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A Revised Analysis of Upper Bounds for the First Zagreb Index: Addressing Errors in Multiple Papers

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Abstract

This commentary addresses some minor errors in the literature concerning the upper bounds of the first Zagreb index, both related to the necessary and sufficient conditions for equality in the associated inequalities. To resolve these issues, we provide corrected derivations and clarify their implications for the validity of the bounds. Furthermore, we conduct a review of recent papers that have incorrectly applied these inequalities, identifying common misuses and providing revised conclusions to ensure accuracy. Additionally, to ensure completeness and accessibility, we present more concise and elementary proofs of the underlying inequalities, which simplifies the original approach.

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1 Introduction

This commentary uses the notation $\mathbb{Z}_{[a,b]}$ to represent the integer interval $\mathbb{Z} \cap [a,b]$, and adopts the term (n,m)-*graph* to describe a graph with n vertices and m edges. Let G be a simple (n,m)-graph with vertex set $V(G) = \{v_1, v_2, \ldots, v_n\}$. For each vertex $v_i \in V(G)$, we denote its degree as $d_i := d_G(v_i)$, and assume without loss of generality that $d_1 \geq d_2 \geq \cdots \geq d_n$. This ordering ensures $d_i \geq 1$ for all $i \in \mathbb{Z}_{[1,n]}$, as connectivity is required for the scope of this work.

The first Zagreb index, denoted $M_1(G)$, was introduced in 1972 [8] by Gutman and Trinajstić as a measure of molecular structure complexity. It is defined as the sum of the squares of vertex degrees in a graph G:

$$M_1(G) = \sum_{i=1}^{n} d_i^2.$$

Over decades, $M_1(G)$ has become a cornerstone in chemical graph theory, with extensive research dedicated to deriving its upper and lower bounds. A comprehensive survey [3] by Borovičanin, Das, Furtula, and Gutman in 2017 systematically summarized these bounds for both the first and second Zagreb indices. However, upon reviewing the literature guided by this survey, we identified minor but critical errors in Theorems 31 and 33 of [3] concerning the first Zagreb index.

According to the survey [3], Theorem 33 originated as Theorem 2 in [9] (with a correction implemented in [11]) and concurrently appeared as Theorem 2 in [12], each accompanied by independently developed proofs. The errors in these distinct papers will be corrected in Sections 2 and 3, respectively. Additionally, Theorem 31 of [3] was first introduced as Theorem 3 in [12]. The correction of it will be presented in Section 4. Subsequent analysis has identified analogous misapplications of related inequalities across other works [5, 7, 10, 13], which will be systematically examined in Section 5.

To ensure clarity and traceability, excerpted content from these sources will be highlighted in boxes throughout the commentary. Within these excerpts, theorem and inequality labels, as well as external citations, have been adjusted to align with the current manuscript's referencing system, facilitating direct comparison and verification.

2 Correction for Theorem 2 in [9] with the version in [11]

2.1 Comments

In [9], from Line 15 to Line 18 on Page 98, authors presented the following theorem (labeled in [9] as Theorem 2, and cited in [3] as Theorem 33):

Theorem 1 (Theorem 2 of [9] with the version in [11]). *Let G be a nontrivial graph of order n and size m. Then*

$$M_1(G) \leq \frac{\alpha(n)(\Delta-\delta)^2 + 4m^2}{n}, \tag{1}$$

where $\alpha(n) = n\left\lfloor \frac{n}{2} \right\rfloor \left(1 - \frac{1}{n}\left\lfloor \frac{n}{2} \right\rfloor\right)$. Further, equality holds if and only if G is a regular graph.

Remark. The function $\alpha(n)$ in the origin manuscript of [9] was incorrectly defined using $\lceil x \rceil$, which was later corrected in [11] by replacing $\lceil x \rceil$ with $\lfloor x \rfloor$. We will adopt this correction by default in the subsequent discussion.

Comments of Theorem 1:

i. A Tedious Expression

The expression "$\alpha(n) = n\left\lfloor \frac{n}{2} \right\rfloor \left(1 - \frac{1}{n}\left\lfloor \frac{n}{2} \right\rfloor\right)$" (replaced $\lceil x \rceil$ with $\lfloor x \rfloor$) is unnecessarily complex (but no mistake) and can be simplified without altering its meaning. Specifically, it can be rewritten as $\alpha(n) = \lfloor n^2/4 \rfloor$, since

$$n\left\lfloor \frac{n}{2} \right\rfloor \left(1 - \frac{1}{n}\left\lfloor \frac{n}{2} \right\rfloor\right) = \left\lfloor \frac{n^2}{4} \right\rfloor. \tag{2}$$

The equality (2) holds trivially when n is even. Therefore, we consider the case where n is odd, i.e., $n = 2k + 1$ for some $k \in \mathbb{Z}_{[0,+\infty)}$. Then,

$$n\left\lfloor\frac{n}{2}\right\rfloor\left(1-\frac{1}{n}\left\lfloor\frac{n}{2}\right\rfloor\right) = (2k+1)k\left(1-\frac{k}{2k+1}\right) = k^2+k.$$

On the other hand,

$$\left\lfloor\frac{n^2}{4}\right\rfloor = \left\lfloor\frac{4k^2+4k+1}{4}\right\rfloor = k^2+k.$$

Thus (2) holds in both cases.

ii. A Minor Error

The necessary and sufficient condition stated in Theorem 1, that the equality in (1) holds if and only if "G is a regular graph" is incorrect.

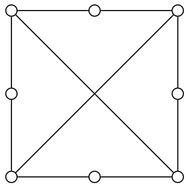

Figure 1. G_1

Consider the graph G_1 depicted Fig. 1. This graph has four vertices of degree three, four vertices of degree two, and ten edges. Consequently, the left-hand side of (1) for G_1 evaluates to $M_1(G_1) = 52$, while the right-hand side of (1) for G_1 is $\frac{1}{8}(16 + 4 \times 10^2) = 52$. Thus, the equality in (1) holds for G_1, despite G_1 not being a regular graph. Next we will present the correction of this minor error.

2.2 Correction

The authors in [9] derived Theorem 1 (Theorem 2 in [9]) from the following theorem (where $\lceil x \rceil$ was replaced by $\lfloor x \rfloor$), originally labeled as Theorem 1 in [9].

Theorem 2 (Theorem 1 of [9]). *Suppose a_i and b_i, $1 \le i \le n$ are positive real numbers, then*

$$\left| n \sum_{i=1}^{n} a_i b_i - \sum_{i=1}^{n} a_i \sum_{i=1}^{n} b_i \right| \le \alpha(n)(A-a)(B-b)$$

where a, b, A and B are real constants, that for each i, $1 \le i \le n$, $a \le a_i \le A$ and $b \le b_i \le B$. Further, $\alpha(n) = n \left\lfloor \frac{n}{2} \right\rfloor \left(1 - \frac{1}{n} \left\lfloor \frac{n}{2} \right\rfloor\right)$.

The authors of [9] omitted the necessary and sufficient condition for equality in Theorem 2, which constitutes the root cause of their error. To trace this issue back to its origin, we refer to [2], the foundational paper where Theorem 2 was first established.

Published in 1950 by Polish mathematicians Biernacki, Pidek and Ryll-Nardzewski, [2] presented a discrete variant of Grüss' inequality, which corresponds exactly to the inequality stated in Theorem 2. The original manuscript [2] was written in French, and the English translation of the key inequality is provided below:

Theorem 3 (Lemma of [2]). *Let $a_1, \ldots, a_n$ and $b_1, \ldots, b_n$ be real numbers that satisfy the inequalities:*

$$a \le a_i \le A \quad \text{and} \quad b \le b_i \le B \quad (i = 1, 2, \ldots, n).$$

Then

$$\begin{aligned} -(A-a)(B-b) \left\lfloor \frac{n}{2} \right\rfloor \left(1 - \frac{1}{n} \left\lfloor \frac{n}{2} \right\rfloor\right) \le& \\ \sum_{i=1}^{n} a_i b_i - \frac{1}{n} \sum_{i=1}^{n} a_i \sum_{i=1}^{n} b_i& \\ \le (A-a)(B-b) \left\lfloor \frac{n}{2} \right\rfloor \left(1 - \frac{1}{n} \left\lfloor \frac{n}{2} \right\rfloor\right).& \end{aligned}$$

The equalities hold when $\left\lfloor \frac{n}{2} \right\rfloor$ or $\left\lfloor \frac{n+1}{2} \right\rfloor$ of the numbers a_i's are equal to A and the remaining a_i's are equal to a. Under these conditions, if $b_i = b$ when $a_i = A$ and $b_i = B$ when $a_i = a$, the equality holds in the left inequality; whereas if $b_i = b$ when $a_i = a$ and $b_i = B$ when $a_i = A$, the equality holds in the right inequality.

It is straightforward to correct Theorem 1 (which corresponds to Theorem 2 of [9]) using Theorem 3, as follows:

Theorem 4 (Correction for Theorem 2 of [9])**.** *Let G be a connected (n, m)-graph. Then*

$$M_1(G) \leq \frac{1}{n} \left\lfloor \frac{n^2}{4} \right\rfloor (\Delta - \delta)^2 + \frac{4m^2}{n}.$$

The equality holds if and only if $\Delta = d_1 = d_2 = \cdots = d_p$ and $\delta = d_{p+1} = \cdots = d_n$ where $p = \lfloor n/2 \rfloor$ or $\lfloor (n+1)/2 \rfloor$.

Noting that G is regular when $\Delta = \delta$, we observe that the condition "G is regular" in Theorem 1 is simply a special case of the necessary and sufficient condition stated in Theorem 4.

Proof. Take $a = b = d_n = \delta$, $A = B = d_1 = \Delta$ and $a_i = b_i = d_i$ for every $i \in \mathbb{Z}_{[1,n]}$. Then from Theorem 3, we have that

$$\begin{aligned}
M_1(G) &= \sum_{i=1}^{n} d_i^2 \\
&\leq \frac{1}{n} \left\lfloor \frac{n^2}{4} \right\rfloor (\Delta - \delta)^2 + \frac{1}{n} \left(\sum_{i=1}^{n} d_i \right)^2 \\
&= \frac{1}{n} \left\lfloor \frac{n^2}{4} \right\rfloor (\Delta - \delta)^2 + \frac{4m^2}{n}.
\end{aligned}$$

By Theorem 3, the equality holds if and only if $\Delta = d_1 = \cdots = d_p$ and $\delta = d_{p+1} = \cdots = d_n$ where $p = \lfloor n/2 \rfloor$ or $\lfloor (n+1)/2 \rfloor$. ■

In fact, we do not require an inequality as strong as Theorem 3. The following lemma offers a more concise and straightforward inequality with a shorter proof, which is sufficient to replace Theorem 3 in the derivation of Theorem 4.

Lemma 1. *If $x_1, x_2, \ldots, x_n \in [a,b]$ and $n \geq 2$, then*

$$n\left(\sum_{i=1}^{n} x_i^2\right) - \left(\sum_{i=1}^{n} x_i\right)^2 \leq \left\lfloor \frac{n^2}{4} \right\rfloor (b-a)^2,$$

where the equality holds if and only if exactly $\lfloor n/2 \rfloor$ or $\lfloor (n+1)/2 \rfloor$ among all of x_i's take the value a and the remaining $n - \lfloor n/2 \rfloor$ or $n - \lfloor (n+1)/2 \rfloor$ take b.

Proof. Denote

$$f(\mathbf{x}) = f(x_1, \ldots, x_n) := n\left(\sum_{i=1}^{n} x_i^2\right) - \left(\sum_{i=1}^{n} x_i\right)^2$$

where every $x_i \in [a,b]$. Then

$$f(x) = \sum_{1 \leq i < j \leq n} (x_i - x_j)^2.$$

Because the Hessian matrix of f is positive semi-definite, f is a convex function. Noting that the domain of f is $[a,b]^n$, which is a bounded and closed convex polyhedron in $\mathbb{R}^n$, the maximum value of f is attained at a vertex of such bounded convex polyhedron $[a,b]^n$. Let $\mathbf{x}^* = (x_1^*, \ldots, x_n^*)$ be the vertex where f attains its maximum value. Then every x_i^* is equal to a or b. Assume that the number of x_i^* equal to a is t. Then the number of x_i^* equal to b is $n-t$. Thus the maximum value $\max\{f\} = t(n-t)(b-a)^2$ for some positive integer $t \in \mathbb{Z}_{[1,n]}$. Noting that t and $n-t \in \mathbb{Z}_+$, we derive that $t(n-t) \leq \lfloor n^2/4 \rfloor$ from mean inequality and $t(n-t)$ reaches its maximum value when $t = \lfloor n/2 \rfloor$ or $\lfloor (n+1)/2 \rfloor$. Further, whether $t = \lfloor n/2 \rfloor$ or $\lfloor (n+1)/2 \rfloor$, it holds that $t(n-t) = \lfloor n^2/4 \rfloor$. Hence,

$$f \leq \left\lfloor \frac{n^2}{4} \right\rfloor (b-a)^2$$

where the equality holds if and only if exactly $\lfloor n/2 \rfloor$ (or $\lfloor (n+1)/2 \rfloor$) numbers among all of x_i's take the value a and the remaining $n - \lfloor n/2 \rfloor$ (or $n - \lfloor (n+1)/2 \rfloor$) take b. ■

Remark. To demonstrate Theorem 4, one can set $a = \delta$, $b = \Delta$, and $x_i = d_i$ for every $i \in \mathbb{Z}_{[1,n]}$. This completes the correction for [9].

3 Correction for Theorem 2 in [12]

3.1 Comments

In [12], Theorem 33 of [3] was wrote as follows:

Theorem 5 (Theorem 2 in [12])**.** *Let G be an undirected connected graph with n, $n \geq 2$, vertices and m edges. Then*

$$M_1 \leq \frac{4m^2}{n} + n(\Delta - \delta)^2 \alpha(n)$$

where

$$\alpha(n) = \frac{1}{4}\left(1 - \frac{1 + (-1)^{n+1}}{2n^2}\right).$$

The equality holds if and only if G is isomorphic with k-regular graph, $1 \leq k \leq n-1$.

Comments of Theorem 5:

i. Theorem 1 and Theorem 5 are equivalent, because $\alpha(n)$ in Theorem 1 corresponds to $n^2\alpha(n)$ in Theorem 5, and it is easy to check that

$$n^2 \cdot \frac{1}{4}\left(1 - \frac{1 + (-1)^{n+1}}{2n^2}\right) = \left\lfloor \frac{n^2}{4} \right\rfloor.$$

ii. The necessary and sufficient condition of the equality still is incorrect with the same counterexample.

3.2 Correction

Next, we explain the source of the error in Theorem 5 (which corresponds to Theorem 2 in [12]). In [12], this theorem was derived from the following lemma (Lemma 6 in [12]):

Lemma 2 (Lemma 6 in [12]). *Let $p_1, p_2, \ldots, p_n$ be non-negative real numbers and $a_1, a_2, \ldots, a_n$ and $b_1, b_2, \ldots, b_n$ be real numbers with the properties $0 < r_1 \leq a_i \leq R_1 < +\infty$ and $0 < r_2 \leq b_i \leq R_2 < +\infty$ for each $i = 1, 2, \ldots, n$. Further, let S be a subset of $\{1, 2, \ldots, n\}$ which minimizes the expression*

$$\left| \sum_{i \in S} p_i - \frac{1}{2} \sum_{i=1}^{n} p_i \right|.$$

Then

$$\left| \sum_{i=1}^{n} p_i \sum_{i=1}^{n} p_i a_i b_i - \sum_{i=1}^{n} p_i a_i \sum_{i=1}^{n} p_i b_i \right| \leq (R_1 - r_1)(R_2 - r_2) \sum_{i \in S} p_i \left(\sum_{i=1}^{n} p_i - \sum_{i \in S} p_i \right).$$

The authors of [12] omitted critical conditions for equality in Lemma 2 (Lemma 6 in [12]), potentially contributing to the error in Theorem 5. Moreover, they cited Lemma 2 (Lemma 6 in [12]) without providing a proof, referring instead to [4]. However, [4] neither explicitly states nor rigorously proves Lemma 2 (Lemma 6 in [12]), despite discussing refined integral-form Grüss' inequalities in measurable spaces. While Lemma 2 (Lemma 6 in [12]) might be inferred as a corollary of [4]'s conclusions, this ambiguity has caused significant confusion.

We resolved this by locating Lemma 2 (Lemma 6 in [12]) in [1]. In 1988, Hungarian mathematicians Andrica and Badea introduced a pivotal discrete variant of Grüss' inequality (Theorem 2 in [1]), later referenced as Lemma 2 (Lemma 6 in [12]) and we will term it the *Andrica-Badea inequality* in this commentary. Notably, the original proof in [1] employed functional analysis terminology, which may obscure its applicability for discrete mathematics researchers. To address this, we present an elementary proof of the Andrica-Badea inequality to ensure both rigor and accessibility.

To contextualize the Andrica-Badea inequality, we introduce a foundational NP-hard problem: the *Number Partitioning Problem* (NPP, [6]). Given a vector $\mathbf{p} = (p_1, p_2, \ldots, p_n) \in \mathbb{R}_+^n$, NPP seeks a partition $(S, \bar{S})$ of $\mathbb{Z}_{[1,n]}$ minimizing the discrepancy:

$$\left| \sum_{i \in S} p_i - \sum_{j \in \bar{S}} p_j \right| \quad \text{or equivalently} \quad \left| \sum_{i \in S} p_i - \frac{1}{2} \sum_{j=1}^{n} p_j \right|.$$

In the following Lemma 3 and Theorem 6, we fix $\mathbf{p} = (p_1, p_2, \ldots, p_n) \in \mathbb{R}_+^n$, denote

$$\eta(S, \bar{S}) := \sum_{i \in S} p_i \sum_{j \in \bar{S}} p_j$$

for a partition $(S, \bar{S})$ of $\mathbb{Z}_{[1,n]}$, use $(S_{\mathbf{p}}, \bar{S}_{\mathbf{p}})$ to denote the optimal solution of NPP with respect to $\mathbf{p}$, and denote

$$\begin{aligned} \psi_{\mathbf{p}}(\mathbf{x}) &:= \left(\sum_{i=1}^{n} p_i \right) \left(\sum_{i=1}^{n} p_i x_i^2 \right) - \left(\sum_{i=1}^{n} p_i x_i \right)^2 \quad \text{and} \\ \phi_{\mathbf{p}}(\mathbf{x}, \mathbf{y}) &:= \left(\sum_{i=1}^{n} p_i \right) \left(\sum_{i=1}^{n} p_i x_i y_i \right) - \left(\sum_{i=1}^{n} p_i x_i \right) \left(\sum_{i=1}^{n} p_i y_i \right) \end{aligned}$$

where $\mathbf{x} := (x_1, x_2, \ldots, x_n)$ and $\mathbf{y} := (y_1, y_2, \ldots, y_n) \in \mathbb{R}^n$.

Lemma 3. *Let $r, R \in \mathbb{R}$ such that $r \leq R$ and $\mathbf{p} \in \mathbb{R}_+^n$. If the domain of $\psi_{\mathbf{p}}$ is $[r, R]^n$, then*

$$\max\{\psi_{\mathbf{p}}(\mathbf{x})\} = (R - r)^2 \eta(S_{\mathbf{p}}, \bar{S}_{\mathbf{p}}).$$

Further $\mathbf{x}^* = (x_1^*, x_2^*, \ldots, x_n^*) \in [r, R]^n$ is the point where $\psi_{\mathbf{p}}$ reaches the maximum value if and only if $x_i^* = R$ for all $i \in S_{\mathbf{p}}$ and simultaneously,

$x_i^* = r$ for all $i \in \bar{S}_{\mathbf{p}}$.

Remark. Within the partition $(S, \bar{S})$, S and $\bar{S}$ exhibit symmetry in their roles. Consequently, the condition for equality in Lemma 3 can be rewritten as: $x_i^* = R$ for all $i \in \bar{S}_{\mathbf{p}}$ and $x_i^* = r$ for all $i \in S_{\mathbf{p}}$. Note that a similar "symmetry" exists in Theorem 6. For the sake of brevity, we omit explicitly stating these symmetries.

Proof. It is easy to check that the Hessian matrix of $\psi_{\mathbf{p}}$ is positive semi-definite. Thus $\psi_{\mathbf{p}}$ is convex. Since the domain is $[r, R]^n$, which is a bounded and closed convex polyhedron, $\psi_{\mathbf{p}}$ attains the maximum value at a vertex of $[r, R]^n$. Take an arbitrary vertex $\mathbf{x}^* = (x_1^*, x_2^*, \dots, x_n^*)$ of $[r, R]^n$. Then $x_i^* \in \{r, R\}$ for every $i \in \mathbb{Z}_{[1,n]}$. Let $S := \{i \in \mathbb{Z}_{[1,n]} : x_i^* = R\}$. Then

$$\begin{aligned}
\psi_{\mathbf{p}}(\mathbf{x}^*) &= \sum_{i=1}^{n}\sum_{j=1}^{n} p_i p_j {x_i^*}^2 - \sum_{i=1}^{n}\sum_{j=1}^{n} p_i p_j x_i^* x_j^* = \sum_{i=1}^{n}\sum_{j=1}^{n} p_i p_j x_i^* (x_i^* - x_j^*) \\
&= \sum_{i\in S}\sum_{j\in\bar{S}} p_i p_j R(R-r) + \sum_{i\in\bar{S}}\sum_{j\in S} p_i p_j r(r-R) \\
&= (R-r)^2 \sum_{i\in S} p_i \sum_{j\in\bar{S}} p_j = (R-r)^2 \eta(S, \bar{S}).
\end{aligned}$$

Thus

$$\max\{\psi_{\mathbf{p}}(\mathbf{x})\} = \max_{\mathbf{x}^*}\{\psi_{\mathbf{p}}(\mathbf{x}^*)\} = (R-r)^2 \max_{(S,\bar{S})}\{\eta(S,\bar{S})\}.$$

By mean inequalities, $\eta(S, \bar{S})$ attains the maximum value if and only if

$$\left| \sum_{i\in S} p_i - \sum_{j\in\bar{S}} p_j \right|$$

attains the minimum value. Hence, by the choice of $(S_{\mathbf{p}}, \bar{S}_{\mathbf{p}})$, we have that $\max\{\psi_{\mathbf{p}}(\mathbf{x})\} = (R-r)^2\eta(S_{\mathbf{p}}, \bar{S}_{\mathbf{p}})$ and $\psi_{\mathbf{p}}$ attains the maximum value at $\mathbf{x}^*$ if and only if $x_i^* = R$ for all $i \in S_{\mathbf{p}}$ and simultaneously, $x_i^* = r$ for all $i \in \bar{S}_{\mathbf{p}}$. ■

Theorem 6 (Andrica-Badea inequality, Theorem 2 in [1])**.** *Let r_1, r_2, R_1, $R_2 \in \mathbb{R}$ such that $r_1 \leq R_1$ and $r_2 \leq R_2$ and $\mathbf{p} = (p_1, p_2, \ldots, p_n) \in \mathbb{R}_+^n$. If $\mathbf{x} = (x_1, x_2, \ldots, x_n) \in [r_1,\, R_1]^n$ and $\mathbf{y} = (y_1, y_2, \ldots, y_n) \in [r_2,\, R_2]^n$, then*

$$|\phi_{\mathbf{p}}(\mathbf{x}, \mathbf{y})| \leq (R_1 - r_1)(R_2 - r_2)\eta(S_{\mathbf{p}}, \bar{S}_{\mathbf{p}}),$$

i.e.,

$$\left| \sum_{i=1}^n p_i \sum_{i=1}^n p_i x_i y_i - \sum_{i=1}^n p_i x_i \sum_{i=1}^n p_i y_i \right| \leq (R_1 - r_1)(R_2 - r_2) \sum_{i \in S} p_i \sum_{j \in \bar{S}} p_j$$

Further, the equality holds if and only if one of the following statements holds:

(i) *$x_i = R_1$ and $y_i = R_2$ for all $i \in S_{\mathbf{p}}$ and simultaneously, $x_i = r_1$ and $y_i = r_2$ for all $i \in \bar{S}_{\mathbf{p}}$, or*

(ii) *$x_i = R_1$ and $y_i = r_2$ for all $i \in S_{\mathbf{p}}$ and simultaneously, $x_i = r_1$ and $y_i = R_2$ for all $i \in \bar{S}_{\mathbf{p}}$.*

Proof. It is easy to check that

$$\begin{aligned}
\psi_{\mathbf{p}}(\mathbf{x}) &= \sum_{i=1}^n \sum_{j=1}^n p_i p_j x_i^2 - \sum_{i=1}^n \sum_{j=1}^n p_i p_j x_i x_j \\
&= \sum_{i=1}^n \sum_{j=1}^n p_i p_j x_i (x_i - x_j) \\
&= \sum_{1 \leq i < j \leq n} p_i p_j (x_i - x_j)^2.
\end{aligned}$$

Then by Cauchy-Schwartz inequality, we have that

$$\begin{aligned}
&[\phi_{\mathbf{p}}(\mathbf{x}, \mathbf{y})]^2 \\
&= \left[\sum_{i=1}^n \sum_{j=1}^n p_i p_j x_i y_i - \sum_{i=1}^n \sum_{j=1}^n p_i p_j x_i y_j \right]^2 \\
&= \left[\sum_{i=1}^n \sum_{j=1}^n p_i p_j x_i (y_i - y_j) \right]^2 = \left[\sum_{1 \leq i < j \leq n} p_i p_j (x_i - x_j)(y_i - y_j) \right]^2
\end{aligned}$$

$$= \left[\sum_{1 \le i < j \le n} \left[\sqrt{p_i p_j}(x_i - x_j) \right] \left[\sqrt{p_i p_j}(y_i - y_j) \right] \right]^2$$
$$\le \sum_{1 \le i < j \le n} p_i p_j (x_i - x_j)^2 \sum_{1 \le i < j \le n} p_i p_j (y_i - y_j)^2 = \psi_{\mathbf{p}}(\mathbf{x}) \psi_{\mathbf{p}}(\mathbf{y}),$$

thus

$$|\phi_{\mathbf{p}}(\mathbf{x}, \mathbf{y})| \le \sqrt{\psi_{\mathbf{p}}(\mathbf{x}) \psi_{\mathbf{p}}(\mathbf{y})} \tag{3}$$

where the equality holds if and only if there exists a constant λ such that $x_i - x_j = \lambda(y_i - y_j)$ for every $i, j \in \mathbb{Z}_{[1,n]}$. By Lemma 3,

$$\psi_{\mathbf{p}}(\mathbf{x}) \le (R_1 - r_1)^2 \eta(S_{\mathbf{p}}, \bar{S}_{\mathbf{p}}) \text{ and } \psi_{\mathbf{p}}(\mathbf{y}) \le (R_2 - r_2)^2 \eta(S_{\mathbf{p}}, \bar{S}_{\mathbf{p}}) \tag{4}$$

where equalities hold simultaneously if and only if one of the following statements holds (for the symmetries):

(i) $x_i = R_1$ and $y_i = R_2$ for all $i \in S_{\mathbf{p}}$ and simultaneously, $x_i = r_1$ and $y_i = r_2$ for all $i \in \bar{S}_{\mathbf{p}}$, or

(ii) $x_i = R_1$ and $y_i = r_2$ for all $i \in S_{\mathbf{p}}$ and simultaneously, $x_i = r_1$ and $y_i = R_2$ for all $i \in \bar{S}_{\mathbf{p}}$.

Noting that the condition for both equalities in (4) to hold satisfies the condition for the equality in (3) to hold, hence the conclusion holds. ■

Remark. By setting $p_i = 1$, $y_i = x_i = d_i$ for all $i \in \mathbb{Z}_{[1,n]}$, $r_1 = r_2 = \delta$, and $R_1 = R_2 = \Delta$ in Theorem 6, it is straightforward to derive Theorem 4 from Theorem 6. Consequently, Theorem 6 can serve as a replacement for Lemma 2 (Lemma 6 in [12]), despite the proof being quite tedious. This concludes our correction for [12].

4 Correction for Theorem 3 in [12]

4.1 Comments

From Line -6 on Page 1020 to Line 5 on Page 1021 of [12], authors presented the following theorem:

Theorem 7 (Theorem 3 in [12]). *Let G be an undirected connected graph with n, $n \geq 2$, vertices and m edges. Further, let S be a subset of $I_n = \{1, 2, \ldots, n\}$ that minimizes the expression*

$$\left| \sum_{i \in S} d_i - m \right| .$$

Then

$$M_1 \leq \frac{4m^2 \left(1 + \left(\sqrt{\frac{\Delta}{\delta}} - \sqrt{\frac{\delta}{\Delta}} \right)^2 \beta(S) \right)}{n} . \tag{5}$$

where

$$\beta(S) = \frac{1}{2m} \sum_{i \in S} d_i \left(1 - \frac{1}{2m} \sum_{i \in S} d_i \right) .$$

Equality in (5) *holds if and only if G is isomorphic with k-regular graph, $1 \leq k \leq n-1$, or bidegreed graph such that $\Delta + \delta$ divides $n\delta$ and there are exactly $p = \frac{n\delta}{\Delta+\delta}$ vertices of degree Δ and $q = \frac{n\Delta}{\Delta+\delta}$ vertices of degree δ.*

Comments of Theorem 7: The necessary and sufficient condition of the equality in (5) is incorrect.

Consider the graph G_2 showed in Fig. 2. G_2 has five vertices of degree four, nine vertices of degree two, and 19 edges. Let $S \subseteq \mathbb{Z}_{[1,n]}$ that minimizes the expression $\left|\sum_{i \in S} d_i - m\right|$. Then $S = \{1, 2, 3, 4, 5\}$ where $d_1 + d_2 + d_3 + d_4 + d_5 - m = 20 - 19 = 1$. Thus the left-hand-side of (5) for G_2 is $M_1(G_2) = 116$, and the right-hand-side of (5) for G_2 is

$$\frac{4 \times 19^2}{14} \left[1 + \frac{1}{2} \left(\frac{20}{38} \times \frac{18}{38} \right) \right] = 116.$$

It follows that the equality of (5) holds on G_2. But G_2 is not regular, and for G_2, the number

$$\frac{n\delta}{\Delta + \delta} = \frac{2 \times 14}{4 + 2} = \frac{14}{3}$$

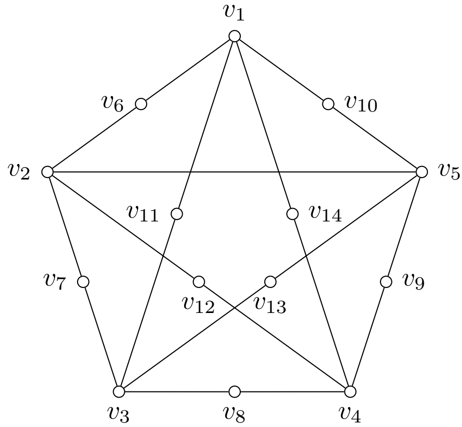

Figure 2. G_2

is not an integer, which contradicts with the condition "$\Delta + \delta$ divides $n\delta$". Thus the necessary and sufficient condition of the equality in (5) is incorrect (consequently, Corollary 1 in [12] is also incorrect).

4.2 Correction

In [12], Theorem 7 (Theorem 3 in [12]) was derived from Lemma 2 (Lemma 6 in [12]), which is precisely why the proof lacks robustness. In Subsection 3.2, we explained that Lemma 2 (Lemma 6 in [12]) should be replaced by Lemma 3 and Theorem 6. In this subsection, we will present the corrected version of Theorem 7 using Lemma 3 and Theorem 6.

Lemma 4. *Let $r, R \in \mathbb{Z}_+$ such that $r \leq R$, $\mathbf{p} := (p_1, p_2, \ldots, p_n)$ such that $p_i \in \mathbb{Z}_{[r,R]}$ for every $i \in \mathbb{Z}_{[1,n]}$, and $\widetilde{\mathbf{p}} := (1/p_1, 1/p_2, \ldots, 1/p_n)$. Then*

$$n\left(\sum_{i=1}^{n} p_i^2\right) - \left(\sum_{i=1}^{n} p_i\right)^2 \leq \frac{(R-r)^2}{Rr}\eta(S_{\mathbf{p}}, \bar{S}_{\mathbf{p}}). \tag{6}$$

where inequality holds if and only if $R = p_1 = p_2 = \cdots = p_n = r$ or the following statements hold simultaneously:

(i) $p_i \in \{R, r\}$ *where $R > r$ for every $i \in \mathbb{Z}_{[1,n]}$;*

(ii) *for the number s of p_i's equal to R, and every $a \in \mathbb{Z}_{[1,s]}$, $b \in \mathbb{Z}_{[1,\,n-s]}$ such that $aR \neq br$,*

$$s \leq \frac{aR - br + nr}{R + r} \text{ when } aR > br\,, \text{ and}$$
$$s \geq \frac{aR - br + nr}{R + r} \text{ when } aR < br.$$

Proof. Let $x = \mathbf{p}$, $y = \widetilde{\mathbf{p}}$. Then by Cauchy-Schwartz inequality, we can get

$$n\left(\sum_{i=1}^{n} p_i^2\right) - \left(\sum_{i=1}^{n} p_i\right)^2 = \left|n\left(\sum_{i=1}^{n} p_i^2\right) - \left(\sum_{i=1}^{n} p_i\right)^2\right| = \left|\phi_{\mathbf{p}}(\mathbf{p}, \widetilde{\mathbf{p}})\right|.$$

Now applying Theorem 6 with $R_1 = R$, $r_1 = r$, $R_2 = 1/r$ and $r_2 = 1/R$, we have that

$$|\phi_{\mathbf{p}}(\mathbf{p}, \widetilde{\mathbf{p}})| \leq \max\{|\phi_{\mathbf{p}}(\mathbf{x}, \mathbf{y})|\} = \frac{(R-r)^2}{Rr}\eta(S_{\mathbf{p}}, \bar{S}_{\mathbf{p}}).$$

Thus (6) holds. Next consider the necessary and sufficient condition of the equality in (6) to hold.

($\Rightarrow$) Suppose that the equality in (6) holds. Then $(\mathbf{p}, \widetilde{\mathbf{p}})$ is one of the points where $|\phi_{\mathbf{p}}(\mathbf{x}, \mathbf{y})|$ attains its maximum value. If $R = r$, then we have obtained the conclusion. Without loss of generality, assume that $R > r$. It is sufficient to show that (i) and (ii) hold.

Since $(\mathbf{p}, \widetilde{\mathbf{p}})$ is one of the points where $|\phi_{\mathbf{p}}(\mathbf{x}, \mathbf{y})|$ attains its maximum value and considering the choice of $\widetilde{\mathbf{p}}$, $(\mathbf{p}, \widetilde{\mathbf{p}})$ satisfies the condition (ii) in Theorem 6. Hence, $p_i = R$ for all $i \in S_{\mathbf{p}}$ and $p_i = r$ for all $i \in \bar{S}_{\mathbf{p}}$. Then (i) holds. Take $s := |S_{\mathbf{p}}|$. Now we can assume that

$$\mathbf{p} = (\underbrace{R, R, \ldots, R}_{s}, \underbrace{r, r, \ldots, r}_{n-s}). \tag{7}$$

It follows that $S_{\mathbf{p}} = \{1, 2, \ldots, s\}$ and $\bar{S}_{\mathbf{p}} = \{s+1, \ldots, n\}$,

Take arbitrary $a \in \mathbb{Z}_{[1,s]}$ and $b \in \mathbb{Z}_{[1,\,n-s]}$ such that $aR \neq br$. Let $S = (S_{\mathbf{p}} \setminus \mathbb{Z}_{[1,a]}) \cup \mathbb{Z}_{[s+1,\,s+b]}$ and $\bar{S} = \mathbb{Z}_{[1,n]} \setminus S$. Then $(S, \bar{S})$ is also a partition of $\mathbb{Z}_{[1,n]}$. Noting $(S_{\mathbf{p}}, \bar{S}_{\mathbf{p}})$ is the optimal partition in NPP with respect to $\mathbf{p}$, we have that

$$\left|\sum_{i\in S_{\mathbf{p}}} p_i - \sum_{j\in \bar{S}_{\mathbf{p}}} p_j\right| \leq \left|\sum_{i\in S} p_i - \sum_{j\in \bar{S}} p_j\right|.$$

It follows that

$$|Rs - r(n-s)| \leq |(Rs - aR + br) - (r(n-s) + aR - br)|.$$

That is

$$|Rs - r(n-s)| \leq |(Rs - r(n-s)) - 2(aR - br)|.$$

Denote $A := Rs - r(n-s)$ and $B := aR - br$. Then $|A| \leq |A - 2B|$. It follows that $A^2 \leq A^2 - 4AB + 4B^2$. Then $AB \leq B^2$. Noting $aR \neq br$, we have $B \neq 0$, thus $A \leq B$ when $B > 0$, and $A \geq B$ when $B < 0$, which derive (ii).

($\Leftarrow$) If $R = r$, the equality in (6) holds clearly. Assume that $R > r$. Suppose that there exists $s \in \mathbb{Z}_+$ such that (i) and (ii) hold. Since (i) holds, we assume that (7) holds. Let $S := \{1, 2, \ldots, s\}$ and $\bar{S} = \{s+1, \ldots, n\}$. Then $(S, \bar{S})$ is a partition of $\mathbb{Z}_{[1,n]}$. Since (ii) holds, it is derived that $(S, \bar{S})$ is the optimal partition with respect to $\mathbf{p}$, i.e., $S = S_{\mathbf{p}}$ and $\bar{S} = \bar{S}_{\mathbf{p}}$. Then by (ii) of Theorem 6, $(\mathbf{p}, \widetilde{\mathbf{p}})$ is one of the points where $|\phi_{\mathbf{p}}(\mathbf{x}, \mathbf{y})|$ attains its maximum value. Thus the equality in (6) holds. ■

By setting $p_i = d_i$ for every $i \in \mathbb{Z}_{[1,n]}$, $r = \delta$, $R = \Delta$, $S_{\mathbf{p}} = S$, and $\eta(S_{\mathbf{p}}, \bar{S}_{\mathbf{p}}) = 4m^2 \cdot \beta(S)$ as per Lemma 4, we immediately obtain the following upper bound.

Theorem 8 (Correction of Theroem 7)**.** *Let G be a connected (n, m)-graph with $n \geq 2$, and S be a subset $\mathbb{Z}_{[1,n]}$ that minimizes $\left|\sum_{i\in S} d_i - m\right|$.*

$$M_1(G) \leq \frac{4m^2}{n}\left[1 + \left(\sqrt{\frac{\Delta}{\delta}} - \sqrt{\frac{\delta}{\Delta}}\right)^2 \beta(S)\right] \tag{8}$$

where

$$\beta(S) = \frac{1}{2m}\sum_{i\in S} d_i \left(1 - \frac{1}{2m}\sum_{i\in S} d_i\right)$$

The equality holds if and only if G is regular, or G is bidegered such that $\Delta = d_1 = d_2 = \cdots = d_s > d_{s+1} = d_{s+2} = \cdots = d_n = \delta$ and for every $a \in \mathbb{Z}_{[1,s]}$ and $b \in \mathbb{Z}_{[1,\,n-s]}$ such that $a\Delta \neq b\delta$, the number s satisfies:

$$s \leq \frac{a\Delta - b\delta + n\delta}{\Delta + \delta} \text{ when } a\Delta > b\delta, \text{ and}$$
$$s \geq \frac{a\Delta - b\delta + n\delta}{\Delta + \delta} \text{ when } a\Delta < b\delta.$$

Remark. The condition for equality to hold in Theorem 8 is satisfied when $\frac{n\delta}{\Delta+\delta} \in \mathbb{Z}$ and $s = \frac{n\delta}{\Delta+\delta}$. Hence the condition in Theorem 7 is a special case of the condition in Theorem 8.

5 Spillover effect of above corrections

According to our investigation, the absence or incorrect statement of the necessary and sufficient conditions for equality in Theorem 2, Theorem 5 and Theorem 7 has led to similar errors in the literature. Conducting an exhaustive review of all papers that have encountered issues in this field is not feasible; therefore, we limit our corrections to a selected subset of these papers.

Error 1. From Line 11 to Line 19 on Page 480 of [13], the following theorem (Theorem 1 in [13]) is presented:

Theorem 9 (Theorem 1 in [13]). *Let $p = (p_i)$ and $a = (a_i)$, $i = 1, 2, \ldots, m$, be real number sequences, with $a = (a_i)$ being monotonic and $0 < r \leq a_i \leq R < +\infty$. Let S be a subset of $I_m = \{1, 2, \ldots, m\}$ which minimizes the expression*

$$\left| \sum_{i \in S} p_i - \frac{1}{2} \sum_{i=1}^{m} p_i \right| .$$

Then

$$\sum_{i=1}^{m} p_i a_i \sum_{i=1}^{m} \frac{p_i}{a_i} \leq \left(1 + \gamma(S) \frac{(R-r)^2}{rR} \right) \left(\sum_{i=1}^{m} p_i \right)^2 , \tag{9}$$

where

$$\gamma(S) = \frac{\sum_{i \in S} p_i}{\sum_{i=1}^{m} p_i} \left(1 - \frac{\sum_{i \in S} p_i}{\sum_{i=1}^{m} p_i} \right) .$$

Equality is attained if $R = a_1 = \cdots = a_m = r$.

Comments.

i. There is an error in the necessary and sufficient condition for equality to hold. We present a counterexample below. Let $p = (3, 3, 3, 2, 2, 2, 2, 2)$, $a = (4, 4, 4, 1, 1, 1, 1, 1)$, $R = 4$, and $r = 1$. Then $S = \{1, 2, 3\}$. Consequently, the right-hand side of equation (9) evaluates to 563.5. Similarly, the left-hand side of equation (9) also equals 563.5. Thus, the equality holds; however, the condition $R = a_1 = \cdots = a_m = r$ does not hold.

ii. The correction can be derived from Theorem 6 (the Andrica-Badea inequality) of this commentary.

Error 2. In Section 3 (Auxiliary Results) of [10], the authors presented the same conclusion as in Theorem 9 above, leading to the same counterexample.

Error 3. From Line 24 to Line 29 on Page 262 (Section 3: Auxiliary Results) of [10], the authors erroneously cited Theorem 2 (rewritten as (12) and (13) in [10]). Additionally, the necessary and sufficient condition for equality to hold is incorrect (the correct condition is given by Theorem 3 of this commentary). It remains unclear whether this error impacts the validity of Theorem 5 in [10]. A detailed verification by the authors is recommended.

Error 4. The authors in [5] cited Theorem 2 (labeled as Lemma 2.1 in [5]). This citation led to an error in the following theorem (labeled as Theorem 2.2 in [5]):

Theorem 10 (Theorem 2.2 in [5])**.** *Let D be a digraph of order n with a arcs having first outdegree Zagreb index $Zg^+(D)$. Let Δ^+ be the maximum outdegree and let k be the largest positive integer such that $d_k^+ > 0$, where $1 \leq k \leq n$. Then*

$$Zg^+(D) \leq \frac{1}{k}\Big(\alpha(k)(\Delta^+ - d_k^+)^2 + a^2\Big).$$

Equality occurs if and only if $d_1^+ = d_2^+ = \cdots = d_k^+$.

Comments.

i. We present a counterexample D, which is a digraph with an outdegree sequence of $(4, 4, 4, 3, 3, 3, 3)$. While parallel arcs (for example, two arcs from v to u) are not allowed in [5], symmetric pairs of arcs (such as (v, u) and (u, v)) are permitted. Consequently, constructing a digraph D with the specified outdegree sequence $(4, 4, 4, 3, 3, 3, 3)$ is straightforward.

ii. The correction can be derived from Theorem 3 of this commentary.

Error 5. In [7], the authors erroneously cited Theorem 2 (labeled as Theorem 2.11 in [7]). However, this error does not affect the validity of Theorem 2.12 in [7], as the proof of Theorem 2.12 relies on the Cauchy-Schwarz inequality, simultaneously.

6 Conclusions

Our investigation reveals that numerous papers have cited the error addressed in this commentary. Fortunately, only a few of them appear to have propagated new errors. In most cases, such as Errors 3 and 5, it is unclear whether the error led to incorrect results or if the flawed reasoning coincidentally yielded correct conclusions. We believe it is appropriate for the authors of these works to conduct independent, careful reviews and issue any necessary corrections.

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