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MAJORIZATION UNDER CONSTRAINTS AND BOUNDS ON THE SECOND ZAGREB INDEX

MONICA BIANCHI, ALESSANDRA CORNARO AND ANNA TORRIERO

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Abstract. In this paper we present a theoretical analysis in order to establish maximal and minimal vectors with respect to the majorization order of particular subsets of $\Re^n$. Afterwards we apply these issues to the calculation of bounds for a topological descriptor of a graph known as the second Zagreb index. Finally, we show how our bounds may improve the results obtained in the literature, providing some theoretical and numerical examples.

1. Introduction

The notion of majorization ordering was introduced by Hardy, Littlewood and Polya ([12]) and is closely connected with the economic theory of disparity indices ([2]). But this concept was first presented by Schur ([21]) who investigated functions which preserve the majorization order, the so-called Schur-convex functions and can be also found in Karamata ([13]). Using this property and characterizing maximal and minimal vectors with respect to majorization order under suitable constraints, many inequalities involving such functions can be derived ([18]). A significant application of this approach concerns the localization of ordered sequences of real numbers as they occur in the problem of finding estimates of eigenvalues of a matrix ([4], [20], [22] and [23]). Another field of interest concerns the network analysis, where the same methodology can be useful applied in order to provide bounds for some topological indicators of graphs which can be usefully expressed as a Schur-convex function, in terms of the degree sequence of the graph (see [7]).

In this paper, after some preliminary definitions and notations, we perform a theoretical analysis aimed at determining maximal and minimal vectors with respect to the majorization order of suitable subsets of $\Re^n$. In Section 3 and 4 we extend the results, obtained by Marshall and Olkin [18] into more specific sets of constraints determining their extremal elements. In Section 5, we provide an application of these results, dealing with the problem of computing bounds for the second Zagreb index, $M_2(G)$ of a particular class of graphs with a given number of pendant vertices. This index is extensively studied in graph theory, as a chemical molecular structure descriptor ([8], [9], [10], [19] and [24]) and, more generally, in network analysis, as a measure of degree-assortativity,

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quantifying how well a network is connected, ([1], [14] and [15]). In the latter context the Zagreb index $M_2(G)$ is renamed $S(G)$. Since determining $S(G)$ requires a specific algorithm ([14]), many bounds have been proposed in the literature ([5], [6], [17], [25] and [26]). Recently Grassi et al. in [7] obtained different bounds through a majorization technique. Using this approach, we derive new bounds in terms of graph degree sequence and present some theoretical and numerical examples comparing our results with the literature. Our conclusions are presented in Section 6.

2. Notations and preliminaries

Let $\mathbf{e^j}$, $j = 1, \ldots n$, be the fundamental vectors of $\mathbb{R}^n$ and set:

$$\mathbf{s^0} = \mathbf{0},\ \mathbf{s^j} = \sum_{i=1}^{j} \mathbf{e^i},\ \ j = 1, \ldots n,$$

$$\mathbf{v^n} = \mathbf{0},\ \mathbf{v^j} = \sum_{i=j+1}^{n} \mathbf{e^i},\ \ j = 0, \ldots (n-1).$$

Recalling that the Hadamard product of two vectors $\mathbf{x}, \mathbf{y} \in \mathbb{R}^n$ is defined as follows:

$$\mathbf{x} \circ \mathbf{y} = [x_1 y_1, x_2 y_2, \ldots, x_n y_n]^T$$

it is easy to verify the following properties, where $\langle \cdot, \cdot \rangle$ denotes the inner product in $\mathbb{R}^n$:

i) $\langle \mathbf{x} \circ \mathbf{y}, \mathbf{z} \rangle = \langle \mathbf{x}, \mathbf{y} \circ \mathbf{z} \rangle$

ii) $\langle \mathbf{s^h}, \mathbf{v^k} \rangle = h - \min\{h, k\}$

iii) $\mathbf{s^k} \circ \mathbf{s^j} = \mathbf{s^h},\ h = \min\{k, j\}$

iv) $\mathbf{v^k} \circ \mathbf{s^j} = \mathbf{s^j} - \mathbf{s^h} = \mathbf{v^h} - \mathbf{v^j},\ h = \min\{k, j\}$

DEFINITION 1. Assuming that the components of the vectors $\mathbf{x}$, $\mathbf{y} \in \mathbb{R}^n$ are arranged in nonincreasing order, the majorization order $\mathbf{x} \trianglelefteq \mathbf{y}$ means:

$$\left\langle \mathbf{x}, \mathbf{s^k} \right\rangle \leqslant \left\langle \mathbf{y}, \mathbf{s^k} \right\rangle,\ k = 1, \ldots, (n-1)$$

and

$$\langle \mathbf{x}, \mathbf{s^n} \rangle = \langle \mathbf{y}, \mathbf{s^n} \rangle.$$

In the sequel $\mathbf{x}^*(S)$ and $\mathbf{x}_*(S)$ will denote the maximal and the minimal elements of a subset $S \subseteq \mathbb{R}^n$ with respect to the majorization order.

Given a positive real number a, it is well known [18] that the maximal and the minimal elements of the set

$$\Sigma_a = \{\mathbf{x} \in \mathbb{R}^n : x_1 \geqslant x_2 \geqslant \ldots \geqslant x_n \geqslant 0, \langle \mathbf{x}, \mathbf{s^n} \rangle = a\}$$

with respect to the majorization order are respectively

$$\mathbf{x}^*(\Sigma_a) = a\mathbf{e}^1 \qquad \text{and} \qquad \mathbf{x}_*(\Sigma_a) = \frac{a}{n}\mathbf{s}^{\mathbf{n}}.$$

Next sections are dedicated to the study of the maximal and the minimal elements, with respect to the majorization order, of the particular subset of Σ_a given by

$$S_a = \Sigma_a \cap \{\mathbf{x} \in \mathbb{R}^n : M_i \geqslant x_i \geqslant m_i,\ i = 1,...n\}, \tag{1}$$

where $\mathbf{m} = [m_1, m_2, ..., m_n]^T$ and $\mathbf{M} = [M_1, M_2, ..., M_n]^T$ are two assigned vectors arranged in nonincreasing order with $0 \leqslant m_i \leqslant M_i$, for all $i = 1,...n$, and a is a positive real number such that $\langle \mathbf{m}, \mathbf{s}^{\mathbf{n}} \rangle \leqslant a \leqslant \langle \mathbf{M}, \mathbf{s}^{\mathbf{n}} \rangle$. Notice that the intervals $[m_i, M_i]$ are not necessarily disjointed unless the additional assumption $M_{i+1} < m_i,\ i = 1,...,(n-1)$ is required. The existence of maximal and minimal elements of S_a are ensured by the compactness of the set S_a and by the closure of the upper and lower level sets:

$$U(\mathbf{x}) = \{\mathbf{z} \in S_a : \mathbf{x} \trianglelefteq \mathbf{z}\},\ L(\mathbf{x}) = \{\mathbf{z} \in S_a : \mathbf{z} \trianglelefteq \mathbf{x}\}.$$

3. The maximal element of S_a

We start computing the maximal element, with respect to the majorization order, of the set S_a.

THEOREM 2. *Let $k \geqslant 0$ be the smallest integer such that*

$$\left\langle \mathbf{M}, \mathbf{s}^{\mathbf{k}} \right\rangle + \left\langle \mathbf{m}, \mathbf{v}^{\mathbf{k}} \right\rangle \leqslant a < \left\langle \mathbf{M}, \mathbf{s}^{k+1} \right\rangle + \left\langle \mathbf{m}, \mathbf{v}^{\mathbf{k+1}} \right\rangle, \tag{2}$$

and $\theta = a - \left\langle \mathbf{M}, \mathbf{s}^{\mathbf{k}} \right\rangle - \left\langle \mathbf{m}, \mathbf{v}^{\mathbf{k+1}} \right\rangle$. Then

$$\mathbf{x}^*(S_a) = \mathbf{M} \circ \mathbf{s}^{\mathbf{k}} + \theta \mathbf{e}^{k+1} + \mathbf{m} \circ \mathbf{v}^{\mathbf{k+1}} \tag{3}$$

Proof. First of all we verify that $\mathbf{x}^*(S_a) \in S_a$. It easy to see that $\langle \mathbf{x}^*(S_a), s^n \rangle = a$ and that $m_i \leqslant \mathbf{x}_i^*(S_a) \leqslant M_i$ for $i \neq k+1$. To prove that $m_{k+1} \leqslant \mathbf{x}_{k+1}^*(S_a) \leqslant M_{k+1}$, notice that from (2)

$$m_{k+1} = \left\langle \mathbf{m}, \mathbf{e}^{\mathbf{k+1}} \right\rangle \leqslant a - \left\langle \mathbf{M}, \mathbf{s}^{\mathbf{k}} \right\rangle - \left\langle \mathbf{m}, \mathbf{v}^{\mathbf{k+1}} \right\rangle = \theta < \left\langle \mathbf{M}, \mathbf{e}^{\mathbf{k+1}} \right\rangle = M_{k+1}.$$

Now we show that $\mathbf{x} \trianglelefteq \mathbf{x}^*(S_a)$ for all $\mathbf{x} \in S_a$. By property i) follows

$$\left\langle \mathbf{x}^*(S_a), \mathbf{s}^{\mathbf{j}} \right\rangle = \left\langle \mathbf{M}, \mathbf{s}^{\mathbf{k}} \circ \mathbf{s}^{\mathbf{j}} \right\rangle + \theta \left\langle \mathbf{e}^{\mathbf{k+1}}, \mathbf{s}^{\mathbf{j}} \right\rangle + \left\langle \mathbf{m}, \mathbf{v}^{\mathbf{k+1}} \circ \mathbf{s}^{\mathbf{j}} \right\rangle,\ j = 1,...(n-1)$$

and by iii) and iv)

$$\left\langle \mathbf{x}^*(S_a), \mathbf{s}^{\mathbf{j}} \right\rangle = \begin{cases} \left\langle \mathbf{M}, \mathbf{s}^{\mathbf{j}} \right\rangle & 1 \leqslant j \leqslant k \\ \left\langle \mathbf{M}, \mathbf{s}^{\mathbf{k}} \right\rangle + \theta + \left\langle \mathbf{m}, \mathbf{s}^{\mathbf{j}} - \mathbf{s}^{\mathbf{k+1}} \right\rangle & (k+1) \leqslant j \leqslant (n-1) \end{cases}.$$

Thus, given a vector $\mathbf{x} \in S_a$, for $1 \leqslant j \leqslant k$ we obtain

$$\left\langle \mathbf{x}, \mathbf{s^j} \right\rangle \leqslant \left\langle \mathbf{M}, \mathbf{s^j} \right\rangle = \left\langle \mathbf{x}^*(S_a), \mathbf{s^j} \right\rangle,$$

while for $(k+1) \leqslant j \leqslant (n-1)$, by iii),

$$\left\langle \mathbf{x}, \mathbf{s^j} \right\rangle = \langle \mathbf{x}, \mathbf{s^n} \rangle - \left\langle \mathbf{x}, \mathbf{v^j} \right\rangle \leqslant a - \left\langle \mathbf{m}, \mathbf{v^j} \right\rangle = \left\langle \mathbf{M}, \mathbf{s^k} \right\rangle + \theta + \left\langle \mathbf{m}, \mathbf{s^j} - \mathbf{s^{k+1}} \right\rangle = \left\langle \mathbf{x}^*(S_a), \mathbf{s^j} \right\rangle$$

and the result follows. □

From this general result, the maximal element of particular subsets of S_a can be deduced. We then focus on a specific case which will be useful in the application we deal with in Section 5. We denote by $\lfloor x \rfloor$ the integer part of the real number x.

COROLLARY 3. *Given $1 \leqslant h \leqslant n$, let us consider the set*

$$S_a^{[h]} = \Sigma_a \cap \{\mathbf{x} \in \mathbb{R}^n : M_1 \geqslant x_1 \geqslant \ldots \geqslant x_h \geqslant m_1, M_2 \geqslant x_{h+1} \geqslant \ldots \geqslant x_n \geqslant m_2\}, \tag{4}$$

where

$$0 \leqslant m_2 \leqslant m_1,\ 0 \leqslant M_2 \leqslant M_1,\ m_i < M_i, \quad i = 1,2$$

and

$$hm_1 + (n-h)m_2 \leqslant a \leqslant hM_1 + (n-h)M_2.$$

Let $a^* = hM_1 + (n-h)m_2$ and

$$k = \begin{cases} \left\lfloor \dfrac{a - h(m_1 - m_2) - nm_2}{M_1 - m_1} \right\rfloor & \text{if } a < a^* \\ \left\lfloor \dfrac{a - h(M_1 - M_2) - nm_2}{M_2 - m_2} \right\rfloor & \text{if } a \geqslant a^* \end{cases}$$

Then

$$\mathbf{x}^*(S_a^{[h]}) = \begin{cases} \left[\underbrace{M_1, \ldots\ldots, M_1}_{k}, \theta, \underbrace{m_1, \ldots\ldots, m_1}_{h-k-1}, \underbrace{m_2, \ldots\ldots, m_2}_{n-h} \right] & \text{if } a < a^* \\ \left[\underbrace{M_1, \ldots\ldots, M_1}_{h}, \underbrace{M_2, \ldots\ldots, M_2}_{k-h}, \theta, \underbrace{m_2, \ldots\ldots m_2}_{n-k-1} \right] & \text{if } a \geqslant a^* \end{cases}$$

where $\mathbf{M} = M_1\mathbf{s^h} + M_2\mathbf{v^h}$, $\mathbf{m} = m_1\mathbf{s^h} + m_2\mathbf{v^h}$ and $\theta = a - \left\langle \mathbf{M}, \mathbf{s^k} \right\rangle - \left\langle \mathbf{m}, \mathbf{v^{k+1}} \right\rangle$.

Proof. Easy computations give:

$$\left\langle \mathbf{M}, \mathbf{s^k} \right\rangle = \begin{cases} hM_1 + M_2(k-h) & \text{if } k \geqslant h \\ kM_1 & \text{if } k < h \end{cases}$$

$$\langle \mathbf{m}, \mathbf{v}^{\mathbf{k}} \rangle = \begin{cases} (n-k)m_2 & \text{if } k \geqslant h \\ (n-h)m_2 + m_1(h-k) & \text{if } k < h \end{cases}$$

and the values are linked for continuity when $k = h$. We distinguish two cases:

i) $k \geqslant h$: from (2) we have

$$k = \left\lfloor \frac{a - h(M_1 - M_2) - nm_2}{M_2 - m_2} \right\rfloor$$

that is acceptable only if $a \geqslant hM_1 + (n-h)m_2 = a^*$. Then, from (3)

$$\mathbf{x}^*(S_a^{[h]}) = \left[\underbrace{M_1, \ldots\ldots, M_1}_{h}, \underbrace{M_2, \ldots\ldots, M_2}_{k-h}, \theta, \underbrace{m_2, \ldots\ldots m_2}_{n-k-1} \right].$$

ii) $k < h$: from (2) we get

$$k = \left\lfloor \frac{a - h(m_1 - m_2) - nm_2}{M_1 - m_1} \right\rfloor$$

that is acceptable only if $a < hM_1 + (n-h)m_2 = a^*$. Then, from (3)

$$\mathbf{x}^*(S_a^{[h]}) = \left[\underbrace{M_1, \ldots\ldots, M_1}_{k}, \theta, \underbrace{m_1, \ldots\ldots, m_1}_{h-k-1}, \underbrace{m_2, \ldots\ldots, m_2}_{n-h} \right]. \quad \square$$

REMARK 4. When $a = a^*$ it is worthwhile to note that $k = h$ and $\theta = m_2$ so that

$$\mathbf{x}^*(S_a^{[h]}) = \left[\underbrace{M_1, \ldots\ldots, M_1}_{h}, \underbrace{m_2, \ldots\ldots, m_2}_{n-h} \right].$$

REMARK 5. The assumption $m_i < M_i$ in Corollary 3 can be relaxed to $m_i \leqslant M_i$. Indeed, if $m_i = M_i, i = 1,2$, the set $S_a^{[h]}$ reduces to the singleton $\{m_1\mathbf{s^h} + m_2\mathbf{v^h}\}$, while if $m_1 = M_1, m_2 < M_2$ the first h components of any $\mathbf{x} \in S_a^{[h]}$ are fixed and equal to m_1 and the maximal element of $S_a^{[h]}$ can be computed by the maximal element of $S_{a-hm_1} \in \mathbb{R}^{n-h}$ (see Corollary 6 below). The case $m_2 = M_2, m_1 < M_1$ is similar.

The next corollary is proved in [18] and it immediately follows from Corollary 3 when $m_1 = m_2 = m$ and $M_1 = M_2 = M$.

COROLLARY 6. *Let* $0 \leqslant m < M$ *and* $m \leqslant \dfrac{a}{n} \leqslant M$. *Given the subset*

$$S_a^1 = \Sigma_a \cap \{\mathbf{x} \in \mathbb{R}^n : M \geqslant x_1 \geqslant x_2 \geqslant \ldots \geqslant x_n \geqslant m\}$$

we have

$$\mathbf{x}^*(S_a^1) = M\mathbf{s}^{\mathbf{k}} + \theta\mathbf{e}^{\mathbf{k+1}} + m\mathbf{v}^{\mathbf{k+1}},$$

where $k = \left\lfloor \dfrac{a-nm}{M-m} \right\rfloor$ *and* $\theta = a - Mk - m(n-k-1)$.

In particular when $m = 0$ *we obtain*

$$\mathbf{x}^*(S_a^1) = M\mathbf{s}^{\mathbf{k}} + \theta\mathbf{e}^{\mathbf{k+1}},$$

where $k = \left\lfloor \dfrac{a}{M} \right\rfloor$ *and* $\theta = a - Mk$.

It is worthwhile to notice that S_a is a subset of S_a^1 where $m = m_n$ and $M = M_1$. Thus, the following inequality holds:

$$x^*(S_a) \trianglelefteq x^*(S_a^1). \tag{5}$$

Finally we recall the following result (see [4]).

COROLLARY 7. *Let* $1 \leqslant h \leqslant n$ *and* $0 < \alpha \leqslant a/h$. *Given the subset*

$$S_a^2 = \Sigma_a \cap \{\mathbf{x} \in \mathbb{R}^n : x_i \geqslant \alpha,\ i = 1, \ldots h\},$$

we have $\mathbf{x}^*(S_a^2) = (a - h\alpha)\mathbf{e}^1 + \alpha\mathbf{s}^{\mathbf{h}}$.

Proof. The set S_a^2 can be obtained by (1) for $m_1 = \alpha$, $m_2 = 0$, $M_1 = M_2 = a$. Since $a^* = ha \geqslant a$, two cases can be distinguished:

i) $h = 1$: we have $a^* = a$ and from Remark 4 it immediately follows that $k = 1$ and $\theta = 0$ so that

$$\mathbf{x}^*(S_a^2) = a\mathbf{e}^1.$$

ii) $h > 1$: we have $a^* > a$ and Corollary 3 implies that $k = \left\lfloor \dfrac{a-h\alpha}{a-\alpha} \right\rfloor = 0$. Thus,

$$\mathbf{x}^*(S_a^2) = \left[\theta, \underbrace{\alpha, \ldots, \alpha}_{h-1}, \underbrace{0, \ldots, 0}_{n-h}\right]$$

where $\theta = a - (h-1)\alpha$, which leads to

$$\mathbf{x}^*(S_a^2) = \theta\mathbf{e}^{\mathbf{1}} + \alpha\mathbf{s}^{\mathbf{h}} - \alpha\mathbf{e}^{\mathbf{1}} = (a - h\alpha)\mathbf{e}^1 + \alpha\mathbf{s}^{\mathbf{h}}. \quad \square$$

4. The minimal element of S_a

In this section we study the structure of the minimal element, with respect to the majorization order, of the set S_a.

THEOREM 8. *Let $k \geqslant 0$ and $d \geqslant 0$ be the smallest integers such that*

1) $k+d<n$

2) $m_{k+1} \leqslant \rho \leqslant M_{n-d}$ *where* $\rho = \dfrac{a-\langle \mathbf{m},\mathbf{s^k}\rangle - \langle \mathbf{M},\mathbf{v^{n-d}}\rangle}{n-k-d}$.

Then

$$\mathbf{x}_*(S_a) = \mathbf{m}\circ\mathbf{s^k} + \rho(\mathbf{s^{n-d}}-\mathbf{s^k}) + \mathbf{M}\circ\mathbf{v^{n-d}}.$$

Proof. The minimal element of the set Σ_a is $\mathbf{x}_\circ(\Sigma_a) = \frac{a}{n}\mathbf{s^n}$. If $m_1 \leqslant \mathbf{x}_*(\Sigma_a) \leqslant M_n$, then $\mathbf{x}_*(\Sigma_a) \in S_a$ and $\mathbf{x}_*(S_a) = \mathbf{x}_*(\Sigma_a)$ (notice that in this case $k=d=0$).

If $\mathbf{x}_*(\Sigma_a) \notin S_a$, let k and d the smallest integers satisfying conditions 1) and 2) above. It is easy to verify that $\mathbf{x}_*(S_a) \in S_a$. In order to prove that it is the minimal element, we must show that for all $\mathbf{x} \in S_a$

$$\langle \mathbf{x}_*(S_a),\mathbf{s^h}\rangle \leqslant \langle \mathbf{x},\mathbf{s^h}\rangle, \quad h=1,\cdots(n-1). \tag{6}$$

We distinguish three cases:

i) $1 \leqslant h \leqslant k$. Since $\langle \mathbf{x}_*(S_a),\mathbf{s^h}\rangle = \langle \mathbf{m},\mathbf{s^h}\rangle$, the inequality (6) is straightforward.

ii) $k+1 \leqslant h \leqslant n-d$. We prove the inequality (6) for $h=k+1$. By induction, similar arguments can be applied to prove the inequality for $h=k+2,\cdots(n-d)$.

By contradiction, let us assume that there exists $\mathbf{x} \in S_a$ such that

$$\langle \mathbf{x}_*(\mathbf{S_a}),\mathbf{s^{k+1}}\rangle = \langle \mathbf{m},\mathbf{s^k}\rangle + \rho > \langle \mathbf{x},\mathbf{s^k}\rangle + x_{k+1}.$$

Then $x_j \leqslant x_{k+1} < \langle \mathbf{m},\mathbf{s^k}\rangle + \rho - \langle \mathbf{x},\mathbf{s^k}\rangle$, for $j=k+2,\cdots n$ and thus,

$$\langle \mathbf{x},\mathbf{s^{n-d}}\rangle = \langle \mathbf{x},\mathbf{s^k}\rangle + \langle \mathbf{x},\mathbf{s^{n-d}}-\mathbf{s^k}\rangle < \langle \mathbf{x},\mathbf{s^k}\rangle + (n-d-k)(\langle \mathbf{m},\mathbf{s^k}\rangle + \rho - \langle \mathbf{x},\mathbf{s^k}\rangle).$$

Taking into account that

$$\langle \mathbf{x},\mathbf{s^{n-d}}\rangle = a - \langle \mathbf{x},\mathbf{v^{n-d}}\rangle \geqslant a - \langle \mathbf{M},\mathbf{v^{n-d}}\rangle,$$

we get

$$a - \langle \mathbf{M},\mathbf{v^{n-d}}\rangle < (1-n+d+k)\langle \mathbf{x},\mathbf{s^k}\rangle + (n-d-k)(\langle \mathbf{m},\mathbf{s^k}\rangle + \rho).$$

Using the expression of ρ, we obtain

$$0 < (1-n+d+k)(\langle \mathbf{x},\mathbf{s^k}\rangle - \langle \mathbf{m},\mathbf{s^k}\rangle).$$

Since $(1-n+d+k) \leqslant 0$ and $\langle \mathbf{x},\mathbf{s^k}\rangle \geqslant \langle \mathbf{m},\mathbf{s^k}\rangle$, the inequality above is false, and we have got the contradiction.

iii) $n-d+1 \leqslant h < n$. For any $\mathbf{x} \in S_a$ we have

$$\begin{aligned}\langle \mathbf{x}_*(S_a), \mathbf{s^h} \rangle &= \langle \mathbf{x}_*(S_a), \mathbf{s^{n-d}} \rangle + \langle \mathbf{x}_*(S_a), \mathbf{s^h} - \mathbf{s^{n-d}} \rangle = \\ &= \langle \mathbf{m}, \mathbf{s^k} \rangle + (n-d-k)\rho + \langle \mathbf{M}, \mathbf{s^h} - \mathbf{s^{n-d}} \rangle = \\ &= a - \langle \mathbf{M}, \mathbf{v^{n-d}} \rangle + \langle \mathbf{M}, \mathbf{s^h} - \mathbf{s^{n-d}} \rangle = \\ &= a - \langle \mathbf{M}, \mathbf{s^n} - \mathbf{s^h} \rangle = \\ &= \langle \mathbf{x}, \mathbf{s^h} \rangle + \langle \mathbf{x}, \mathbf{s^n} - \mathbf{s^h} \rangle - \langle \mathbf{M}, \mathbf{s^n} - \mathbf{s^h} \rangle \\ &\leqslant \langle \mathbf{x}, \mathbf{s^h} \rangle. \quad \square\end{aligned}$$

Now we analyze the minimal element of particular subsets of S_a. We start considering the intervals $[m_i, M_i]$, $i = 1, \cdots, n$ disjointed. Notice that this additional assumption does not modify the choice of the maximal element, while it simplifies the choice of the minimal element.

COROLLARY 9. *Let us consider the set S_a and assume*

$$M_{i+1} < m_i \quad \text{for } i = 1, \ldots (n-1). \tag{7}$$

Let $k \geqslant 0$ be the smallest integer such that

$$\left\langle \mathbf{m}, \mathbf{s^{k+1}} \right\rangle + \left\langle \mathbf{M}, \mathbf{v^{k+1}} \right\rangle \leqslant a < \left\langle \mathbf{m}, \mathbf{s^k} \right\rangle + \left\langle \mathbf{M}, \mathbf{v^k} \right\rangle \tag{8}$$

and $\rho = a - \left\langle \mathbf{m}, \mathbf{s^k} \right\rangle - \left\langle \mathbf{M}, \mathbf{v^{k+1}} \right\rangle$. Then

$$\mathbf{x}_*(S_a) = \mathbf{m} \circ \mathbf{s^k} + \rho \mathbf{e^{k+1}} + \mathbf{M} \circ \mathbf{v^{k+1}}$$

Proof. By condition 2) in Theorem 8 and assumption (7), we get

$$M_{k+2} < m_{k+1} \leqslant \rho \leqslant M_{n-d}.$$

Thus, $k > n-d-2$. Since k is an integer such that $k < n-d$, we have necessarily $k = n-d-1$ and the thesis follows. $\square$

Another case of practical interest regards the set studied in Corollary 3.

COROLLARY 10. *Given $1 \leqslant h \leqslant n$, let us consider the set*

$$S_a^{[h]} = \Sigma_a \cap \{\mathbf{x} \in \mathbb{R}^n : M_1 \geqslant x_1 \geqslant \ldots \geqslant x_h \geqslant m_1, M_2 \geqslant x_{h+1} \geqslant \ldots \geqslant x_n \geqslant m_2\},$$

where $0 \leqslant m_2 \leqslant m_1$, $0 \leqslant M_2 \leqslant M_1$, $m_i < M_i$, $i = 1, 2$ and

$$hm_1 + (n-h)m_2 \leqslant a \leqslant hM_1 + (n-h)M_2.$$

If $m_1 \leqslant \dfrac{a}{n} \leqslant M_2$ *we have* $x_*(S_a^{[h]}) = \frac{a}{n}\mathbf{s^n}$. *Otherwise, let* $\widetilde{a} = hm_1 + (n-h)M_2$.
If $\begin{cases} a < m_1 n \\ a \leqslant \widetilde{a} \end{cases}$, *given* $\rho = \dfrac{a - hm_1}{n-h}$, *we have*

$$\mathbf{x}_*(S_a^{[h]}) = m_1\mathbf{s^h} + \rho\mathbf{v^h} = \left[\underbrace{m_1, \ldots\ldots, m_1}_{h}, \underbrace{\rho, \ldots\ldots, \rho}_{n-h}\right].$$

If $\begin{cases} a > M_2 n \\ a \geqslant \widetilde{a} \end{cases}$, *given* $\rho = \dfrac{a - M_2(n-h)}{h}$, *we have*

$$\mathbf{x}_*(S_a^{[h]}) = \rho\mathbf{s^h} + M_2\mathbf{v^h} = \left[\underbrace{\rho, \ldots, \rho}_{h}, \underbrace{M_2, \ldots, M_2}_{n-h}\right].$$

Proof. Let us investigate when the best choice $k = d = 0$ is admissible. Under this assumption, from condition 2) in Theorem 8 we have

$$m_1 \leqslant \rho = \frac{a}{n} \leqslant M_n = M_2. \tag{9}$$

If the condition above holds, the minimal element is $\mathbf{x}_*(S_a^{[h]}) = \dfrac{a}{n}\mathbf{s^n}$.

Otherwise if condition (9) does not hold, we begin with the case $k = 0$. We have

$$\rho = \frac{a - \langle \mathbf{M}, \mathbf{v^{n-d}} \rangle}{n-d}$$

and

$$\mathbf{x}_*(S_a^{[h]}) = \rho\mathbf{s^{n-d}} + \mathbf{M} \circ \mathbf{v^{n-d}}.$$

From condition 2) in Theorem 8, we have $m_1 \leqslant \rho \leqslant M_{n-d}$ and, taking into account that the elements in $\mathbf{x}_*(S_a^{[h]})$ are in nonincreasing order, $\rho \geqslant M_{n-d+1}$. We distinguish three cases:

i) if $n - d > h$ then necessarily $\rho = M_2$, but this contradicts (9).

ii) if $n - d < h$ then $\rho = M_1$ and this is admissible only if $a = M_1 h + M_2(n-h)$, so that

$$\mathbf{x}_*(S_a^{[h]}) = \left[\underbrace{M_1, \ldots\ldots, M_1}_{h}, \underbrace{M_2, \ldots\ldots, M_2}_{n-h}\right].$$

iii) if $n - d = h$, then $\rho = \dfrac{a - M_2 d}{n-d}$ and

$$\mathbf{x}_*(S_a^{[h]}) = \left[\underbrace{\rho, \ldots\ldots, \rho}_{h}, \underbrace{M_2, \ldots\ldots, M_2}_{n-h}\right].$$

This result is admissible only if $\rho > M_2$ and $m_1 \leqslant \rho \leqslant M_1$, i.e., if $\begin{cases} a > M_2 n \\ a \geqslant \widetilde{a} \end{cases}$.

A symmetric case occurs when $d = 0$, so we have

$$\rho = \frac{a - \langle \mathbf{m}, \mathbf{s}^{\mathbf{k}} \rangle}{n-k}$$

and

$$\mathbf{x}_*(S_a^{[h]}) = \mathbf{m} \circ \mathbf{s}^{\mathbf{k}} + \rho \mathbf{v}^{\mathbf{k}}.$$

From condition 2) in Theorem 8, we have that $m_{k+1} \leqslant \rho \leqslant M_2$ and, taking into account that the elements in $\mathbf{x}_*(S_a^{[h]})$ are in nonincreasing order, $\rho \leqslant m_k$. We distinguish three cases:

i) if $k < h$ then necessarily $\rho = m_1$, but this contradicts (9).

ii) if $k > h$, then $\rho = m_2$ and this is possible only if $a = hm_1 + m_2(n-h)$, so that

$$\mathbf{x}_*(S_a^{[h]}) = \left[\underbrace{m_1, \ldots\ldots, m_1}_{h}, \underbrace{m_2, \ldots\ldots, m_2}_{n-h} \right].$$

iii) if $k = h$, then $\rho = \dfrac{a - hm_1}{n-h}$ and

$$\mathbf{x}_*(S_a^{[h]}) = \left[\underbrace{m_1, \ldots\ldots, m_1}_{h}, \underbrace{\rho, \ldots\ldots, \rho}_{n-h} \right].$$

This result is admissible only if $m_2 \leqslant \rho \leqslant M_2$ and $\rho < m_1$, i.e., only if $\begin{cases} a < m_1 n \\ a \leqslant \widetilde{a} \end{cases}$.

□

Corollary 10 distinguishes the minimal element of $S_a^{[h]}$ whether

$$\begin{cases} a < m_1 n \\ a \leqslant \widetilde{a} \end{cases} \quad \text{or} \quad \begin{cases} a > M_2 n \\ a \geqslant \widetilde{a} \end{cases}.$$

We note that, if $m_1 \leqslant M_2$, the first inequality in the systems above is always stronger than the second one, while, if $M_2 < m_1$, the second one is stronger than the first. Thus, we can summarize the minimal element of $S_a^{[h]}$ in a more accessible way according to the following scheme:

i) If $m_1 \leqslant M_2$ then

$$\mathbf{x}_*(S_a^{[h]}) = \begin{cases} \dfrac{a}{n}\mathbf{s}^{\mathbf{n}} & \text{if } m_1 \leqslant \dfrac{a}{n} \leqslant M_2 \\ m_1 \mathbf{s}^{\mathbf{h}} + \dfrac{a - hm_1}{n-h}\mathbf{v}^{\mathbf{h}} & \text{if } \dfrac{a}{n} < m_1 \\ \dfrac{a - M_2(n-h)}{h}\mathbf{s}^{\mathbf{h}} + M_2 \mathbf{v}^{\mathbf{h}} & \text{if } \dfrac{a}{n} > M_2 \end{cases} \tag{10}$$

and the vectors are linked for continuity.

ii) If $M_2 < m_1$ then

$$\mathbf{x}_*(S_a^{[h]}) = \begin{cases} m_1\mathbf{s^h} + \dfrac{a-hm_1}{n-h}\mathbf{v^h} & \text{if } a < \widetilde{a} \\ \dfrac{a-M_2(n-h)}{h}\mathbf{s^h} + M_2\mathbf{v^h} & \text{if } a \geqslant \widetilde{a}. \end{cases} \tag{11}$$

REMARK 11. When $a = \widetilde{a}$ it is worthwhile to note that

$$\mathbf{x}_*(S_a^{[h]}) = m_1\mathbf{s^h} + M_2\mathbf{v^h} = \left[\underbrace{m_1,\ldots\ldots,m_1}_{h},\underbrace{M_2,\ldots\ldots,M_2}_{n-h}\right].$$

REMARK 12. We note that the minimal element of the set $S_a^{[h]}$ does not necessarily have integer components, while this is not the case for the maximal element. For some applications, it is meaningful to find the minimal vector in $S_a^{[h]}$ with integer components. We illustrate below the procedure to follow. Let us consider, for instance, the vector $\mathbf{x}_*(S_a^{[h]}) = \dfrac{a}{n}\mathbf{s^n}$ which corresponds to the case $m_1 \leqslant \dfrac{a}{n} \leqslant M_2$ (see (10)). If $\dfrac{a}{n}$ is not an integer, let us find the index k, $1 \leqslant k \leqslant n$, such that

$$\left(\left\lfloor\frac{a}{n}\right\rfloor + 1\right)k + \left\lfloor\frac{a}{n}\right\rfloor(n-k) = a$$

i.e., $k = a - \left\lfloor\dfrac{a}{n}\right\rfloor n$. The vector

$$\mathbf{x}_*^{\mathbf{1}} = \left(\left\lfloor\frac{a}{n}\right\rfloor + 1\right)\mathbf{s^k} + \left\lfloor\frac{a}{n}\right\rfloor\mathbf{v^k}$$

is the minimal element of $S_a^{[h]}$ with integer components.

With slight modification, the same procedure can be applied also in the other cases illustrated in (10) or (11), where only some of the components of $\mathbf{x}_*(S_a^{[h]})$ can be non integer.

To complete our analysis, we show how from Corollary 10, particular cases can be deduced. More precisely, assuming in Corollary 10 $m_1 = m_2$, $M_1 = M_2$ or $h = n$ we obtain the results proved in [18].

COROLLARY 13. *Let $0 \leqslant m < M$ and $m \leqslant \dfrac{a}{n} \leqslant M$. Given the subset*

$$S_a^1 = \Sigma_a \cap \{\mathbf{x} \in \mathbb{R}^n : M \geqslant x_1 \geqslant \ldots \geqslant x_{n-1} \geqslant x_n \geqslant m\}$$

we have $\mathbf{x}_*(S_a^1) = \dfrac{a}{n}\mathbf{s^n}$.

As we did with the maximal element, it is clear that the vector provided by Corollary 10 majorizes the vector in Corollary 13, i.e., the following inequality holds:

$$\mathbf{x}_*(S_a^1) \trianglelefteq \mathbf{x}_*(S_a). \tag{12}$$

Assuming $m_1 = \alpha$, $m_2 = 0$, $M_1 = M_2 = a$ or $m_1 = m_2 = 0$ and $M_2 = \alpha$, $M_1 = a$ we easily obtain the following two corollaries (see [4]).

COROLLARY 14. *Let $1 \leqslant h \leqslant n$ and $0 < \alpha \leqslant a/h$. Given the subset*

$$S_a^2 = \Sigma_a \cap \{\mathbf{x} \in \mathbb{R}^n : x_i \geqslant \alpha,\ i = 1, \ldots h\},$$

we have

$$\mathbf{x}_*(S_a^2) = \begin{cases} \dfrac{a}{n}\mathbf{s^n} & \text{if } \alpha \leqslant \dfrac{a}{n} \\ \alpha\mathbf{s^h} + \rho\mathbf{v^h} \text{ with } \rho = \dfrac{a - \alpha h}{n - h} & \text{if } \alpha > \dfrac{a}{n} \end{cases}$$

COROLLARY 15. *Let $1 \leqslant h \leqslant (n-1)$ and $0 < \alpha < a$. Given the subset*

$$S_a^3 = \Sigma_a \cap \{\mathbf{x} \in \mathbb{R}^n : x_i \leqslant \alpha,\ i = h+1, \ldots n\},$$

we have

$$\mathbf{x}_*(S_a^3) = \begin{cases} \dfrac{a}{n}\mathbf{s^n} & \text{if } \alpha \geqslant \dfrac{a}{n} \\ \rho\mathbf{s^h} + \alpha\mathbf{v^h} \text{ with } \rho = \dfrac{a - (n-h)\alpha}{h} & \text{if } \alpha < \dfrac{a}{n} \end{cases}$$

5. New bounds for the second Zagreb index

Let $G = (V, E)$ a simple, connected, undirected graph with fixed order $|V| = n$ and fixed size $|E| = m$. Denote by $\pi = (d_1, d_2, .., d_n)$ the degree sequence of G, being d_i the degree of vertex v_i, arranged in nonincreasing order $d_1 \geqslant d_2 \geqslant \cdots \geqslant d_n$. We recall that the sequences of integers which are degree sequences of a simple graph were characterized by Erdős and Gallai (see [11]). The second Zagreb index is defined as

$$S(G) = \sum_{(v_i, v_j) \in E} d_i d_j$$

or equivalently ([7])

$$S(G) = \frac{\sum\limits_{(v_i, v_j) \in E} (d_i + d_j)^2 - \sum\limits_{i=1}^{n} d_i^3}{2}. \tag{13}$$

In order to compute upper and lower bounds for $S(G)$ we refer to [7], where a methodology based on majorization order was proposed. Before presenting our results, we briefly describe the procedure we will follow.

Let π be a fixed degree sequence and $\mathbf{x} \in \mathbb{R}^m$ the vector whose components are $d_i + d_j$, $(v_i, v_j) \in E$. In [16] it is shown that

$$\sum_{(v_i,v_j)\in E} (d_i + d_j) = \sum_{i=1}^{n} d_i^2$$

and thus, $\sum_{i=1}^{m} x_i = \sum_{i=1}^{n} d_i^2$ is a constant. Given a suitable subset S of

$$\Sigma_a = \left\{ \mathbf{x} \in \mathbb{R}^m : x_1 \geqslant x_2 \geqslant \ldots \geqslant x_m \geqslant 0, \sum_{i=1}^{m} x_i = a \right\},$$

where $a = \sum_{i=1}^{n} d_i^2$, the Schur-convex function $f(\mathbf{x}) = \sum_{i=1}^{m} x_i^2$ attains its minimum and maximum on S at $f(\mathbf{x}_*(S))$ and $f(\mathbf{x}^*(S))$ respectively, being $\mathbf{x}_*(S)$ and $\mathbf{x}^*(S)$ the extremal vectors of S with respect to the majorization order (see [18]). Hence from (13) the maximum and the minimum of $S(G)$ can be easily deduced.

Let C_π be the class of graphs $G = (V, E)$ with h pendant vertices and degree sequence

$$\pi = (\underbrace{d_1, d_2, .., d_{n-h-1}, d_{n-h}}_{n-h}, \underbrace{1, \ldots, 1}_{h}), \quad n \geqslant 4, n-h \geqslant 2, h \geqslant 1$$

and let us consider graphs $G \in C_\pi$ with maximum vertex degree upper bounded by $d_{n-h} + d_{n-h-1}$, i.e.,, $d_1 < d_{n-h} + d_{n-h-1}$, or equivalently

$$1 + d_1 \leqslant d_{n-h} + d_{n-h-1}. \tag{14}$$

For $G \in C_\pi$, we note that this constraint is always satisfied, for example, if the maximum vertex degree is at most three, as for some graphs of chemical interest where the maximum degree is four.

We observe that for $i, j = 1, \ldots, n-h$ and $(v_i, v_j) \in E$:

$$d_{n-h} + d_{n-h-1} \leqslant d_i + d_j \leqslant d_1 + d_2,$$

while for $i = n-h+1, \ldots, n$, $j = 1, \ldots, n-h$ and $(v_i, v_j) \in E$:

$$1 + d_{n-h} \leqslant d_i + d_j \leqslant 1 + d_1.$$

Furthermore, inequality (14) assures that the above intervals are concatenated so that the vector $\mathbf{x} \in \mathbb{R}^m$ can be arranged in nonincreasing order with the h pendant vertices in the last h positions.

Setting $m_1 = d_{n-h} + d_{n-h-1}$, $m_2 = 1 + d_{n-h}$, $M_1 = d_1 + d_2$, $M_2 = 1 + d_1$, let us consider the set

$$S_a^{m-h} = \Sigma_a \cap \{\mathbf{x} \in \mathbb{R}^n : M_1 \geqslant x_1 \geqslant \ldots x_{m-h} \geqslant m_1, M_2 \geqslant x_{m-h+1} \geqslant \ldots x_m \geqslant m_2\}.$$

Applying Corollaries 3 and 10 we can compute maximal and minimal elements of S_a^{m-h} with respect to the majorization order and from (13) we obtain:

$$\frac{\left\|\mathbf{x}_*(S_a^{m-h})\right\|_2^2 - \sum_{i=1}^{n} d_i^3}{2} \leqslant S(G) \leqslant \frac{\left\|\mathbf{x}^*(S_a^{m-h})\right\|_2^2 - \sum_{i=1}^{n} d_i^3}{2}, \tag{15}$$

where $\|\cdot\|_2$ stands for the euclidean norm.

In spite of inequalities (5) and (12), these bounds can't be worse than those in [7], and they are often sharper.

It is noteworthy that both equalities in (15) are attained if and only if the set $S_a^{[h]}$ reduces to a singleton, that is, by Remark 5, $m_i = M_i, i = 1,2$.

The condition $m_2 = 1 + d_{n-h} = M_2 = 1 + d_1$ implies that in $G = (V,E)$ all non-pendant vertices have the same degree. Some examples of this kind of graphs are:

$i)$ all trees with degree sequence

$$\pi = \left(\underbrace{k,\ldots,k}_{r}, \underbrace{1,\ldots,1}_{rk-2r+2}\right), \tag{16}$$

including, as particular case, for $k = 2$, the path.

$ii)$ graphs obtained by adding the same number s of pendant vertices to each vertex of a $k-$regular graph on r vertices, being kr even, $2 \leqslant k \leqslant r-1$, i.e.,

$$\pi = \left(\underbrace{k+s,\ldots,k+s}_{r}, \underbrace{1,\ldots,1}_{sr}\right).$$

Computing $S(G)$, from Remark 5 and (15), we get $k(2kr-2r-k+2)$ and $\frac{1}{2}r\left(2s+ks+k^2\right)(k+s)$ respectively.

In the following we provide some significant examples, computing bounds for graphs belonging to C_π and satisfying (14). Furthermore, a comparison with some other known bounds (see [5], [6], [17], [25] and [26]) are provided.

EXAMPLE 1. Let us consider the classes of trees $T_{t,s}$ with degree sequences π_i $(i = 1,2,3)$ given by:

$i)$ $\pi_1 = \left(t, \underbrace{s,\ldots,s}_{t}, \underbrace{1,\ldots,1}_{t(s-1)}\right)$, $2 \leqslant s < t < 2s$

$ii)$ $\pi_2 = \left(\underbrace{s,\ldots,s}_{t}, t, \underbrace{1,\ldots,1}_{t(s-1)}\right)$, $s > t \geqslant 2$

$iii)$ $\pi_3 = \left(\underbrace{t,\ldots,t}_{t+1}, \underbrace{1,\ldots,1}_{t(t-1)} \right)$, $t \geqslant 2$

Case $i)$.

$M_1 = t+s$	$m_1 = 2s$
$M_2 = t+1$	$m_2 = s+1$
$m = ts$	$h = t(s-1)$

Applying Corollary 3 and Remark 4 it follows that:

$$\mathbf{x}^*(T_{t,s}) = \left[\underbrace{(t+s),\ldots,(t+s)}_{t}, \underbrace{(s+1),\ldots,(s+1)}_{st-t} \right]$$

while from (10), (11) and Remark 12 we get

$$\mathbf{x}_*(T_{t,s}) = \begin{cases} \left[\underbrace{2s,\ldots,2s}_{t}, \underbrace{s+2,\ldots,s+2}_{t(t-s)}, \underbrace{s+1,\ldots,s+1}_{t(2s-t-1)} \right] & \text{if } t < 2s-1 \\ \left[\underbrace{2s,\ldots,2s}_{t}, \underbrace{s+2,\ldots,s+2}_{st-t} \right] & \text{if } t = 2s-1 \end{cases}. \tag{17}$$

Taking into account (15), the following inequalities hold:

$$\begin{cases} \frac{1}{2}t\left(3t-t^2-5s+2st+3s^2\right) \leqslant S(T_{t,s}) \leqslant ts(s+t-1) & \text{if } t < 2s-1 \\ \frac{1}{2}(2s-1)\left(3s+3s^2-4\right) \leqslant S(T_{t,s}) \leqslant s(2s-1)(3s-2) & \text{if } t = 2s-1 \end{cases}. \tag{18}$$

We note that in (17) the right-hand equality holds if $T_{t,s}$ is the tree obtained by the union of t stars, each one of order s (see Figure 1).

Case $ii)$.

$M_1 = 2s$	$m_1 = t+s$
$M_2 = s+1$	$m_2 = t+1$
$m = ts$	$h = t(s-1)$

By Corollary 3 follows

$$\mathbf{x}^*(T_{t,s}) = \left[\underbrace{2s,\ldots,2s}_{t}, \underbrace{(s+1),\ldots,(s+1)}_{st-2t}, \underbrace{(t+1),\ldots,(t+1)}_{t} \right]$$

while from Remark (11) we get

$$\mathbf{x}_*(T_{t,s}) = \left[\underbrace{s+t,\ldots,s+t}_{t}, \underbrace{(s+1),\ldots,(s+1)}_{st-t} \right].$$

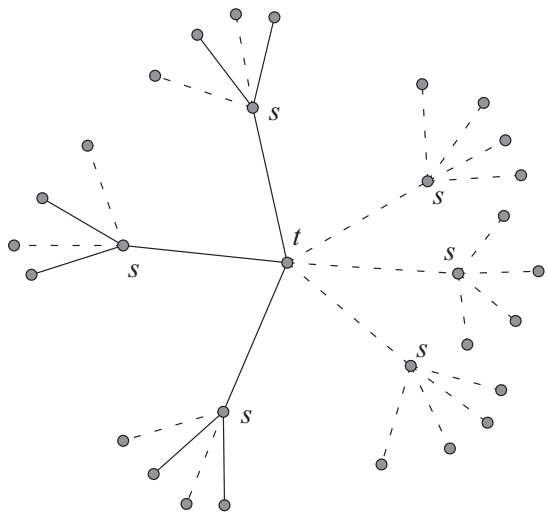

Figure 1: *Example illustrating tree* $T_{t,s}$ *for* $2 \leqslant s < t < 2s$.

Taking into account (15), the following inequalities hold:

$$ts(s+t-1) \leqslant S(T_{t,s}) \leqslant t(t-2s+2s^2) \tag{19}$$

We note that the left-hand equality holds if $T_{t,s}$ is the tree obtained by the union of t stars each one of order s (see Figure 2).

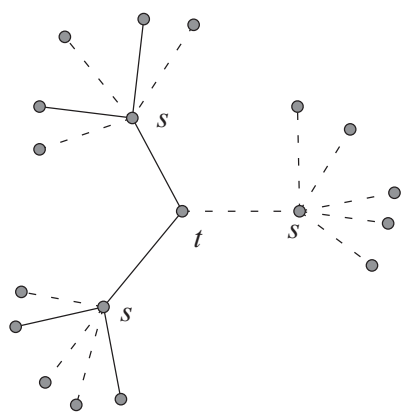

Figure 2: *Example illustrating tree* $T_{t,s}$ *for* $s > t \geqslant 2$.

Case $iii)$. This is a particular case of (16), for $k = t$ and $r = t+1$, such that

$$S(T_{t,s}) = 2t^3 - t^2. \tag{20}$$

Finally we observe that for the class of trees with degree sequence π_1, π_2 or π_3, our upper bounds always perform better than those in [6]. Indeed, in the presence of pendant vertices and with $m = ts$ and $n = ts + 1$, the bound in [6] becomes:

$$S(G) \leqslant 2m^2 - (n-1)m = t^2 s^2 \tag{21}$$

which is always greater than the upper bound in (18), (19), (20).

EXAMPLE 2. Let us consider a unicyclic graph G, i.e., a graph with $n = m$ having the following degree sequence

$$\pi = (3,3,3,3,2,2,2,2,2,1,1,1,1).$$

Being (14) satisfied, by Remark 12, (15) gives

$$64 \leqslant S(G) \leqslant 74.$$

The comparison (see Table 1) with bounds in [5], [6], [7], [17] and [25] shows that our bounds always perform better. Indeed, we obtain:

Bounds	Lower	Upper
ours	64	74
[5]	x	277.9
[6]	x	182
[7]	61.462	77
[17]	28	76
[25]	64	92

Table 1: *Lower and upper bounds for* $S(G)$

EXAMPLE 3. Consider the graphs G and H with degree sequences $\pi_1 = (3,2,2,1)$ and $\pi_2 = (3,3,3,3,2,1,1)$ respectively, as in Examples 2.2 and 2.3 in [7]. Besides the bounds discussed in [7], we add the comparison with those in [6], [25] and [26]. Observing that G is a unicyclic graph $(m = n)$ and H is a bicyclic graph $(m = n+1)$, both with pendant vertices, bounds in [25] and [26] can also be respectively properly applied.

Bounds for $S(G)$ are shown in Table 2.

Our bounds are sharper than [5], [7] and [17]. The best one is provided by [25] and has been specifically constructed for this class of graph.

Bounds for $S(G)$ are shown in Table 3.

Note that our bounds perform better than all the others and in particular better than [26] which is properly designed for bicyclic graphs as H is.

Ref.	Lower	Upper
ours	19	20
[5]	x	22.511
[6]	x	20
[7]	18.5	20
[17]	18	22
[25]	19	19

Table 2: *Lower and upper bounds for* $S(G)$.

ref.	lower	upper
ours	54	58
[5]	x	99.75
[6]	x	80
[7]	51.25	58
[17]	40	59
[26]	50	68

Table 3: *Lower and upper bounds for* $S(H)$.

6. Conclusion

The purpose of this paper is to establish maximal and minimal vectors with respect to the majorization order under sharper constraints than those presented by Marshall and Olkin in [18]. We have shown how these results can provide a simple methodology for localizing the second Zagreb index of a particular class of graphs. Some numerical examples have been discussed, showing that our bounds often provide sharper bounds than those in the literature. Moreover, in network analysis, there are a variety of potential applications for this kind of approach, considering other topological indices which can be defined by a suitable Schur-convex function.

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Monica Bianchi
Department of Mathematics and Econometrics
Catholic University
Milan, Italy
e-mail: monica.bianchi@unicatt.it

Alessandra Cornaro
Department of Mathematics and Econometrics
Catholic University
Milan, Italy
e-mail: alessandra.cornaro@unicatt.it

Anna Torriero
Department of Mathematics and Econometrics
Catholic University
Milan, Italy
e-mail: anna.torriero@unicatt.it