Comparing Variable Zagreb Indices of Graphs *

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Abstract

The variable first and second Zagreb indices are defined to be $\lambda M_1(G) = \sum_{u \in V}(d(u))^{2\lambda}$ and $\lambda M_2(G) = \sum_{uv \in E}(d(u)d(v))^{\lambda}$, where $\lambda$ is any real number. In this paper, we prove that when $\lambda \in [0, 1]$ (resp. $\lambda \in (-\infty, 0)$), $\lambda M_1(G)/n \leq \lambda M_2(G)/m$ (resp. $\lambda M_1(G)/n \geq \lambda M_2(G)/m$) holds for graphs $G$ satisfying one of the following conditions: $\Delta(G) - \delta(G) \leq 2$; $\Delta(G) - \delta(G) \leq 3$ and $\delta(G) \neq 2$; $G$ is a chemical graph. When $\lambda \in (1, +\infty)$, the relationship of numerical value between $\lambda M_1(G)/n$ and $\lambda M_2(G)/m$ is indefinite for distinct graphs $G$ even if $\Delta(G) - \delta(G) \leq 2$.

1 Introduction

A molecular graph is a representation of the structural formula of a chemical compound in terms of graph theory, whose vertices correspond to the atoms of the compound and edges correspond to chemical bonds. The first Zagreb index $M_1(G)$ and the second Zagreb index $M_2(G)$ are usually used in the study of molecular graphs, and they are defined in [2] as follows:

$$M_1(G) = \sum_{u \in V}(d(u))^2 \text{ and } M_2(G) = \sum_{uv \in E}d(u)d(v),$$

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where $V$ is the set of vertices, $E$ is the set of edges and $d(u)$ is degree of the vertex $u$ of $G$. The research of Zagreb indices and their generalization are often found in chemistry and mathematical chemistry.

A natural issue is to compare the values of the Zagreb indices on the same graph. In [1], the AutoGraphiX system proposed the following conjecture:

**Conjecture 1.1 ([1])** For all simple connected graphs $G$,

$$\frac{M_1(G)}{n} \leq \frac{M_2(G)}{m}$$

and the bound is tight for complete graphs.

However, this conjecture does not hold for all general graphs ([3]), while it is proved to be true for chemical graphs ([3]), trees ([10]) and unicyclic graphs([7]), and connected bicyclic graphs except one class ([9]). Besides, its generalization to the variable Zagreb indices has already been discussed (see e.g. [5, 6, 13]). The variable first and the variable second Zagreb indices are defined as:

$$\lambda M_1(G) = \sum_{u \in V} (d(u))^2$$

and

$$\lambda M_2(G) = \sum_{uv \in E} (d(u)d(v))^\lambda,$$

where $\lambda$ is any real number. Clearly, $\frac{1}{2} M_1(G) = M_1(G)$ and $\frac{1}{2} M_2(G) = M_2(G)$.

Similarly as Conjecture 1.1, many mathematicians showed that

$$\frac{\lambda M_1(G)}{n} \leq \frac{\lambda M_2(G)}{m}$$

is true for the following cases: all chemical graphs and $\lambda \in [0, 1]$ ([11]), all trees and $\lambda \in [0, 1]$ ([12]), all unicyclic graphs and $\lambda \in [0, 1]$ ([4]).

On the other hand, the inequality

$$\frac{\lambda M_1(G)}{n} \geq \frac{\lambda M_2(G)}{m}$$

is true for the following cases: all unbalanced bipartite graphs and $\lambda \in R \setminus [0, 1]$ ([11]), all unicyclic graphs and $\lambda \in (-\infty, 0]$ ([14]).

Let $G$ be an undirected, simple graph. Let $\Delta(G)$ and $\delta(G)$ denote the maximum and minimum degrees of $G$, respectively. A graph $G$ is called a chemical graph if $\Delta(G) \leq 4$. A graph $G$ is called $k$-regular if $d(v) = k$ for all $v \in V(G)$.

It is known to all that there are many molecular graphs with small difference between the maximum and minimum degrees. In [8], it has been proved that $M_1(G)/n \leq M_2(G)/m$ holds for graphs $G$ with small difference between the maximum and minimum degrees, which implies the results in [3].
In this paper, we investigate the relationship of $\lambda M_1(G)/n$ and $\lambda M_2(G)/m$ in the graphs $G$ with small difference between the maximum and minimum degrees for $\lambda \in R$. When $\lambda \in [0, 1]$ (resp. $\lambda \in (-\infty, 0)$), we show that (1) (resp. (2)) holds for graphs satisfying one of the following conditions: $\Delta(G) - \delta(G) \leq 3$ and $\delta(G) \neq 2$; all chemical graphs. Moreover, the extremal graphs (with the equality (1) or (2) holds) are characterized completely. When $\lambda \in (1, +\infty)$, the relationship of numerical value between $\lambda M_1(G)/n$ and $\lambda M_2(G)/m$ is indefinite for distinct graphs even if $\Delta(G) - \delta(G) \leq 2$.

2 Preliminaries

In this section, we introduce some notations and lemmas which are useful in the presentations and proofs of our main results.

Let $\{i, j\}, \{k, l\} \in (Z^+)^2$ and $\lambda \in R$. Suppose

$$f_{\lambda}^1(i, j, k, l) = i^{k+1}j^{l+1} + j^{k+1}i^{l+1} + f_{\lambda}^1 k + j f_{\lambda}^1 l + i f_{\lambda}^1 k + i j k l l - i j k l l.$$

In the following lemmas, let $a, b, c, d$ be distinct positive integers.

**Lemma 2.1** $f_{\lambda}^1(a, a, a, a) = 0$.

**Proof.** Obviously, we have $f_{\lambda}^1(a, a, a, a) = 4a^{2+3} - 4a^{2+3} = 0$. □

**Lemma 2.2** $f_{\lambda}^1(a, a, a, b) = \begin{cases} > 0, & \text{if } 0 < \lambda \leq 1, \\ < 0, & \text{if } \lambda < 0. \end{cases}$

**Proof.** Note that $f_{\lambda}^1(a, a, a, b) = a^{2+2}b + a^{2+3} + 2a^{1+2}b^{1+1} - 3a^{2+2}b - a^2b^2$

$$= a^2(b^2 - a^2)(b - a)a^2 + ab(a^{a-1} - b^{a-1}).$$

**Case 1.** $0 \leq \lambda \leq 1$.

If $b > a > 0$, then $b^4 - a^4 > 0$, $(b - a)a^4 + ab(a^{a-1} - b^{a-1}) > 0$.

If $a > b > 0$, then $b^4 - a^4 < 0$, $(b - a)a^4 + ab(a^{a-1} - b^{a-1}) < 0$.

Therefore, we always have $f_{\lambda}^1(a, a, a, b) > 0$.

**Case 2.** $\lambda < 0$.

If $b > a > 0$, then $b^4 - a^4 < 0$, $(b - a)a^4 + ab(a^{a-1} - b^{a-1}) > 0$.

If $a > b > 0$, then $b^4 - a^4 > 0$, $(b - a)a^4 + ab(a^{a-1} - b^{a-1}) < 0$.

It can be seen that $f_{\lambda}^1(a, a, a, b) < 0$. □
Lemma 2.3  \( f_{(a, b), (b, b)} \) \[
\begin{aligned}
&< 0, \quad \text{if } \lambda < 0, \\
&> 0, \quad \text{if } 0 < \lambda \leq 1,
\end{aligned}
\]

Proof. Note that \( f_{(a, a), (b, b)} = 2a^{2t+2}b + 2ab^{2t+2} - 2a^{2t+1}b^2 - 2a^2b^{2t+1} \)

\[= 2ab(b - a)(b^{2t} - a^{2t}). \]

Case 1. \( 0 < \lambda \leq 1 \). Without loss of generality, suppose \( b > a > 0 \). Then

\[b - a > 0, \quad b^{2t} - a^{2t} > 0.\]

Thus we have \( f_{(a, a), (b, b)} > 0 \).

Case 2. \( \lambda < 0 \). Without loss of generality, suppose \( b > a > 0 \). Then

\[b - a > 0, \quad b^{2t} - a^{2t} < 0.\]

It follows that \( f_{(a, a), (b, b)} < 0. \)

Lemma 2.4  \( f_{(a, b), (a, b)} \) \[
\begin{aligned}
&< 0, \quad \text{if } \lambda < 0, \\
&> 0, \quad \text{if } 0 < \lambda < 1,
\end{aligned}
\]

Proof. Note that \( f_{(a, b), (a, b)} = 2a^{t+1}b^{t+2} + 2a^{t+2}b^{t+1} - 2a^{t+1}b^2 - 2a^2b^{2t+1} \)

\[= 2a^2b^2(b^t - a^t)(a^{t-1} - b^{t-1}). \]

Without loss of generality, suppose \( b > a > 0 \).

Case 1. \( \lambda = 1 \). Then \( b^{t} - a^{t} > 0, \quad a^{t-1} - b^{t-1} = 0 \). Hence \( f_{(a, b), (a, b)} = 0 \).

Case 2. \( 0 < \lambda < 1 \). Then \( b^{t} - a^{t} > 0, \quad a^{t-1} - b^{t-1} > 0 \). So \( f_{(a, b), (a, b)} > 0 \).

Case 3. \( \lambda < 0 \). Then \( b^{t} - a^{t} < 0, \quad a^{t-1} - b^{t-1} > 0 \). Thus \( f_{(a, b), (a, b)} < 0. \)

Lemma 2.5  \( f_{(a, b), (a, c)} \) \[
\begin{aligned}
&< 0, \quad \text{if } \lambda < 0, \\
&> 0, \quad \text{if } 0 < \lambda \leq 1,
\end{aligned}
\]

Proof. Notice that \( f_{(a, b), (a, c)} \)

\[= a^{t+1}b^{t+1}c + a^{t+2}b^{t+1} + a^{t+1}bc^{t+1} + a^{t+2}c^{t+1} - 2a^{t+1}bc - a^2b^2c - a^2bc^{2t} \]

\[= a^2bc[(a^{t-1} - b^{t-1})(b^t - a^t) + (a^{t-1} - c^{t-1})(c^t - a^t)] + a^{t+2}(c - b)(c^t - b^t). \]

Case 1. \( 0 < \lambda \leq 1 \). Without loss of generality, suppose \( c > b > 0 \).
If $c > b > a > 0$, then
\[ a^{d-1} - b^{d-1} \geq 0, \ b^1 - a^1 > 0, \ a^{d-1} - c^{d-1} \geq 0, \ c^d - a^d > 0, \ c^d - b^d > 0. \]

If $a > c > b > 0$, then
\[ a^{d-1} - b^{d-1} \leq 0, \ b^1 - a^1 < 0, \ a^{d-1} - c^{d-1} \leq 0, \ c^d - a^d < 0, \ c^d - b^d > 0. \]

If $c > a > b > 0$, then
\[ a^{d-1} - b^{d-1} \leq 0, \ b^1 - a^1 < 0, \ a^{d-1} - c^{d-1} \geq 0, \ c^d - a^d > 0, \ c^d - b^d > 0. \]

All in all, we always have $f^1_{[a, b], [a, c]} > 0$.

**Case 2.** $\lambda < 0$. Without loss of generality, suppose $c > b > 0$.

If $c > b > a > 0$, then
\[ a^{d-1} - b^{d-1} > 0, \ b^1 - a^1 < 0, \ a^{d-1} - c^{d-1} > 0, \ c^d - a^d < 0, \ c^d - b^d < 0. \]

If $a > c > b > 0$, then
\[ a^{d-1} - b^{d-1} < 0, \ b^1 - a^1 > 0, \ a^{d-1} - c^{d-1} < 0, \ c^d - a^d > 0, \ c^d - b^d < 0. \]

If $c > a > b > 0$, then
\[ a^{d-1} - b^{d-1} < 0, \ b^1 - a^1 > 0, \ a^{d-1} - c^{d-1} > 0, \ c^d - a^d < 0, \ c^d - b^d < 0. \]

Therefore, it can be conclude that $f^1_{[a, b], [a, c]} < 0$. \(\square\)

**Lemma 2.6** Let $c > b > 0$. If $c > a > b$, we suppose $bc \leq a^2$. Then
\[ f^1_{[a, a], [b, c]} \begin{cases} \geq 0, & \text{if } \lambda = 1, \\ > 0, & \text{if } 0 < \lambda < 1, \\ < 0, & \text{if } \lambda < 0. \end{cases} \]

**Proof.**
\[
f^1_{[a, a], [b, c]} = a^{2d+2} + a^{2d+2} b + 2ab^{d+1} c^{d+1} - 2a^{2d+1} bc - a^2 b^2 c - a^2 bc^{2d-1}
= a^2 bc(c^d - b^d)(b^{d-1} - c^{d-1}) + a(2bc - ab - ac)(b^d c^d - a^{2d}). \]

**Case 1.** $0 < \lambda \leq 1$.

If $c > b > a > 0$, then
\[ c^d - b^d > 0, \ b^{d-1} - c^{d-1} \geq 0, \ 2bc - ab - ac > 0, \ b^d c^d - a^{2d} > 0. \]
If $a > c > b > 0$, then
\[ c^4 - b^4 > 0, \quad b^{d-1} - c^{d-1} \geq 0, \quad 2bc - ab - ac < 0, \quad b^4c^4 - a^{2d} < 0. \]

If $c > a > b > 0$, then
\[ c^4 - b^4 > 0, \quad b^{d-1} - c^{d-1} \begin{cases} > 0, & \text{if } 0 < \lambda < 1, \\ = 0, & \text{if } \lambda = 1. \end{cases} \]

Since $bc \leq a^2$. Hence $b^4c^4 - a^{2d} \leq 0$, and
\[ 2bc - ab - ac \leq bc + a^2 - ab - ac = (c - a)(b - a) < 0. \]

It can be seen that $f^{\lambda}_{\{a, a\}, \{b, c\}} \begin{cases} > 0, & \text{if } 0 < \lambda < 1, \\ = 0, & \text{if } \lambda = 1. \end{cases}$

**Case 2.** $\lambda < 0$.
If $c > b > a > 0$, then
\[ c^4 - b^4 < 0, \quad b^{d-1} - c^{d-1} > 0, \quad 2bc - ab - ac > 0, \quad b^4c^4 - a^{2d} < 0. \]

If $a > c > b > 0$, then
\[ c^4 - b^4 < 0, \quad b^{d-1} - c^{d-1} > 0, \quad 2bc - ab - ac < 0, \quad b^4c^4 - a^{2d} > 0. \]

If $c > a > b > 0$, then $c^4 - b^4 < 0, \quad b^{d-1} - c^{d-1} > 0.$

Note that $bc \leq a^2$. Hence $b^4c^4 - a^{2d} \geq 0$, and
\[ 2bc - ab - ac \leq bc + a^2 - ab - ac = (c - a)(b - a) < 0. \]

Consequently, we conclude that $f^{\lambda}_{\{a, a\}, \{b, c\}} < 0$. \(\square\)

**Lemma 2.7** Let $c > b > 0$. If $c > a > b$, we suppose $a, \quad b, \quad c \in \{p, \quad p + 1, \quad p + 2, \quad p + 3\}$ and $p \neq 2$. Then
\[
\begin{align*}
f^{\lambda}_{\{a, a\}, \{b, c\}} & \begin{cases} \geq 0, & \text{if } \lambda = 1, \\ > 0, & \text{if } 0 < \lambda < 1, \\ < 0, & \text{if } \lambda < 0. \end{cases}
\end{align*}
\]

**Proof.** From the proof of Lemma 2.6, we need to discuss the case $c > a > b$.

**Case 1.** $0 < \lambda \leq 1$. Thus
\[
\begin{align*}
c^4 - b^4 & > 0, \quad b^{d-1} - c^{d-1} \begin{cases} > 0, & \text{if } 0 < \lambda < 1, \\ = 0, & \text{if } \lambda = 1. \end{cases}
\end{align*}
\]

**Subcase 1.1** $a = p + 1, \quad b = p, \quad c = p + 2$.
**Subcase 1.2** $a = p + 2, \quad b = p, \quad c = p + 3$.
**Subcase 1.3** $a = p + 2, \quad b = p + 1, \quad c = p + 3$. 
For Subcase 1.1-1.3, since $bc \leq a^2$, by Lemma 2.6, the results are obtained.

**Subcase 1.4** $a = p + 1$, $b = p$, $c = p + 3$. Then

$$b^4c^4 - a^2 = p^4(p + 3)^4 - (p + 1)^2 \begin{cases} > 0, & \text{if } p \geq 3; \\ = 0, & \text{if } p = 1. \end{cases}$$

$$2bc - ab - ac = p - 3 \geq 0 \text{ if } p \geq 3.$$

All in all, we obtain the results as desired.

**Case 2.** $\lambda < 0$. Then $c^4 - b^4 < 0$, $b^{l-1} - c^{l-1} > 0$.

Similarly, for Subcase 1.1-1.3, since $bc \leq a^2$, it follows from Lemma 2.6 that the results are obtained as desired.

If $a = p + 1$, $b = p$, $c = p + 3$, then

$$b^4c^4 - a^2 = p^4(p + 3)^4 - (p + 1)^2 \begin{cases} < 0, & \text{if } p \geq 3; \\ = 0, & \text{if } p = 1. \end{cases}$$

$$2bc - ab - ac = p - 3 \geq 0 \text{ if } p \geq 3.$$

Therefore, we always have $f_{\lambda}^4(a, b, c) < 0$ if $\lambda < 0$. □

**Lemma 2.8** Let $d > c$ and $a = \min\{a, b, c, d\}$. If $b > d > c > a$, we suppose $a + b \geq c + d$, $ab \leq cd$. Thus

$$f_{\lambda}^4(a, b, c, d) \begin{cases} \geq 0, & \text{if } \lambda = 1, \\ > 0, & \text{if } 0 < \lambda < 1, \\ < 0, & \text{if } \lambda < 0. \end{cases}$$

**Proof.** Note that $f_{\lambda}^4(a, b, c, d)$

$$= a^{l+1}b^{l+1}d + a^{l+1}b^{l+1}c + bc^{l+1}d^{l+1} + ac^{l+1}d^{l+1} - a^{2l+1}bcd - ab^{2l+1}c - abc^{2l+1}d - abcd^{2l+1}$$

$$= abcd[(a^{l-1} - b^{l-1})(b^{l} - a^{l}) + (c^{l-1} - d^{l-1})(d^{l} - c^{l})] + [ac(d - b) + bd(c - a)](c^{l}d^{l} - a^{l}b^{l}).$$

**Case 1.** $0 < \lambda \leq 1$.

If $d > c > b > a > 0$ or $d > b > c > a > 0$, then

$$a^{l-1} - b^{l-1} \geq 0, b^{l} - a^{l} > 0, c^{l-1} - d^{l-1} \geq 0, d^{l} - c^{l} > 0,$$

$$ac(d - b) + bd(c - a) > 0, c^{l}d^{l} - a^{l}b^{l} > 0.$$
If \( b > d > c > a > 0 \), since \( a + b \ge c + d \) and \( ab \le cd \), then
\[
a^{t_1} - b^{t_1} = \begin{cases} 
0, & \text{if } 0 < \lambda < 1, \\
> 0, & \text{if } \lambda = 1.
\end{cases}
\]
\[
c^4 d^4 - a^4 b^4 \ge 0, \quad ac(d - b) + bd(c - a) = cd(a + b) - ab(c + d) = ab(a + b - c - d) \ge 0.
\]
Therefore, we always have \( f^{t_1}_{(a, b), (c, d)} \ge 0, \) if \( 0 < \lambda < 1 \).

**Case 2.** \( \lambda < 0 \).
If \( d > c > b > a > 0 \) or \( d > b > c > a > 0 \), then
\[
a^{t_1} - b^{t_1} > 0, \quad b^4 - a^4 < 0, \quad c^{t_1} - d^{t_1} > 0, \quad d^4 - c^4 < 0,
\]
\[
ac(d - b) + bd(c - a) > 0, \quad c^4 d^4 - a^4 b^4 < 0.
\]
If \( b > d > c > a > 0 \), note that \( a + b \ge c + d \) and \( ab \le cd \), then
\[
a^{t_1} - b^{t_1} > 0, \quad b^4 - a^4 < 0, \quad c^{t_1} - d^{t_1} > 0, \quad d^4 - c^4 < 0,
\]
\[
c^4 d^4 - a^4 b^4 \le 0, \quad ac(d - b) + bd(c - a) \ge ab(a + b - c - d) \ge 0.
\]
Therefore, it can be seen that \( f^{t_1}_{(a, b), (c, d)} < 0. \)

### 3 Main results

Let \( G \) be a finite, undirected and simple graph. If \( xy \in E(G) \), we say that \( y \) is a neighbor of \( x \) and denote by \( N(x) \) the set of neighbors of \( x \). And \( d(x) = |N(x)| \) is called the degree of \( x \). We denote the number of vertices of degree \( i \) in \( G \) by \( n_i \) and the number of edges that connect vertices of degree \( i \) and \( j \) by \( m_{ij} \), where we do not distinguish \( m_{ij} \) and \( m_{ji} \). Similarly as in paper [11] we show that:

**Lemma 3.1** Let \( G \) be a graph with \( n \) vertices and \( m \) edges. Let \( N \) denote the set of the degrees of vertices in \( G \). Let \( \mu = \sum_{k \leq n} m_{kl} \cdot \sum_{k \leq n} m_{kl}(\frac{1}{k} + \frac{1}{l}) \). Then
\[
\lambda M_2(G) / m - \lambda M_1(G) / n = \frac{1}{\mu} \cdot \sum_{i, j, k, l \leq n} \left( f_{(i, j), (k, l)}^{t_1} \cdot \frac{m_{ij} m_{kl}}{i \cdot j \cdot k \cdot l} \right).
\]
Theorem 3.2 Let $G$ be a graph with $n$ vertices, $m$ edges and $\Delta(G) - \delta(G) \leq 2$.

If $\lambda \in [0, 1]$, then $\lambda M_1(G)/n \leq \lambda M_2(G)/m$. \hfill (3)

If $\lambda \in (-\infty, 0)$, then $\lambda M_1(G)/n \geq \lambda M_2(G)/m$. \hfill (4)

Moreover, if $\lambda = 0$, the equality of (3) always holds.

If $\lambda = 1$, the equality of (3) holds if and only if all edges $ij$ have the same pair $(d_i, d_j)$ of degrees.

If $\lambda \in (0, 1)$ (resp. $\lambda \in (-\infty, 0)$), the equality of (3) (resp. (4)) holds if and only if $G$ is a regular graph.

Proof. For simplicity, let $\delta(G) = p$ and $N = \{p, p + 1, p + 2\}$.

Case 1. If $\lambda = 0$, it is obvious that

$$0 M_1(G)/n = (\sum_{v \in V} \lambda^2)/n = 1 = (\sum_{u \in E} \lambda^0)/m = 0 M_2(G)/m.$$ 

Case 2. If $\lambda \in (0, 1)$ (resp. $\lambda \in (-\infty, 0)$), by Lemma 3.1,

$$\lambda M_2(G)/m - \lambda M_1(G)/n = \frac{1}{\mu} \sum_{i, j, k, l \in N^2} (f_{i, j, k, l}) \cdot \frac{m_{ij}m_{kl}}{i \cdot j \cdot k \cdot l}.$$ 

Note that all $i, j, k$ and $l$ can not be distinct numbers, we need to show that $f_{i, j, k, l} \geq 0$ (resp. $\leq 0$) for each $(i, j), (k, l) \subseteq N^2$. Let $a, b, c$ be distinct elements of $N$. Then we have the following subcases.

Subcase 2.1 $\{(i, j), (k, l)\} = \{(a, a), (a, a)\}$. By Lemma 2.1, $f_{i, j, k, l} = 0$.

Subcase 2.2 $\{(i, j), (k, l)\} = \{(a, a), (a, b)\}$. By Lemma 2.2,

$$f_{i, j, k, l} \begin{cases} > 0, & \text{if } 0 < \lambda \leq 1, \\ < 0, & \text{if } \lambda < 0. \end{cases}$$ 

Subcase 2.3 $\{(i, j), (k, l)\} = \{(a, a), (b, b)\}$. By Lemma 2.3,

$$f_{i, j, k, l} \begin{cases} > 0, & \text{if } 0 < \lambda \leq 1, \\ < 0, & \text{if } \lambda < 0. \end{cases}$$ 

Subcase 2.4 $\{(i, j), (k, l)\} = \{(a, b), (a, b)\}$. By Lemma 2.4,

$$f_{i, j, k, l} \begin{cases} = 0, & \text{if } \lambda = 1, \\ > 0, & \text{if } 0 < \lambda < 1, \\ < 0, & \text{if } \lambda < 0. \end{cases}$$
Subcase 2.5 \{\{i, j\}, \{k, l\}\} = \{\{a, b\}, \{a, c\}\}. By Lemma 2.5,

\[
\begin{align*}
 f_{\{i, j\}, \{k, l\}}^\lambda &> 0, \quad \text{if } 0 < \lambda \leq 1, \\
 &< 0, \quad \text{if } \lambda < 0.
\end{align*}
\]

Subcase 2.6 \{\{i, j\}, \{k, l\}\} = \{\{a, a\}, \{b, c\}\}. Without loss of generality, suppose \(i = j\) and \(l > k\). If \(k < i = j < l\), since \(N = \{p, p + 1, p + 2\}\), then \(kl = p(p + 2) \leq (p + 1)^2 = l^2\). By Lemma 2.6,

\[
\begin{align*}
 f_{\{i, j\}, \{k, l\}}^\lambda &\geq 0, \quad \text{if } \lambda = 1, \\
 &> 0, \quad \text{if } 0 < \lambda < 1, \\
 &< 0, \quad \text{if } \lambda < 0.
\end{align*}
\]

All in all, the inequality (3) (resp. (4)) is proved.

Moreover, if \(\lambda = 0\), then the equality of (3) always holds.

If \(\lambda = 1\), from the proof of Case 2, the equality of (3) holds if and only if \(f_{\{i, j\}, \{k, l\}}^\lambda = 0\) for all \(m_{ij} \cdot m_{kl} > 0\), which implies that all edges \(ij\) have the same pair \((d_i, d_j)\) of degrees (also see [8]).

If \(\lambda \in (0, 1)\) (resp. \(\lambda \in (-\infty, 0)\)), from the foregoing proof, the equality of (3) (resp. (4)) holds if and only if \(f_{\{i, j\}, \{k, l\}}^\lambda = 0\) for all \(m_{ij} \cdot m_{kl} > 0\), which means \(i = j = k = l\) for each \(\{i, j\}, \{k, l\} \subseteq N^2\), that is, \(G\) is a regular graph. \(\Box\)

From Theorem 3.2, we obtain the main result in [8] immediately.

**Corollary 3.3** ([8]) Let \(G\) be a graph with \(n\) vertices, \(m\) edges and \(\Delta(G) - \delta(G) \leq 2\). Then \(\frac{M_1(G)}{n} \leq \frac{M_2(G)}{m}\), with the equality holds if and only if all edges \(ij\) have the same pair \((d_i, d_j)\) of degrees.

Let \(G^*\) denote the graphs with each edge connecting a 3-degree vertex and a 6-degree vertex. The star graph \(S_n\) is a tree on \(n\) vertices with one vertex having degree \(n - 1\) and the other vertices having degree 1.

**Theorem 3.4** Let \(G\) be a graph with \(n\) vertices and \(m\) edges such that \(\Delta(G) - \delta(G) \leq 3\) and \(\delta(G) \neq 2\).

If \(\lambda \in [0, 1]\), then \(\frac{\lambda M_1(G)}{n} \leq \frac{\lambda M_2(G)}{m}\). \hspace{1cm} (5)

If \(\lambda \in (-\infty, 0)\), then \(\frac{\lambda M_1(G)}{n} \geq \frac{\lambda M_2(G)}{m}\). \hspace{1cm} (6)

Moreover, if \(\lambda = 0\), the equality of (5) always holds.
If \( \lambda = 1 \), the equality of (5) holds if and only if all edges \( ij \) have the same pair \((d_i, d_j)\) of degrees or if the graph is composed of disjoint stars \( S_5 \) and cycles of any length or if the graph is composed of disjoint \( G^2 \) and 4-regular graphs ([8]).

If \( \lambda \in (0, 1) \) (resp. \( \lambda \in (-\infty, 0) \)), the equality of (5) (resp. (6)) holds if and only if \( G \) is a regular graph.

**Proof.** For simplicity, let \( \delta(G) = p \) and \( N = \{p, p+1, p+2, p+3\} \). Let \( a, b, c, d \) be distinct elements of \( N \). If \( \lambda = 0 \), it is obvious that \( ^0M_1(G)/n = ^0M_2(G)/m \).

If \( \lambda \in (0, 1) \) (resp. \( \lambda \in (-\infty, 0) \)), by Lemma 3.1, we just need to show that \( f_{[i, \ j], \ [k, \ l]} = 0 \) (resp. \( \leq 0 \)) for each \( \{i, \ j\}, \{k, \ l\} \subseteq N^2 \) \((i \leq j, k \leq l)\).

In the proof of Theorem 3.2, we found that \( f_{[i, \ j], \ [k, \ l]} = 0 \) holds for the case
\[
\begin{cases}
\geq 0, & \text{if } \lambda = 1, \\
\geq 0, & \text{if } 0 < \lambda < 1, \\
< 0, & \text{if } \lambda < 0
\end{cases}
\]

of \( \{i, \ j\}, \{k, \ l\} = \{\{a, a\}, \{a, a\}\} \), and \( f_{[i, \ j], \ [k, \ l]} > 0 \), \( if \ 0 < \lambda < 1 \), holds for the case \( \{i, \ j\}, \{k, \ l\} \) \( \geq 0 \) if \( \lambda = 1 \), \( \geq 0 \) if \( 0 < \lambda < 1 \), \( < 0 \) if \( \lambda < 0 \)

cases \( \{i, \ j\}, \{k, \ l\} = \{\{a, a\}, \{a, b\}\}, \{\{a, a\}, \{b, b\}\}, \{\{a, b\}, \{a, b\}\} \) and \( \{\{a, b\}, \{a, c\}\} \). We only need to discuss the following two cases.

**Case 1.** \( \{i, \ j\}, \{k, \ l\} = \{\{a, a\}, \{a, b\}\} \). Without loss of generality, suppose \( i = j \) and \( l > k \). It follows from Lemma 2.7 that
\[
\begin{cases}
\geq 0, & \text{if } \lambda = 1, \\
> 0, & \text{if } 0 < \lambda < 1, \\
< 0, & \text{if } \lambda < 0
\end{cases}
\]

Case 2. \( \{i, \ j\}, \{k, \ l\} = \{\{a, b\}, \{c, d\}\} \). Without loss of generality, suppose \( l > k \) and \( i = \min\{i, j, k, l\} \). If \( i < k < l < j \), then \( i = p, k = p + 1, l = p + 2, j = p + 3 \), and it follows that \( i + j = 2p + 3 = k + l \), and \( ij = p^2 + 3p \leq p^2 + 3p + 2 = kl \).

Then by Lemma 2.8, we obtain that \( f_{[i, \ j], \ [k, \ l]} \)
\[
\begin{cases}
\geq 0, & \text{if } \lambda = 1, \\
> 0, & \text{if } 0 < \lambda < 1, \\
< 0, & \text{if } \lambda < 0
\end{cases}
\]

Therefore, the inequality (5) and (6) are proved.

Moreover, if \( \lambda = 0 \), the equality of (5) always holds.

If \( \lambda = 1 \), the equality of (5) in this case had been proved in [8].

If \( \lambda \in (0, 1) \) (resp. \( \lambda \in (-\infty, 0) \)), from the foregoing proof, the equality of (5) (resp. (6)) holds if and only if \( f_{[i, \ j], \ [k, \ l]} = 0 \) for all \( m_{ij} \cdot m_{kl} > 0 \), which means \( i = j = k = l \) for each \( \{i, j\}, \{k, l\} \subseteq N^2 \), that is, \( G \) is a regular graph. \( \square \)
If $\lambda = 1$, Hansen and Vukičević in [3] proved that $M_1(G)/n \leq M_2(G)/m$ for chemical graphs. Now we consider the case $\lambda \in (0, 1)$ (resp. $\lambda \in (-\infty, 0)$).

**Corollary 3.5** Let $G$ be a chemical graph with $n$ vertices and $m$ edges.

If $\lambda \in (0, 1)$, then $\lambda M_1(G)/n \leq \lambda M_2(G)/m$. ([11])

(7)

If $\lambda \in (-\infty, 0)$, then $\lambda M_1(G)/n \geq \lambda M_2(G)/m$.

(8)

Moreover, if $\lambda \in (0, 1)$ (resp. $\lambda \in (-\infty, 0)$), the equality of (7) (resp. (8)) holds if and only if $G$ is a regular graph.

**Proof.** Note that $G$ is a chemical graph, thus $\Delta \leq 4$. If $\delta = 1$, then $\Delta - \delta \leq 3$, by Theorem 3.4, the results are proved. If $\delta \geq 2$, we have $\Delta - \delta \leq 2$, and it follows from Theorem 3.2 that the results are obtained as desired. □

Let $e_i, e_j \in E$, where the degrees of their end vertices are $\{d_{i_1}, d_{i_2}\}$ ($d_{i_1} \leq d_{i_2}$) and $\{d_{j_1}, d_{j_2}\}$ ($d_{j_1} \leq d_{j_2}$), respectively. A pair of edges $[e_i, e_j]$ is called a degrees-nested edges pair if $d_{i_1} < d_{j_1} \leq d_{j_2} < d_{i_2}$ or $d_{j_1} < d_{i_1} \leq d_{i_2} < d_{j_2}$.

**Corollary 3.6** Let $G$ be a graph with $n$ vertices, $m$ edges, and $G$ contains no degrees-nested edges pairs.

If $\lambda \in (0, 1)$, then $\lambda M_1(G)/n \leq \lambda M_2(G)/m$.

(9)

If $\lambda \in (-\infty, 0)$, then $\lambda M_1(G)/n \geq \lambda M_2(G)/m$.

(10)

Moreover, if $\lambda \in (0, 1)$ (resp. $\lambda \in (-\infty, 0)$), the equality of (9) (resp. (10)) holds if and only if $G$ is a regular graph.

**Proof.** If $\lambda \in (0, 1]$ (resp. $\lambda \in (-\infty, 0)$), by Lemma 3.1, we just need to show that $f_{\lambda}^{i, j, k, l} \geq 0$ (resp. $\leq 0$) for each $\{i, j\}, \{k, l\} \subseteq \mathbb{N}^2$ ($i \leq j, k \leq l$) (*)

Since $G$ contains no degrees-nested edges pairs, from the proof of Lemma 2.1-2.8, we conclude that (*) always holds, and this completes the proof. □

Finally, we consider the relationship of $\lambda M_1(G)/n$ and $\lambda M_2(G)/m$ for $\lambda > 1$. A simple graph on $n$ vertices in which each pair of distinct vertices is joined by an edge is called a complete graph, and denoted by $K_n$. A complete bipartite graph is a simple bipartite graph with bipartition $(X, Y)$ in which each vertex of $X$ is joined to each vertex of $Y$; if $|X| = n_1$ and $|Y| = n_2$, such a graph is denoted by $K_{n_1, n_2}$. The disjoint union of $k$ copies of $G$ is often written by $kG$. 
Example 1 Let $G_1$ be a graph of order 9 created from $K_3$ and $3K_2$ by connecting each vertex of $K_3$ to a vertex of a $K_2$. Thus $\Delta(G_1) - \delta(G_1) = 3 - 1 = 2$, and

$$\lambda M_2(G_1)/m - \lambda M_1(G_1)/n = \frac{6^4 + 2^4 - 4^4 - 1}{3} > 0 \text{ for } \lambda > 1.$$ 

Example 2 Let $G_2 = K_{4, 5}$. Obviously, $\Delta(G_2) - \delta(G_2) = 5 - 4 = 1$, and

$$\lambda M_2(G_2)/m - \lambda M_1(G_2)/n = \frac{9 \cdot 20^4 - 4 \cdot 25^4 - 5 \cdot 16^4}{9} < 0 \text{ for } \lambda > 1.$$ 

Remark 1 It is known that the inequality $\lambda M_2(G)/m - \lambda M_1(G)/n < 0$ is true for all unbalanced bipartite graphs $G$ and $\lambda \in \mathbb{R}\setminus[0, 1]$ ([11]).

Combining Example 1 and 2, when $\lambda > 1$, we can find a suitable graph $G_1$ such that $\lambda M_2(G_1)/m - \lambda M_1(G_1)/n > 0$, and a suitable graph $G_2$ such that $\lambda M_2(G_2)/m - \lambda M_1(G_2)/n < 0$. Besides, note that $\Delta(G_i) - \delta(G_i) \leq 2$ ($i = 1, 2$) and $|V(G_i)| = |V(G_2)|$, we conclude that when $\lambda \in (1, +\infty)$, the relationship of $\lambda M_1(G)/n$ and $\lambda M_2(G)/m$ is indefinite for distinct graphs $G$ even if $\Delta(G) - \delta(G) \leq 2$.

References


