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The Nordhaus–Gaddum-type inequalities for the Zagreb index and co-index of graphs

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ABSTRACT

Let $k \geq 2$ be an integer, a *k-decomposition* $(G_1, G_2, \dots, G_k)$ of the complete graph K_n is a partition of its edge set to form k spanning subgraphs $G_1, G_2, \dots, G_k$. In this contribution, we investigate the Nordhaus–Gaddum-type inequality of a k-decomposition of K_n for the general Zagreb index and a 2-decomposition for the Zagreb co-indices, respectively. The corresponding extremal graphs are characterized.

1. Introduction

Throughout this paper, we consider only finite simple connected graphs, i.e., connected graphs without loops and multiple edges. Let G be a graph with vertex set $V(G)$ and edge set $E(G)$, and $|G|$ and $|E|$ denote its order and size, respectively.

The *degree* of a vertex u is the number of edges incident to it in G, denoted by $\deg_G(u)$, or $\deg(u)$ when no confusion is possible. Such a minimal number is called the minimal degree $\delta(G)$ of G. The *distance* $d_G(u, v)$ between vertices u and v is the length of the shortest path connecting them in G. Such maximal distance between any two vertices is called the *diameter* $\mathrm{diam}(G)$ of G. The *complement* of G, denoted by $\overline{G}$, is a simple graph on the same set of vertices $V(G)$ in which two vertices u and v are adjacent if and only if they are not adjacent in G. For the sake of simplicity, we let $m = |E|$ and $\overline{m} = |\overline{E}|$, hence $\overline{m} + m = \binom{n}{2}$, and the degree of the same vertex u in $\overline{G}$ is then given by $\deg_{\overline{G}}(u) = n - 1 - \deg_G(u)$, respectively.

Let $k \geq 2$ be an integer, a *k-decomposition* $\mathcal{D}_k = (G_1, G_2, \dots, G_k)$ of the complete graph K_n is a partition of its edge set to form k spanning subgraphs $G_1, G_2, \dots, G_k$. In other words, graphs $G_1, G_2, \dots, G_k$ are pairwise edge disjoint, such that $\cup_{i=1}^{k} E(G_i) = E(K_n)$ and $V(G_i) = V(K_n)$ $(i = 1, 2, \dots, k)$, each of the G_i is said to be a *cell* of K_n. In particular, (G_1, G_2) is a 2-decomposition of the complete graph K_n if and only if G_1 is the complement of G_2. Other terminology and notations needed will be introduced as it naturally occurs in the following and we use [1] for those not defined here.

A graph invariant is a function on a graph that does not depend on the labeling of its vertices. Hundreds of graph invariants have been considered in quantitative structure–activity relationship (QSAR) and quantitative structure–property relationship (QSPR) researches. We refer the reader to monograph [2]. Among those useful invariants, we will present several ones that are relevant for our contribution.

The Zagreb indices have been introduced in 1972 in the report of Gutman and Trinajstić on the topological basis of the π-electron energy—two terms appeared in the topological formula for the total π-energy of alternant hydrocarbons, which

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were in 1975 used by Gutman et al. as branching indices, and later employed as molecular descriptors in QSAR and QSPR. The first Zagreb index equals to the sum of squares of the vertex degrees:

$$M_1(G) = \sum_{u \in V(G)} \left[\deg(u)\right]^2$$

and the second Zagreb index equals to the sum of product of degree of pairs of adjacent vertices:

$$M_2(G) = \sum_{uv \in E(G)} \left[\deg(u)\deg(v)\right].$$

We encourage the interested reader to [3–5] for more information and details.

The general Randić index was proposed 26 years later by Bollobás and Erdös [6] and Amic [7] independently, for a parameter $\alpha \in R - \{0\}$:

$$R_\alpha(G) = \sum_{uv \in E(G)} \left[\deg(u)\deg(v)\right]^\alpha.$$

This index generalized the second Zagreb index and it has been extensively studied by both mathematicians and theoretical chemists [8]. Many important mathematical properties have been established in [9].

By observing the common appearance of the general Randić index and the second Zagreb index, Li and Zhao [10] introduced the first general Zagreb index:

$$M_\alpha(G) = \sum_{u \in V(G)} \left[\deg(u)\right]^\alpha.$$

The first and second Zagreb co-indices are a pair of recently introduced graph invariants [11], which were originally defined as follows:

$$\overline{M}_1(G) = \sum_{uv \notin E(G)} \left[\deg(u) + \deg(v)\right] \quad \text{and} \quad \overline{M}_2(G) = \sum_{uv \notin E(G)} \left[\deg(u)\deg(v)\right].$$

The Zagreb co-indices can be viewed as sums of contributions depend on the degrees of *non-adjacent* vertices over all edges of a given graph, and we encourage the interested reader to [12,13] for some recent results on Zagreb co-indices.

Let I be an invariant of G, we denote by $\bar{I}$ the same invariant but in $\overline{G}$. Nordhaus and Gaddum-type inequalities for the graph invariant I are as follows:

$$L_1(n) \le I + \bar{I} \le U_1(n) \quad \text{and} \quad L_2(n) \le I \cdot \bar{I} \le U_2(n),$$

where $L_1(n)$ and $L_2(n)$ are the lower bounding functions of the order n, and $U_1(n)$ and $U_2(n)$ upper bounding functions of the order n. These types of inequalities are named after Nordhaus and Gaddum [14], who were the first authors to give such relations, namely, the following theorem.

Theorem A (*Nordhaus and Gaddum [14]*). *Let G be a graph with order n and $\overline{G}$ be its complement. Then*

$$2\sqrt{n} \le \chi + \overline{\chi} \le n + 1 \quad \textit{and} \quad n \le \chi \cdot \overline{\chi} \le \left\lfloor \left(\frac{n+1}{2}\right)^2 \right\rfloor,$$

where χ denotes the chromatic number of graph G.

The extremal graphs for the inequalities in Theorem A were characterized by Finck. Since then many graph theorists have been interested in finding such inequalities for various graph invariants. We refer the reader to [15] for review of early results of Nordhaus–Gaddum type.

The following result is a Nordhaus–Gaddum type inequality of k-decomposition of K_n for the diameter [16].

Theorem B (*An et al. [16]*). *Let $\mathcal{D}_k = (G_1, G_2, \ldots, G_k)$ be a k-decomposition of the complete graph K_n. Then for any sufficiently large n with respect to k, we have*

$$2k \le \mathrm{diam}(G_1) + \mathrm{diam}(G_2) + \cdots + \mathrm{diam}(G_k) \le (k-1)(n-1) + 2.$$

The lower and upper bounds are sharp.

Motivated by Theorems A and B, in this paper we consider the Nordhaus–Gaddum-type inequality of a k-decomposition of K_n for the general Zagreb index in Section 3. The Nordhaus–Gaddum-type inequalities for the first and second Zagreb co-indices of a 2-decomposition of K_n are also investigated in Section 4.

Table 1
The $\overline{M}_1$- and $\overline{M}_2$-values of some graph classes.

G	K_n	$\overline{K}_n$	P_n	C_n	Q_k	$K_{s,t}$
$\overline{M}_1$	0	0	$2n^2 - 8n + 8$	$2n^2 - 6n$	$k2^k(2^k - k - 1)$	$st(s + t - 2)$
$\overline{M}_2$	0	0	$2n^2 - 10n + 13$	$2n^2 - 6n$	$k^2 2^{k-1}(2^k - k - 1)$	$s^2t^2 - 2^{-1}s^2t - 2^{-1}st^2$

2. Preliminary lemmas

In this section, we list or prove some lemmas as basic but necessary preliminaries, which will be used in the subsequent proofs.

Recall that if a real valued function $G(x)$ defined on an interval has a second derivative $G''(x)$, then a necessary and sufficient condition for it to be convex (concave, resp.) on that interval is that $G''(x) \geq 0$ ($G''(x) \leq 0$, resp.).

The fundamental discrete Jensen's inequalities show the following lemma.

Lemma 2.1 (*Hairer and Wanner [17]*)**.** *Let $\mathbb{C}$ be a convex subset of a real vector space $\mathbb{X}$, let $x_i \in \mathbb{C}$ and $\sigma_i \geq 0$ $(i = 1, 2, \dots, n)$ with $\sum_{i=1}^{n} \sigma_i = 1$. Then*

$$\text{(a) } \Phi\left(\sum_{i=1}^{k} \sigma_i x_i\right) \leq \sum_{i=1}^{k} \sigma_i \Phi(x_i) \quad \text{if } \Phi(x) : \mathbb{C} \to \mathbb{R} \text{ is a convex function}$$

$$\text{(b) } \Phi\left(\sum_{i=1}^{k} \sigma_i x_i\right) \geq \sum_{i=1}^{k} \sigma_i \Phi(x_i) \quad \text{if } \Phi(x) : \mathbb{C} \to \mathbb{R} \text{ is a concave function.}$$

The following conclusion is the well-known Newton's binomial theorem in integrable-differential.

Lemma 2.2 (*Generalized Binomial Theorem of Newton [18]*)**.** *For any real number α, we have for $x(|x| < 1)$,*

$$(1 + x)^{\alpha} = \sum_{r=0}^{\infty} \binom{\alpha}{r} x^r$$

where

$$\binom{\alpha}{r} = \frac{\alpha(\alpha - 1) \cdots (\alpha - r + 1)}{r!}.$$

Ashrafi and his co-workers established the following relations in [12].

Lemma 2.3 (*Ashrafi et al. [12]*)**.** *Let G be a graph with order n and size m. Then $\overline{M}_1(G) = 2m(n - 1) - M_1(G)$.*

Lemma 2.4 (*Ashrafi et al. [12]*)**.** *Let G be a graph with order n and size m. Then $\overline{M}_2(G) = M_2(\overline{G}) - (n - 1)M_1(\overline{G}) + \overline{m}(n - 1)^2$.*

Lemma 2.5 (*Zhang and Wu [19]*)**.** *Let G be a graph with order n. Then $2^{-2\alpha-1}n(n-1)^{2\alpha+1} \leq R_{\alpha}(G) + R_{\alpha}(\overline{G}) \leq 2^{-1}n(n-1)^{2\alpha+1}$ for $\alpha \in (0, +\infty)$.*

Lemma 2.6. *Let G be a graph with two non-adjacent vertices $u, v \in V(G)$. Then $M_{\alpha}(G+uv) > M_{\alpha}(G)$ for $\alpha \in (0, 1) \cup (1, +\infty)$ and $M_{\alpha}(G + uv) < M_{\alpha}(G)$ for $\alpha \in (-\infty, 0)$.*

Proof. Let $W = V - \{u, v\}$; then by definition and Lagrange's mean-value theorem

$$\begin{aligned} &M_{\alpha}(G + uv) - M_{\alpha}(G) \\ &\quad = \sum_{u \in W} \left[\deg_G(u)\right]^{\alpha} + \left[\deg_G(u) + 1\right]^{\alpha} + \left[\deg_G(v) + 1\right]^{\alpha} - \sum_{u \in W} \left[\deg_G(u)\right]^{\alpha} - \left[\deg_G(u)\right]^{\alpha} - \left[\deg_G(v)\right]^{\alpha} \\ &\quad = \left[\deg_G(u) + 1\right]^{\alpha} - \left[\deg_G(u)\right]^{\alpha} + \left[\deg_G(v) + 1\right]^{\alpha} - \left[\deg_G(v)\right]^{\alpha} = \alpha\left[\xi^{\alpha-1} + \eta^{\alpha-1}\right], \end{aligned}$$

where $\deg_G(u) < \xi < \deg_G(u) + 1$ and $\deg_G(v) < \eta < \deg_G(v) + 1$. This completes the proof. □

Before concluding this section, we present the explicit formulas of several families of graphs for the first and second co-indices in terms of the number of vertices.

Let K_n, P_n and C_n be the complete, path and cycle graph with order n. Let $K_{s,t}$ be the complete bipartite graph with s and t vertices in its two partite sets, and Q_k, $k \geq 2$, the hypercube graph as usual.

3. The general Zagreb index of graphs

Let k be an positive integer not less than 2; we define two classes

$$\mathcal{P}_k^n = \{\mathcal{D}_k | \mathcal{D}_k = (G_1, G_2, \ldots, G_k) \text{ is a } k\text{-decomposition of } K_n \text{ such that each cell } G_i \text{ is connected and } \delta(G_i) \geq 2\}$$

and

$$\mathcal{Q}_k^n = \{\mathcal{D}_k | \mathcal{D}_k = (G_1, G_2, \ldots, G_k) \text{ is a } k\text{-decomposition of } K_n \text{ such that each cell } G_i \text{ is connected and } \delta(G_i) \geq 1\}.$$

Now we state our main result of this section.

Theorem 3.1. *Let $k \geq 2$ and t be integers, $D_k = (G_1, G_2, \ldots, G_k)$ be a k-decomposition of K_n. Then*

(a) $n(n-1)^\alpha k^{1-\alpha} \leq M_\alpha(G_1) + M_\alpha(G_2) + \cdots + M_\alpha(G_k) \leq n(n-1)^\alpha, \quad \text{if } \alpha > 1$

(b) $n(n-1)^\alpha \leq M_\alpha(G_1) + M_\alpha(G_2) + \cdots + M_\alpha(G_k) \leq n(n-1)^\alpha k^{1-\alpha}, \quad \text{if } 0 < \alpha < 1$

(c) $n(n-1)^\alpha k^{1-\alpha} \leq M_\alpha(G_1) + M_\alpha(G_2) + \cdots + M_\alpha(G_k) \leq kn, \quad \text{if } \alpha < 0 \text{ and } \mathcal{D}_k \in \mathcal{Q}_k^n$

(d) $n(n-1)^\alpha k^{1-\alpha} \leq M_\alpha(G_1) + M_\alpha(G_2) + \cdots + M_\alpha(G_k) \leq n\big[t + t(n-2)^\alpha\big], \quad \text{if } \alpha < 0,\ k = 2t \text{ and } \mathcal{D}_k \in \mathcal{P}_k^n$

(e) $n(n-1)^\alpha k^{1-\alpha} \leq M_\alpha(G_1) + M_\alpha(G_2) + \cdots + M_\alpha(G_k) \leq n\big[t + (t+1)(n-2)^\alpha\big], \quad \text{if } \alpha < 0,\ k = 2t+1 \text{ and } \mathcal{D}_k \in \mathcal{P}_k^n.$

Proof. From the definition of the general Zagreb index, we have

$$\begin{aligned} M_\alpha(G_1) + M_\alpha(G_2) + \cdots + M_\alpha(G_k) &= \sum_{u \in V(G_1)} [\deg_{G_1}(u)]^\alpha + \sum_{u \in V(G_2)} [\deg_{G_2}(u)]^\alpha + \cdots + \sum_{u \in V(G_k)} [\deg_{G_k}(u)]^\alpha \\ &= \sum_{u \in V(G)} \Big[[\deg_{G_1}(u)]^\alpha + [\deg_{G_2}(u)]^\alpha + \cdots + [\deg_{G_k}(u)]^\alpha\Big]. \end{aligned}$$

Let $\rho(x) = x^\alpha$ for $x \geq 0$ and $\alpha \in R - \{0, 1\}$. Easy verification shows that $\rho(x)$ is a convex function if $\alpha \in (-\infty, 0) \cup (1, +\infty)$ and is a concave one otherwise. We distinguish the following three separate cases.

Case 1. $\alpha > 1$.

Noticing $\rho(x)$ is a convex function in the case of $\alpha > 1$, and then we have by Lemma 2.1

$$[\deg_{G_1}(u)]^\alpha + [\deg_{G_2}(u)]^\alpha + \cdots + [\deg_{G_k}(u)]^\alpha \geq k\left[\frac{\deg_{G_1}(u) + \deg_{G_2}(u) + \cdots + \deg_{G_k}(u)}{k}\right]^\alpha = \frac{(n-1)^\alpha}{k^{\alpha-1}},$$

which implies that

$$M_\alpha(G_1) + M_\alpha(G_2) + \cdots + M_\alpha(G_k) \geq \frac{n(n-1)^\alpha}{k^{\alpha-1}}.$$

On the other hand, $\deg_{G_1}(u) + \deg_{G_2}(u) + \cdots + \deg_{G_k}(u) = n - 1$ and

$$\begin{aligned} \frac{\sum_{i=1}^{k}\big[\deg_{G_i}(u)\big]^\alpha}{\Big[\deg_{G_1}(u) + \deg_{G_2}(u) + \cdots + \deg_{G_k}(u)\Big]^\alpha} &= \sum_{i=1}^{k}\left[\frac{\deg_{G_i}(u)}{\deg_{G_1}(u) + \deg_{G_2}(u) + \cdots + \deg_{G_k}(u)}\right]^\alpha \\ &\leq \sum_{i=1}^{k}\left[\frac{\deg_{G_i}(u)}{\deg_{G_1}(u) + \deg_{G_2}(u) + \cdots + \deg_{G_k}(u)}\right]^1 = \frac{n-1}{n-1} = 1. \end{aligned}$$

Then, we have

$$[\deg_{G_1}(u)]^\alpha + [\deg_{G_2}(u)]^\alpha + \cdots + [\deg_{G_k}(u)]^\alpha \leq \Big[\deg_{G_1}(u) + \deg_{G_2}(u) + \cdots + \deg_{G_k}(u)\Big]^\alpha.$$

This gives us the proof of (a)

$$M_\alpha(G_1) + M_\alpha(G_2) + \cdots + M_\alpha(G_k) \leq \sum_{u \in V(G)}\Big[\deg_{G_1}(u) + \deg_{G_2}(u) + \cdots + \deg_{G_k}(u)\Big]^\alpha = n(n-1)^\alpha.$$

Case 2. $0 < \alpha < 1$.

By analogous reasoning as used in Case 1 we can prove (b), and we omit the proof here, respectively.

Case 3. $\alpha < 0$.

For sake of simplicity, let $x_1 = \deg_{G_1}(u), x_2 = \deg_{G_2}(u), \ldots, x_k = \deg_{G_k}(u)$. Easy verification shows that each cell G_i must be connected when $\alpha < 0$, otherwise there would produce a contradiction to the definition of M_α. Without loss of generality we assume $x_1 \geq x_2 \geq \cdots \geq x_k \geq 1$.

Subcase 3.1. $\mathcal{D}_k \in \mathcal{Q}_k^n$.

Let $\Phi_1(x_1, x_2, \ldots, x_k) = x_1^\alpha + x_2^\alpha + \cdots + x_k^\alpha$. If $x_1 \geq x_2 \geq \cdots \geq x_{k-l} \geq 2 > x_{k-l+1} = \cdots = x_k = 1$; then

$$\begin{aligned}\Phi_1(x_1, x_2, \ldots, x_k) &= x_1^\alpha + x_2^\alpha + \cdots + x_{k-l}^\alpha + x_{k-l+1}^\alpha + x_{k-l+2}^\alpha + \cdots + x_k^\alpha \\ &= x_1^\alpha + x_2^\alpha + \cdots + x_{k-l}^\alpha + \underbrace{1^\alpha + 1^\alpha + \cdots + 1^\alpha}_{l \text{ times}} \quad (\text{Since } \rho(x) = x^\alpha \text{ is decreasing for } \alpha < 0) \\ &< \underbrace{1^\alpha + 1^\alpha + \cdots + 1^\alpha}_{k-l \text{ times}} + \underbrace{1^\alpha + 1^\alpha + \cdots + 1^\alpha}_{l \text{ times}} = k,\end{aligned}$$

this implies that $M_\alpha(G_1) + M_\alpha(G_2) + \cdots + M_\alpha(G_k) < kn$.

If $x_1 = x_2 = \cdots = x_k$, then $\Phi_1(x_1, x_2, \ldots, x_k) = x_1^\alpha + x_2^\alpha + \cdots + x_k^\alpha = k$. Easy verification shows that there exists a k-decomposition $(\frac{n}{2}K_2, \frac{n}{2}K_2, \ldots, \frac{n}{2}K_2)$ of K_n which attains the maximum M_α-value kn when n is even. This completes the upper bound of (c). Note that $\rho(x)$ is a convex function when $\alpha < 0$, then by Lemma 2.1 we obtain the lower bound of (c).

Subcase 3.2. $\mathcal{D}_k \in \mathcal{P}_k^n$.

Let $\Phi_2(x_1, x_2, \ldots, x_k) = \Phi_1(x_1 + 1, \ldots, x_i + 1, x_{i+1} - 1, \ldots, x_{2i+1} - 1, x_{2i+2}, \ldots, x_k)$.

We first need to prove the following claim.

Claim 1. $\Phi_1(x_1, x_2, \ldots, x_k) < \Phi_2(x_1, x_2, \ldots, x_k)$.

Proof of Claim 1. By using Lagrange's mean-value theorem and Lemma 2.6, we conclude that

$$\begin{aligned}&\Phi_2(x_1, x_2, \ldots, x_k) - \Phi_1(x_1, x_2, \ldots, x_k) \\ &\quad = \left[(x_1+1)^\alpha + \cdots + (x_i+1)^\alpha + (x_{i+1}-1)^\alpha + \cdots + (x_{2i}-1)^\alpha + x_{2i+1}^\alpha + x_{2i+2}^\alpha + \cdots + x_k^\alpha\right] \\ &\qquad - \left[x_1^\alpha + x_2^\alpha + \cdots + x_i^\alpha + x_{i+1}^\alpha + x_{i+2}^\alpha + \cdots + x_{2i}^\alpha + x_{2i+1}^\alpha + x_{2i+2}^\alpha + x_{2i+3}^\alpha + \cdots + x_k^\alpha\right] \\ &\quad = \left[(x_1+1)^\alpha - x_1^\alpha\right] + \cdots + \left[(x_i+1)^\alpha - x_i^\alpha\right] + \left[(x_{i+1}-1)^\alpha - x_{i+1}^\alpha\right] + \cdots + \left[(x_{2i}-1)^\alpha - x_{2i}^\alpha\right] \\ &\quad = \alpha\xi_1^{\alpha-1} + \alpha\xi_2^{\alpha-1} + \cdots \alpha\xi_i^{\alpha-1} - \alpha\eta_1^{\alpha-1} - \alpha\eta_2^{\alpha-1} - \cdots - \alpha\eta_i^{\alpha-1} \\ &\quad = \alpha\left[\left(\xi_1^{\alpha-1} - \eta_1^{\alpha-1}\right) + \left(\xi_2^{\alpha-1} - \eta_2^{\alpha-1}\right) + \cdots + \left(\xi_i^{\alpha-1} - \eta_i^{\alpha-1}\right)\right] \\ &\quad = \alpha(\alpha-1)\left[\zeta_1^{\alpha-2}(\xi_1 - \eta_1) + \zeta_2^{\alpha-2}(\xi_2 - \eta_2) + \cdots + \zeta_i^{\alpha-2}(\xi_i - \eta_i)\right],\end{aligned}$$

where $\xi_1 \in (x_1, x_1 + 1), \xi_2 \in (x_2, x_2 + 1), \ldots, \xi_i \in (x_i, x_i + 1)$; $\eta_1 \in (x_{i+1} - 1, x_{i+1}), \eta_2 \in (x_{i+2} - 1, x_{i+2}), \ldots, \eta_i \in (x_{2i} - 1, x_{2i})$; $\zeta_1 \in (\xi_1, \eta_1), \zeta_2 \in (\xi_2, \eta_2), \ldots, \zeta_i \in (\xi_i, \eta_i)$. In view of the facts that $x_1 \geq x_2 \geq \cdots \geq x_k, x_l < \xi_l < x_l + 1$ and $x_{2l} - 1 < \eta_l < x_{2l}$, we obtain $\xi_l - \eta_l > x_l - x_{2l} \geq x_l - x_l = 0$, this implies $\Phi_1(x_1, x_2, \ldots, x_k) < \Phi_2(x_1, x_2, \ldots, x_k)$ for $\alpha < 0$. □

From Claim 1 we know that the M_α-value of a graph will increase when replacing the degree consequence $(x_1, x_2, \ldots, x_k)$ by $(x_1 + 1, \ldots, x_i + 1, x_{i+1} + 1, \ldots, x_{2i+1} - 1, x_{2i+2}, \ldots, x_k)$.

To obtain the proof of (d) and (e), it is sufficient to consider the following two claims. Note that the equality $x_1 + x_2 + \cdots + x_k = n - 1$ always holds.

Claim 2. $\Phi_1(x_1, x_2, \ldots, x_k) \leq t(n-2)^\alpha + t$, *if* $k = 2t$.

Proof of Claim 2. Actually, from Claim 1 we obtain that

$$\begin{aligned}\Phi_1(x_1, x_2, \ldots, x_{2t}) &= x_1^\alpha + x_2^\alpha + \cdots + x_t^\alpha + x_{t+1}^\alpha + x_{t+2}^\alpha + \cdots + x_{2t}^\alpha \\ &\leq (x_1+1)^\alpha + (x_2+1)^\alpha + \cdots + (x_t+1)^\alpha + (x_{t+1}-1)^\alpha + (x_{t+1}-1)^\alpha + \cdots + (x_{2t}-1)^\alpha \\ &\leq (x_1+2)^\alpha + (x_2+2)^\alpha + \cdots + (x_t+2)^\alpha + (x_{t+1}-2)^\alpha + (x_{t+1}-2)^\alpha + \cdots + (x_{2t}-2)^\alpha \\ &\cdots \\ &\leq \underbrace{(n-2)^\alpha + (n-2)^\alpha + \cdots + (n-2)^\alpha}_{t \text{ times}} + \underbrace{1^\alpha + 1^\alpha + \cdots + 1^\alpha}_{t \text{ times}} \\ &= t(n-2)^\alpha + t.\end{aligned}$$

This completes the proof of Claim 2. □

Now we use Claim 2 to prove (d). By taking the sum over all vertices of G for two sides of Claim 2, we obtain the upper bound of (d). Note that $\rho(x)$ is a convex function when $\alpha < 0$, then by Lemma 2.1 we obtain the lower bound of (d).

Claim 3. $\Phi_1\big(x_1, x_2, \ldots, x_k\big) \le t(n-2)^\alpha + t,$ *if* $k = 2t + 1$.

Proof of Claim 3. By the same reasoning, one can obtain

$$\begin{aligned}
&\Phi_1\big(x_1, x_2, \ldots, x_{2t+1}\big)\\
&= x_1^\alpha + x_2^\alpha + \cdots + x_t^\alpha + x_{t+1}^\alpha + x_{t+2}^\alpha + \cdots + x_{2t}^\alpha + x_{2t+1}^\alpha\\
&\le (x_1+1)^\alpha + (x_2+1)^\alpha + \cdots + (x_t+1)^\alpha + (x_{t+1}-1)^\alpha + (x_{t+1}-1)^\alpha + \cdots + (x_{2t}-1)^\alpha + x_{2t+1}^\alpha\\
&\le (x_1+2)^\alpha + (x_2+2)^\alpha + \cdots + (x_t+2)^\alpha + (x_{t+1}-2)^\alpha + (x_{t+1}-2)^\alpha + \cdots + (x_{2t}-2)^\alpha + x_{2t+1}^\alpha\\
&\cdots\\
&\le \underbrace{(n-2)^\alpha + (n-2)^\alpha + \cdots + (n-2)^\alpha}_{t \text{ times}} + \underbrace{1^\alpha + 1^\alpha + \cdots + 1^\alpha}_{t \text{ times}} + x_{2t+1}^\alpha\\
&= t(n-2)^\alpha + t\cdot 1^\alpha + (n-2)^\alpha\\
&= (t+1)(n-2)^\alpha + t.
\end{aligned}$$

This completes the proof of Claim 3. □

Taking the sum over all vertices of G for two sides of Claim 2, we obtain the upper bound of (e). The lower bound of (e) can be verified by Lemma 2.1 since $\rho(x)$ is a convex function when $\alpha < 0$.

Note that the bounds are best possible. The upper bound of (a) and the lower bound of (b) are the same and are attained uniquely if one of the cells G_i is the complete graph K_n and the others are empty graphs with order n. On the other hand, the lower bound of (a), (c), (d) and (e) and the upper bound of (b) are the same and are attained on the $\frac{n-1}{k}$-regular graphs, since for any $n = \beta k + 1$, $\beta \ge 1$, there exist a graph G_i with G_i and all the $k-1$ graphs $G_1, G_2, \ldots, G_{i-1}, G_{i+1}, \ldots, G_k$ are $\frac{n-1}{k}$-regular and with n orders. The upper bound of (d) attained on the graph H_n is obtained from K_n by deleting a perfect matching, so this occurs only if n is even. □

The following consequence is obvious, just taking $k = 2$ in the following. Theorem 3.1.

Corollary 3.2 (*Zhang and Wu [19]*). *Let G be a graph with order n and $\overline{G}$ its complement. Then*

(a) $n(n-1)^\alpha 2^{1-\alpha} \le M_\alpha(G) + M_\alpha(\overline{G}) \le n(n-1)^\alpha$, *if* $\alpha > 1$;
(b) $n(n-1)^\alpha \le M_\alpha(G) + M_\alpha(\overline{G}) \le n(n-1)^\alpha 2^{1-\alpha}$, *if* $0 < \alpha < 1$;
(c) $n(n-1)^\alpha 2^{1-\alpha} \le M_\alpha(G) + M_\alpha(\overline{G}) \le n\big[1 + (n-2)^\alpha\big]$, *if* $\alpha < 0$.

Theorem 3.3. *Let G be a graph with order n and $\overline{G}$ be its complement. Then*

$$M_\alpha(\overline{G}) = \sum_{r=0}^{\infty}(-1)^r \frac{\alpha(\alpha-1)\cdots(\alpha-r+1)}{r!}(n-1)^{\alpha-r}M_r(G).$$

Proof. From the definition of the general Zagreb index, we obtain

$$M_\alpha(\overline{G}) = \sum_{u\in V(\overline{G})}\Big[\deg_{\overline{G}}(u)\Big]^\alpha = \sum_{u\in V(G)}\Big[n-1-\deg_G(u)\Big]^\alpha = (n-1)^\alpha \sum_{u\in V(G)}\left[1 - \frac{\deg_G(u)}{n-1}\right]^\alpha.$$

By applying Lemma 2.2 to the last equality above, we have

$$M_\alpha(\overline{G}) = (n-1)^\alpha \sum_{u\in V(G)}\sum_{r=0}^{\infty}\binom{\alpha}{r}\left[-\frac{\deg_G(u)}{n-1}\right]^r = \sum_{r=0}^{\infty}(-1)^r(n-1)^{\alpha-r}\binom{\alpha}{r}\sum_{u\in V(G)}\Big[\deg_G(u)\Big]^r.$$

This completes the proof of Theorem 3.3. □

As an immediate corollary of Theorem 3.3, we obtain the following.

Corollary 3.4 (*Ashrafi et al. [12]*). *Let G be a graph with order n and $\overline{G}$ be its complement. Then* $M_1(\overline{G}) = M_1(G) + 2(n-1)\big(\overline{m} - m\big)$.

4. The Zagreb co-index of graphs

The main results of this section show the following theorem.

Theorem 4.1. *Let G be a graph with order n; then $0 \leq \overline{M}_1(G) + \overline{M}_1(\overline{G}) \leq 2^{-1}n(n-1)^2$, the lower bound attains on K_n, and the upper bound attains on the $\frac{n-1}{2}$-regular graphs.*

Proof. By applying Lemma 2.3 to the complement graph $\overline{G}$, one obtains $\overline{M}_1(\overline{G}) = 2\overline{m}(n-1) - M_1(\overline{G})$. Now plugging in the expression for $\overline{M}_1(G)$, we have $\overline{M}_1(G) + \overline{M}_1(\overline{G}) = n(n-1)^2 - [M_1(G) + M_1(\overline{G})]$. From Corollary 3.2, we have $2^{-1}n(n-1)^2 \leq M_1(G) + M_1(\overline{G}) \leq n(n-1)^2$. The theorem follows immediately.

Note that the bounds are best possible. In view of Table 1in Section 2, $\overline{M}_1(K_n) + \overline{M}_1(\overline{K}_n) = 0$, the lower bound attains on K_n. The upper bound attains on the $\frac{n-1}{2}$-regular graphs, so $n = 4\beta + 1$ for some integer β. □

Theorem 4.2. *Let G be a graph with order n; then $0 \leq \overline{M}_2(G) + \overline{M}_2(\overline{G}) \leq 2^{-1}n(n-1)^3$, the lower bound attains on K_n, and the upper bound attains on the $2k$-regular graphs.*

Proof. By applying Lemma 2.4 to the complement graph $\overline{G}$, one obtains $\overline{M}_2(\overline{G}) = M_2(G) - (n-1)M_1(G) + m(n-1)^2$, thus $\overline{M}_2(G) + \overline{M}_2(\overline{G}) = [M_2(G) + M_2(\overline{G})] + 2^{-1}n(n-1)^3 - (n-1)[M_1(G) + M_1(\overline{G})]$. From Corollary 3.2 and Lemma 2.5, we have $2^{-1}n(n-1)^2 \leq M_1(G) + M_1(\overline{G}) \leq n(n-1)^2$ and $2^{-3}n(n-1)^3 \leq M_2(G) + M_2(\overline{G}) \leq 2^{-1}n(n-1)^3$. Easy verification completes the proof.

Note that the bounds are best possible. In view of Table 1 in Section 2, $\overline{M}_2(K_n) + \overline{M}_2(\overline{K}_n) = 0$, the lower bound attains on K_n. The upper bound attains on the $2k$-regular graphs. □

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References

[1] J.A. Bondy, U.S.R. Murty, Graph Theory with Applications, American Elsevier, New York, 1976, [M].
[2] R. Todeschini, V. Consonni, Handbook of Molecular Descriptors, Wiley-VCH, Weinheim, 2000.
[3] I. Gutman, N. Trinajstic, Graph theory and molecular orbitals. Total π-electron energy of alternant hydrocarbons, Chem. Phys. Lett. 17 (1972) 535–538.
[4] L.B. Kier, L.H. Hall, Molecular Connectivity in Structure Activity Analysis, Research Studies Press, Wiley, Chichester, UK, 1986.
[5] S. Nikolic, G. Kovacevic, A. Milicevic, N. Trinajstić, The Zagreb indices 30 years after, Croat. Chem. Acta 76 (2003) 113–124.
[6] B. Bollobás, P. Erdös, Graphs of extremal weights, Ars Combin. 50 (1998) 225–233.
[7] D. Amic, D. Lucic, S. Nikolic, N. Trinajstić, The vertex-connectivity index revisited, J. Chem. Inf. Comput. Sci. 38 (1998) 819–822.
[8] M.H. Khalifeh, H. Yousefi-Azari, A.R. Ashrafi, The first and second Zagreb indices of graph operations, Discrete Appl. Math. 157 (2009) 804–811.
[9] G. Caporossi, I. Gutman, P. Hansen, L. Pavlović, Graphs with maximum connectivity index, Comput. Biol. Chem. 27 (2003) 85–90.
[10] X. Li, H. Zhao, Trees with the first three smallest and largest generalizated topological indices, MATCH Commun. Math. Comput. Chem. 50 (2004) 57–62.
[11] T. Došlić, Vertex-weighted Wiener polynomials for composite graphs, Ars Math. Contemp. 1 (2008) 66–80.
[12] A.R. Ashrafi, T. Došlić, A. Hamzeh, The Zagreb coindices of graph operations, Discrete Appl. Math. 158 (2010) 1571–1578.
[13] A.R. Ashrafi, T. Došlić, A. Hamzeh, Extremal graphs with repect to the Zagreb coindices, MATCH Commun. Math. Comput. Chem. 65 (2011) 85–92.
[14] E.A. Nordhaus, J.W. Gaddum, On complementary graphs, Amer. Math. Monthly 63 (1956) 175–177.
[15] S.J. Xu, Some parameters of graph and its complement, in: Theory of Graphs, in: Proc. Coll. Tihany, 1968, pp. 99–113.
[16] Z. An, B. Wu, D. Bin, Y. Wang, G. Su, Nordhaus–Gaddum-type theorem for diameter of graphs when decomposing into many parts, Discrete Math. Algor. Appl. 3 (2011) 305–310.
[17] E. Hairer, G. Wanner, Analysis by its History, Springer, 2008.
[18] G.H. Hardy, J.E. Littlewood, G. Pólya, Inequalities, in: Cambridge Mathematical Library Series, Cambridge University Press, 1967.
[19] L. Zhang, B. Wu, The Nordhaus–Gaddum-type inequalities for some chemical indices, MATCH Commun. Math. Comput. Chem. 54 (2005) 189–194.