

More examples on the application of majorization theorem to the extremal problem of graph spectrum can be referred to [25, 54, 55].

**3. The majorization theorem of topological index.** In this section, we will explain how the theory of majorization can be applied to face other problems in different branches of graph theory; in particular we will focus on some theorems concerning topological indices.

The first and second Zagreb indices are, respectively, defined as

$$M_1(G) = \sum_{v \in V(G)} d^2(v), \quad M_2(G) = \sum_{uv \in E(G)} d(u)d(v).$$
The first and second Zagreb indices are two important topological indices, which were first introduced by Gutman and Trinajstić in 1972 [22]. Before 2009, similar with the case of (signless Laplacian) spectral radii, many papers concerned with the ordering of $M_1(G)$ and $M_2(G)$ among some given graph categories were published [15, 51], but a simple and general method has not yet been obtained.

In 2009, Liu [29] proved that the majorization theorem holds for the first Zagreb index for any c-cyclic graphs. That is

**Theorem 3.1.** [29] Let $\pi$ and $\pi'$ be two different non-increasing degree sequences with $\pi < \pi'$. If $G \in S(\pi)$ and $G' \in S(\pi')$, then $M_1(G) < M_1(G')$.

By applying Theorem 3.1, Liu extended [29] almost all known results before 2009 on the ordering of the first Zagreb index in some given graph categories like c-cyclic graphs. Note that the proof of Theorem 3.1 follows easily from Corollary 1.7, since the function $\varphi(x) = x^2$ is strictly convex. A similar approach allowed Liu and Liu to extend Theorem 3.1 in [32] to the first general Zagreb index $M_1^c(G) = \sum_{v \in V} d(v)^\alpha$ [27], where $\alpha$ is a given real number not equal to 0 and 1.

**Theorem 3.2.** [32] Let $\pi$ and $\pi'$ be two different non-increasing degree sequences with $\pi < \pi'$. Suppose $G \in S(\pi)$ and $G' \in S(\pi')$.

1. If $0 < \alpha < 1$, then $M_1^c(G) > M_1^c(G')$.
2. If $0 < \alpha < 1$, then $M_1^c(G) > M_1^c(G')$.

Motivated from the definition of $M_1(G)$ and $M_2(G)$, Došljić [16] defined two new graphical invariants $\overline{M}_1(G)$ and $\overline{M}_2(G)$, where

$$\overline{M}_1(G) = \sum_{uv \in E(G)} (d(u) + d(v)),$$

$$\overline{M}_2(G) = \sum_{uv \in E(G)} d(u)d(v).$$

Došljić called $\overline{M}_1(G)$ and $\overline{M}_2(G)$, the first and second Zagreb coindices of $G$, respectively. For the relationship between $M_1(G)$ and $\overline{M}_1(G)$, it is well-known that $M_1(G) = 2m(n - 1) - M_1(G)$ [2]. Thus, from Theorem 3.1 we have

**Theorem 3.3.** [31] Let $\pi$ and $\pi'$ be two different non-increasing degree sequences with $\pi < \pi'$. If $G \in S(\pi)$ and $G' \in S(\pi')$, then $\overline{M}_1(G) > \overline{M}_1(G')$.

The first and second multiplicative Zagreb indices of a connected graph $G$, are defined as $\prod_1(G) = \prod_{v \in V(G)} d^2(v)$ and $\prod_2(G) = \prod_{uv \in E(G)} d(u)d(v)$, respectively [21]. Recently, by applying Corollary 1.7, Eliasi proved that

**Theorem 3.4.** [17] Let $\pi$ and $\pi'$ be two different non-increasing degree sequences with $\pi < \pi'$. If $G \in S(\pi)$ and $G' \in S(\pi')$, then $\prod_1(G) > \prod_1(G')$ and $\prod_2(G) < \prod_2(G')$. 
While the proofs of Theorem 3.1–3.4 are essentially based on Corollary 1.7, it is not evident how $M_2(G)$ can be expressed as a suitable Schur-convex function in order to apply Corollary 1.7. To this point we can refer the reader to Bianchi et al. [5]. However, up to now, the following majorization theorem holds for $M_2(G)$.

**Theorem 3.5.** [28, 30, 52] Let $\pi$ and $\pi'$ be two different non-increasing tree (respectively, unicyclic, bicyclic) degree sequences with $\pi \prec \pi'$. Let $G$ and $G'$ be the trees (respectively, unicyclic graphs, bicyclic graphs) with the maximal second Zagreb indices in $S(\pi)$ and $S(\pi')$, respectively. Then, $M_2(G) < M_2(G')$.

In Ashrafi et al. [2], it was proved that $M_2(G) = 2m^2 - M_2(G) - \frac{1}{2}M_1(G)$, and hence, by Theorem 3.5, we have:

**Theorem 3.6.** [31] Let $\pi$ and $\pi'$ be two different non-increasing tree (respectively, unicyclic, bicyclic) degree sequences with $\pi \prec \pi'$. Suppose $G$ and $G'$ have the minimal second Zagreb coindices in $S(\pi)$ and $S(\pi')$, respectively. If $\pi \prec R_1 \pi'$, then $M_2(G) > M_2(G')$.

Similar to the proofs of the majorization theorems for (signless Laplacian) spectral radii, the proof of Theorem 3.5 also mainly depends on the structure of the extremal graphs with maximal second Zagreb indices in $S(\pi)$. In 2008, Zhang and Xiang [30] used this method (as to our best knowledge, [50] is the first literature applying the majorization theorem to topological index theory) to prove the majorization theorem for the Wiener index $W(G)$, where $W(G)$ is the sum of topological distances between all pairs of vertices in $G$. If we use $d(u, v)$ to denote the distance of $u$ and $v$, then $W(G) = \sum_{(u, v) \subseteq V(G)} d(u, v)$.

**Theorem 3.7.** [50] Let $\pi$ and $\pi'$ be two different non-increasing tree degree sequences with $\pi \prec \pi'$. Suppose $T$ and $T'$ have the minimal Wiener indices in $S(\pi)$ and $S(\pi')$, respectively. Then, $W(T) > W(T')$, and $T$ and $T'$ are the unique BFS-trees of $S(\pi)$ and $S(\pi')$, respectively.

Let $P_r(T)$ be the number of pairs $(u, v)$ of vertices such that $d(u, v) \leq r$. Recently, as an extension of Theorem 3.4, Wagner et al. [147] showed that

**Theorem 3.8.** [147] Let $\pi$ and $\pi'$ be two different non-increasing tree degree sequences with $\pi \prec \pi'$. Suppose $T$ and $T'$ have the maximal number of pairs $(u, v)$ of vertices such that $d(u, v) \leq r$ in $S(\pi)$ and $S(\pi')$, respectively, where $r$ is an arbitrary positive integer. Then, $P_r(T) < P_r(T')$, and $T$ and $T'$ are the unique BFS-trees of $S(\pi)$ and $S(\pi')$, respectively.

Let $\gamma(T)$ denote the number of subtrees of $T$. The following majorization theorem for $\gamma(T)$ was proved by Zhang et al. [57].

**Theorem 3.9.** [57] Let $\pi$ and $\pi'$ be two different non-increasing tree degree
sequences with \( \pi \triangleleft \pi' \). Suppose \( T \) and \( T' \) have the maximal number of subtrees in \( S(\pi) \) and \( S(\pi') \), respectively. Then, \( \gamma(T) < \gamma(T') \), and \( T \) and \( T' \) are the unique BFS-trees of \( S(\pi) \) and \( S(\pi') \), respectively.

As shown in Example 2.26 by Theorem 2.2, we can easily determine the first five largest spectral radii in \( U_n \), but it become much more complicated to deal with the smallest case. The crucial problem is that it is a difficult problem to determine the exact value of spectral radius of a given graph. Analogous with the spectral theory, the majorization theorem of topological index can be applied to deal with the ordering or extremal problems of the corresponding topological indices in some given graph categories. Moreover, since the exact values of many topological indices of a given graph can be determined easily, we can obtain a better result when we employ the majorization theorem to deal with the ordering problem of topological indices. For instance,

**Example 3.10.** Let \( \pi_1 = (2, 2, 2, \ldots, 2) \), \( \pi_2 = (3, 2, 2, \ldots, 2, 1) \) and \( \pi_3 = (3, 3, 2, \ldots, 2, 1, 1) \). Suppose \( U \in U_n \). If \( \pi(U) \not\in \{\pi_1, \pi_2, \pi_3\} \), then \( \pi_1 \triangleleft \pi_2 \triangleleft \pi_3 \triangleleft \pi(U) \).

By Theorem 3.1, the cycle has the smallest first Zagreb index in \( U_n \), the unicyclic graphs of \( S(\pi_2) \) have the second smallest first Zagreb index in \( U_n \), and the unicyclic graphs of \( S(\pi_3) \) have the third smallest first Zagreb index in \( U_n \).

By applying Corollary 1.7 we can obtain good bounds for some topological indices. For instance, by Corollary 1.7 bounds for the sum of the \( \alpha \)-th power of the non-zero Laplacian eigenvalues of \( G \) were given in \([34, 58]\), for the sum of the \( \alpha \)-th power of the non-zero signless Laplacian eigenvalues of \( G \) were given in Liu and Liu \([36]\), and for the sum of power of Laplacian Estrada index of \( G \) were given in Zhou \([59]\).

Recently, Bianchi et al. \([5]\) presented a unified approach for localizing some relevant graph topological indices via majorization techniques. Furthermore, via characterizing \( c \)-cyclic graphs \( (0 \leq c \leq 6) \) as those whose degree sequence belongs to particular subsets of \( \mathbb{R}^n \), Bianchi et al. \([6]\) identified the maximal and minimal vectors of these subsets with respect to the majorization order. They also employed a majorization technique for a suitable class of graphs to derive upper and lower bounds for some topological indices depending on the degree sequence over all vertices. Through this method, old and new bounds can be easily reobtained and improved \([5, 6]\). If the reader is interested in this topic, he can refer to \([5, 6, 7]\) and the references therein.

**4. Further discussion.** As referred in the former sections, the majorization theorem has important application in graph spectrum and topological index theory. Actually, lots of open problems were solved by this tool \([1, 51, 17, 57]\). Thus, we hope
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that more scholars can pay their attention to this interesting research field.

Though several majorization theorems have been proved, a number of questions have been left unsolved. Here, we present two problems for further study.

Problem 4.1. Does there exist some other majorization theorem for graph spectrum (of the orientated or unorientated graph, the hypergraph and so on) or for other topological indices?

Problem 4.2. Give more accurate description of the maximal extremal graphs of $S(\pi)$ or $\Gamma(\pi)$. Furthermore, prove or disprove Conjecture 23.

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REFERENCES


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