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New bounds of degree-based topological indices for some classes of c-cyclic graphs

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ABSTRACT

Making use of a majorization technique for a suitable class of graphs, we derive upper and lower bounds for some topological indices depending on the degree sequence over all vertices, namely the first general Zagreb index and the first multiplicative Zagreb index. Specifically, after characterizing c-cyclic graphs ($0 \leq c \leq 6$) as those whose degree sequence belongs to particular subsets of $\mathbb{R}^n$, we identify the maximal and minimal vectors of these subsets with respect to the majorization order. This technique allows us to determine lower and upper bounds of the above indices recovering some existing results in the literature as well as obtaining new ones.

1. Introduction

Many topological indices in Mathematical Chemistry are based on the degree sequence of a finite graph $G = (V, E)$ over all vertices. One of the most famous among these is the *first Zagreb index* defined as $M_1(G) = \sum_{i=1}^{n} d_i^2$ where $d_i (i = 1, \ldots, n)$ stands for the degree of the vertex i and $n = |V|$ (see [21,20,27]). The notion of $M_1(G)$ was extended by Li and Zheng [25] as the *first general Zagreb index* $M_1^{\alpha}(G) = \sum_{i=1}^{n} d_i^{\alpha}$, for α an arbitrary real number different from 0 and 1, that coincides with the zeroth-order general Randić index (see [23]). For $\alpha = 2$ we recover the first Zagreb index while for $\alpha = -1$ we get the *inverse degree* $\rho(G) = M_1^{-1} = \sum_{j=1}^{n} \frac{1}{d_j}$ which has generated increased attentions motivated by conjectures of the computer program Graffiti (see [15]). We refer to [1,11,14,16,22,30] for additional references.

In this paper we are concerned precisely with those indices depending on the degree sequence over all vertices of G, for which we adopt a unified approach aimed to determine new lower and upper bounds. This fruitful methodology, synthetically introduced in Section 2, is based on the majorization order and Schur-convexity [26], and has already been used by some of the authors [7,17] in other contexts, as well as for localizing some relevant topological indicators of a graph [5,6,2–4,9,10], which is also the aim of the present article. We restrict our attention to a particular class of graphs, the c-cyclic graphs for $0 \leq c \leq 6$. In Section 3 we provide a new characterization of c-cyclic graphs, needed to determine their extremal degree sequences with respect to the majorization order discussed in Section 4. In Section 5 we determine upper and lower bounds for some degree-based topological indices. Section 6 concludes with a summary and some final comments.

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2. Notations and preliminaries results on majorization

In this section we recall some basic notions on majorization, referring for more details to [5,26]. In the sequel we denote by $[x_1^{\alpha_1}, x_2^{\alpha_1}, \dots, x_p^{\alpha_p}]$ a vector in $\mathbb{R}^n$ with α_i components equal to x_i, where $\sum_{i=1}^{p} \alpha_i = n$. If $\alpha_i = 1$ we use for convenience x_i instead of x_i^1, while x_i^0 means that the component x_i is not present.

Definition 1. Given two vectors $\mathbf{y}, \mathbf{z} \in D = \{\mathbf{x} \in \mathbb{R}^n : x_1 \geq x_2 \geq \cdots \geq x_n\}$, the majorization order $\mathbf{y} \trianglelefteq \mathbf{z}$ means:

$$\begin{cases} \langle \mathbf{y}, \mathbf{s^k} \rangle \leq \langle \mathbf{z}, \mathbf{s^k} \rangle, & k = 1, \dots, (n-1) \\ \langle \mathbf{y}, \mathbf{s^n} \rangle = \langle \mathbf{z}, \mathbf{s^n} \rangle, & \end{cases}$$

where $\langle \cdot, \cdot \rangle$ is the inner product in $\mathbb{R}^n$ and $\mathbf{s^j} = [1^j, 0^{n-j}],\ j = 1, 2, \dots, n$.

In what follows we will consider some subsets of

$$\Sigma_a = D \cap \{\mathbf{x} \in \mathbb{R}_+^n : \langle \mathbf{x}, \mathbf{s^n} \rangle = a\},$$

where a is a positive real number. Given a closed subset $S \subseteq \Sigma_a$, a vector $\mathbf{x}^*(S) \in S$ is said to be maximal for S with respect to the majorization order if $\mathbf{x} \trianglelefteq \mathbf{x}^*(S)$ for each $\mathbf{x} \in S$. Analogously, a vector $\mathbf{x}_*(S) \in S$ is said to be minimal for S with respect to the majorization order if $\mathbf{x}_*(S) \trianglelefteq \mathbf{x}$ for each $\mathbf{x} \in S$. Notice that if $S \subseteq T$, then $\mathbf{x}^*(S) \trianglelefteq \mathbf{x}^*(T)$ and $\mathbf{x}_*(T) \trianglelefteq \mathbf{x}_*(S)$.

In [5] some of the authors derived the maximal and minimal elements, with respect to the majorization order, of the set

$$S_a = \Sigma_a \cap \left\{\mathbf{x} \in \mathbb{R}^n : M_i \geq x_i \geq m_i,\ i = 1, \dots, n\right\}, \tag{1}$$

where $\mathbf{m} = [m_1, m_2, \dots, m_n]$ and $\mathbf{M} = [M_1, M_2, \dots, M_n]$ are two fixed vectors arranged in nonincreasing order with $0 \leq m_i \leq M_i$, for all $i = 1, \dots, n$, and a is a positive real number such that $\langle \mathbf{m}, \mathbf{s^n} \rangle \leq a \leq \langle \mathbf{M}, \mathbf{s^n} \rangle$. For the sake of completeness we recall the main results we will use in Section 4. We start discussing the maximal element. Let $\mathbf{v^j} = [0^j, 1^{n-j}]$, $j = 0, \dots, n$.

Theorem 2. *Let $k \geq 0$ be the smallest integer such that*

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

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

$$\mathbf{x}^*(S_a) = [M_1, M_2, \dots, M_k, \theta, m_{k+2}, \dots, m_n]. \tag{3}$$

From this general result, the maximal element of particular subsets of S_a can be deduced. In what follows we will often focus on sets of the type

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

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

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

In this case, given $a^* = hM_1 + (n-h)m_2$, let

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

where $\lfloor x \rfloor$ denote the integer part of the real number x. In Corollary 3 in [5] it has been shown that

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

where θ is evaluated in order to entail $\mathbf{x}^*(S_a^{[h]}) \in \Sigma_a$.

The computation of the minimal element of the set S_a is more tangled. The minimal element of Σ_a is $x_*(\Sigma_a) = [(\frac{a}{n})^n]$. If it belongs to S_a then it is its minimal element, too. Otherwise we will use the following theorem

Theorem 3. *Let $k \geq 0$ and $d \geq 0$ be the smallest integers such that*

(1) $k + d < n$

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

Then

$$\mathbf{x}_*(S_a) = [m_1, \dots, m_k, \rho^{n-d-k}, M_{n-d+1} \cdots, M_n].$$