

On Comparing Variable Zagreb Indices for Unicyclic Graphs

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Abstract

Recently, the first and second Zagreb indices are generalized into the variable Zagreb indices which are defined by ${}^{\lambda}M_1(G) = \sum_{u \in V} (d(u))^{2\lambda}$ and ${}^{\lambda}M_2(G) = \sum_{uv \in E} (d(u)d(v))^{\lambda}$, where λ is any real number. In this paper, we prove that ${}^{\lambda}M_1(G)/n \geq {}^{\lambda}M_2(G)/m$ for all unicyclic graphs and all $\lambda \in (-\infty, 0]$. And we also show that the relationship of numerical value between ${}^{\lambda}M_1(G)/n$ and ${}^{\lambda}M_2(G)/m$ is indefinite in the distinct unicyclic graphs for each $\lambda \in (1, +\infty)$. With the conclusion in [4], we finish discussing the relationship of ${}^{\lambda}M_1(G)/n$ and ${}^{\lambda}M_2(G)/m$ in unicyclic graphs for $\lambda \in R$.

1 Introduction

The first and second Zagreb indices are among the oldest and the most famous topological indices, which are defined as:

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

where V is the set of vertices, E is the set of edges and $d(u)$ is degree of vertex u . $|V| = n$, $|E| = m$.

Recently, the system AutoGraphiX proposed the following conjecture:

Conjecture 1.1 *For all simple connected graph G ,*

$$M_1(G)/n \leq M_2(G)/m$$

and the bound is tight for complete graphs.

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But, in paper [5], this conjecture is proved not true, while it is proved true for chemical graphs([5]), trees([3]) and unicyclic graphs([1]). The generalization of this claim to the variable Zagreb indices has been analyzed. The variable first and second Zagreb indices are defined as:

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

where λ is any real number, with the following theorems from paper [2–4].

Theorem 1.2 For all chemical graphs G and all $\lambda \in [0, 1]$, it holds that ${}^\lambda M_1(G)/n \leq {}^\lambda M_2(G)/m$.

Theorem 1.3 For all trees G and all $\lambda \in [0, 1]$, it holds that ${}^\lambda M_1(G)/n \leq {}^\lambda M_2(G)/m$.

Theorem 1.4 Let $\lambda \in R \setminus [0, 1]$ and G be any unbalanced bipartite graph. Then, ${}^\lambda M_1(G)/n > {}^\lambda M_2(G)/m$.

Theorem 1.5 For all graphs G and all $\lambda \in [0, 1/2]$, it holds that ${}^\lambda M_1(G)/n \leq {}^\lambda M_2(G)/m$.

Theorem 1.6 Let $\lambda \in (\sqrt{2}/2, 1)$. Then, there is a graph G such that ${}^\lambda M_1(G)/n > {}^\lambda M_2(G)/m$.

Theorem 1.7 For all unicyclic graphs G and all $\lambda \in [0, 1]$, it holds that ${}^\lambda M_1(G)/n \leq {}^\lambda M_2(G)/m$.

It is known to all that the variable Zagreb indices are often used in the study of unicyclic molecules. In this paper, we show that the relationship of numerical value between ${}^\lambda M_1(G)/n$ and ${}^\lambda M_2(G)/m$ for $\lambda \in R \setminus [0, 1]$. With the conclusion in [4], we finish discussing the relationship of the variable first and second Zagreb indices in unicyclic graphs for $\lambda \in R$.

2 Comparing Variable Zagreb Indices for Unicyclic Graphs for $\lambda \leq 0$

Theorem 2.1 Let G be a connected unicyclic graph with n vertices and m edges. Then

$${}^\lambda M_1(G)/n \geq {}^\lambda M_2(G)/m, \lambda \in (-\infty, 0]$$

Moreover, if $\lambda \in (-\infty, 0)$, then ${}^\lambda M_1(G)/n = {}^\lambda M_2(G)/m$ holds if and only if G is a cycle.

Proof. If G is a cycle, it is easy to see that ${}^\lambda M_1(G)/n = {}^\lambda M_2(G)/m, \lambda \in (-\infty, 0]$. So we may assume that G is not a cycle in the following proof.

Since G is a connected unicyclic graph, we have $n = m$. Moreover, by the definition of ${}^\lambda M_1(G)$ and ${}^\lambda M_2(G)$, it is obvious that ${}^0 M_1(G) = \sum_{u \in V} (d(u))^{2 \cdot 0} = n = m = {}^0 M_2(G) = \sum_{uv \in E} (d(u)d(v))^{0 \cdot 0}$. So we only need to prove ${}^\lambda M_1(G) > {}^\lambda M_2(G), \lambda \in (-\infty, 0)$. We prove this conclusion by induction on n .

If $n = 4$, since G is not a cycle, G is a connected unicyclic graph that has a triangle and a pendant vertex. Then we have

$${}^{\lambda}M_1(G) = 2^{2\lambda} + 2^{2\lambda} + 3^{2\lambda} + 1^{2\lambda} = 4^{\lambda} + 4^{\lambda} + 9^{\lambda} + 1,$$

$${}^{\lambda}M_2(G) = (2 \times 2)^{\lambda} + (2 \times 3)^{\lambda} + (3 \times 2)^{\lambda} + (3 \times 1)^{\lambda} = 4^{\lambda} + 6^{\lambda} + 6^{\lambda} + 3^{\lambda}.$$

Then

$$\begin{aligned} {}^{\lambda}M_1(G) - {}^{\lambda}M_2(G) &= 4^{\lambda} + 4^{\lambda} + 9^{\lambda} + 1 - 4^{\lambda} - 6^{\lambda} - 6^{\lambda} - 3^{\lambda} \\ &> 1 + 9^{\lambda} - 4^{\lambda} - 3^{\lambda}. \end{aligned}$$

Suppose $f_1(\lambda) = 1 + 9^{\lambda} - 4^{\lambda} - 3^{\lambda}$, $\lambda \in (-\infty, 0)$. Then

$$\begin{aligned} f_1'(\lambda) &= 9^{\lambda} \ln 9 - 4^{\lambda} \ln 4 - 3^{\lambda} \ln 3 \\ &= 2 \cdot 9^{\lambda} \ln 3 - 4^{\lambda} \ln 4 - 3^{\lambda} \ln 3 \\ &= (9^{\lambda} - 3^{\lambda}) \ln 3 + (9^{\lambda} \ln 3 - 4^{\lambda} \ln 4) \\ &< 0. \end{aligned}$$

Note that $f_1(\lambda)$ is decreasing on $(-\infty, 0)$ in λ . We have $f_1(\lambda) > f_1(0) = 1 + 9^0 - 4^0 - 3^0$. Therefore, ${}^{\lambda}M_1(G) - {}^{\lambda}M_2(G) > 0$, $\lambda \in (-\infty, 0)$.

Suppose that it holds for all connected unicyclic graphs with vertices less than n . Since G is not a cycle, there exists a pendant vertex v and its unique neighbor vertex u . Denote by $N_G(u)$ the set of the neighbor vertices of u . Let $N_G(u) = \{v, v_1, v_2, \dots, v_k\}$, ($k \geq 1$) and $N_G[u] = N_G(u) \cup \{u\}$, where $v_i \in V(G)$, ($1 \leq i \leq k$). Let $V(G) = N_G[u] \cup \{x_1, x_2, \dots, x_{n-k-2}\}$.

Case 1 When $k = 1$.

Then $N_G(u) = \{v, v_1\}$. Denote $N_G(v_1) = \{u, u_1, \dots, u_p\}$, ($p \geq 1$), where $u_i \in V(G)$, ($1 \leq i \leq p$).

Subcase 1.1 When $p = 1$.

Let $G' = G - v$. Then G' is a connected unicyclic graph with $n - 1$ vertices. Since u is a pendant vertex in G' , G' is not a cycle. By the induction hypothesis, we have ${}^{\lambda}M_1(G') > {}^{\lambda}M_2(G')$, $\lambda \in (-\infty, 0)$. Now we compare ${}^{\lambda}M_1(G)$ and ${}^{\lambda}M_2(G)$.

$${}^{\lambda}M_1(G) = {}^{\lambda}M_1(G') + 2^{2\lambda} - 1 + 1 = {}^{\lambda}M_1(G') + 4^{\lambda},$$

$${}^{\lambda}M_2(G) = {}^{\lambda}M_2(G') + 4^{\lambda} - 2^{\lambda} + 2^{\lambda} = {}^{\lambda}M_2(G') + 4^{\lambda}.$$

Then

$${}^{\lambda}M_1(G) - {}^{\lambda}M_2(G) = {}^{\lambda}M_1(G') + 4^{\lambda} - {}^{\lambda}M_2(G') - 4^{\lambda} > 0.$$

Subcase 1.2 When $p \geq 2$.

Suppose $V(G) = \{v\} \cup N_G[v_1] \cup \{y_1, y_2, \dots, y_{n-k-3}\}$, where $y_i \in V(G)$, $(1 \leq i \leq n-k-3)$. Let $G'' = G - v - u$. Then G'' is a connected unicyclic graph with $n-2$ vertices. If G'' is a cycle, ${}^\lambda M_1(G'') = {}^\lambda M_2(G'')$. If G'' is not a cycle, by the induction hypothesis, ${}^\lambda M_1(G'') > {}^\lambda M_2(G'')$. Now we compare ${}^\lambda M_1(G)$ and ${}^\lambda M_2(G)$.

$$\begin{aligned} {}^\lambda M_1(G) &= {}^\lambda M_1(G'') + (p+1)^{2\lambda} - p^{2\lambda} + 2^{2\lambda} + 1, \\ {}^\lambda M_2(G) &= {}^\lambda M_2(G'') + [2(p+1)]^\lambda + 2^\lambda - [p^\lambda - (p+1)^\lambda] \sum_{i=1}^p (d_G(u_i))^\lambda. \end{aligned}$$

Then

$$\begin{aligned} {}^\lambda M_1(G) - {}^\lambda M_2(G) &= {}^\lambda M_1(G'') - {}^\lambda M_2(G'') + (p+1)^{2\lambda} - p^{2\lambda} + 2^{2\lambda} + 1 - [2(p+1)]^\lambda - 2^\lambda \\ &\quad + [p^\lambda - (p+1)^\lambda] \sum_{i=1}^p (d_G(u_i))^\lambda \\ &> (p+1)^{2\lambda} - p^{2\lambda} + 2^{2\lambda} + 1 - [2(p+1)]^\lambda - 2^\lambda. \end{aligned}$$

Suppose $g_1(x) = (x+1)^{2\lambda} - x^{2\lambda} + 2^{2\lambda} + 1 - [2(x+1)]^\lambda - 2^\lambda$, $(x \geq 2)$. Then

$$\begin{aligned} g'_1(x) &= 2\lambda(x+1)^{2\lambda-1} - 2\lambda x^{2\lambda-1} - 2\lambda[2(x+1)]^{\lambda-1} \\ &= 2\lambda\{(x+1)^{2\lambda-1} - x^{2\lambda-1} - [2(x+1)]^{\lambda-1}\} \\ &> 0. \end{aligned}$$

Note that $g_1(x)$ is increasing in $x \geq 2$. We have $g_1(x) \geq g_1(2) = 1 + 9^\lambda - 2^\lambda - 6^\lambda$. Suppose $f_2(\lambda) = 1 + 9^\lambda - 2^\lambda - 6^\lambda$, $\lambda \in (-\infty, 0)$. Then

$$\begin{aligned} f'_2(\lambda) &= 9^\lambda \ln 9 - 2^\lambda \ln 2 - 6^\lambda \ln 6 \\ &= 2 \cdot 9^\lambda \ln 3 - 2^\lambda \ln 2 - 6^\lambda \ln 2 - 6^\lambda \ln 3 \\ &= (9^\lambda - 6^\lambda) \ln 3 + (9^\lambda \ln 3 - \frac{2^\lambda + 6^\lambda}{2} \ln 4) \\ &< (9^\lambda - 6^\lambda) \ln 3 + \frac{(9^\lambda - 2^\lambda) + (9^\lambda - 6^\lambda)}{2} \ln 4. \\ &< 0. \end{aligned}$$

Note that $f_2(\lambda)$ is decreasing on $(-\infty, 0)$ in λ . We have $f_2(\lambda) > f_2(0) = 1 + 9^0 - 2^0 - 6^0 = 0$. It can be seen that $g_1(x) \geq g_1(2) = 1 + 9^\lambda - 2^\lambda - 6^\lambda = f_2(\lambda) > f_2(0) = 0$. Then we know that ${}^\lambda M_1(G) - {}^\lambda M_2(G) > 0$, $\lambda \in (-\infty, 0)$.

Therefore, ${}^\lambda M_1(G) - {}^\lambda M_2(G) > 0$, $\lambda \in (-\infty, 0)$ when $k = 1$.

Case 2 When $k \geq 2$.

Since $G' = G - v$, G' is a connected unicyclic graph with $n-1$ vertices. If G' is a cycle, ${}^\lambda M_1(G') = {}^\lambda M_2(G')$. If G' is not a cycle, by the induction hypothesis, ${}^\lambda M_1(G') > {}^\lambda M_2(G')$. Now we compare ${}^\lambda M_1(G)$ and ${}^\lambda M_2(G)$.

$${}^\lambda M_1(G) = {}^\lambda M_1(G') + (k+1)^{2\lambda} - k^{2\lambda} + 1,$$

$${}^{\lambda}M_2(G) = {}^{\lambda}M_2(G') - [k^{\lambda} - (k+1)^{\lambda}] \sum_{i=1}^k (d_G(v_i))^{\lambda} + (k+1)^{\lambda}.$$

Then

$$\begin{aligned} {}^{\lambda}M_1(G) - {}^{\lambda}M_2(G) &= {}^{\lambda}M_1(G') - {}^{\lambda}M_2(G') + (k+1)^{2\lambda} - k^{2\lambda} + 1 - (k+1)^{\lambda} \\ &\quad + [k^{\lambda} - (k+1)^{\lambda}] \sum_{i=1}^k (d_G(v_i))^{\lambda} \\ &> (k+1)^{2\lambda} - k^{2\lambda} + 1 - (k+1)^{\lambda}. \end{aligned}$$

Suppose $g_2(x) = (x+1)^{2\lambda} - x^{2\lambda} + 1 - (x+1)^{\lambda}$, ($x \geq 2$). Then

$$\begin{aligned} g_2'(x) &= 2\lambda(x+1)^{2\lambda-1} - 2\lambda x^{2\lambda-1} - \lambda(x+1)^{\lambda-1} \\ &= \lambda[2(x+1)^{2\lambda-1} - 2x^{2\lambda-1} - (x+1)^{\lambda-1}] \\ &> 0. \end{aligned}$$

Note that $g_2(x)$ is increasing in $x \geq 2$. We have $g_2(x) \geq g_2(2) = 1 + 9^{\lambda} - 4^{\lambda} - 3^{\lambda} = f_1(\lambda)$. From the foregoing proof, it has been know that $f_1(\lambda) > 0$. It can be seen that $g_2(x) \geq g_2(2) = 1 + 9^{\lambda} - 4^{\lambda} - 3^{\lambda} = f_1(\lambda) > 0$. Therefore, we have ${}^{\lambda}M_1(G) - {}^{\lambda}M_2(G) > 0$, $\lambda \in (-\infty, 0)$ when $k \geq 2$.

This completes the proof of theorem. □

3 Comparing Variable Zagreb Indices for Unicyclic Graphs for $\lambda > 1$

Now we discuss the changing situation of the Zagreb indices when $\lambda > 1$.

Case 1

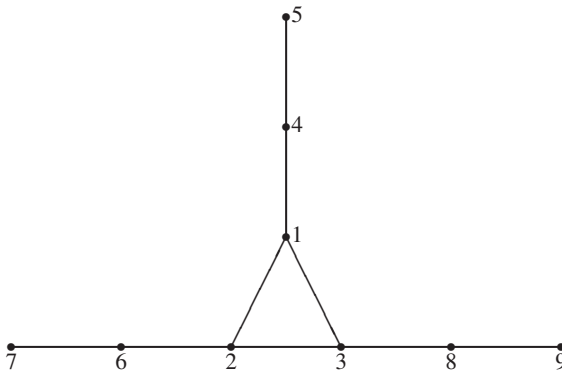


Figure 1. G_1

Since $G = G_1$ (see Fig.1),

$${}^\lambda M_2(G_1) - {}^\lambda M_1(G_1) = 3(6^\lambda + 2^\lambda - 4^\lambda - 1).$$

Suppose $h_1(\lambda) = 3(6^\lambda + 2^\lambda - 4^\lambda - 1)$, $(\lambda > 1)$. Then

$$h'_1(\lambda) = 3(6^\lambda \ln 6 + 2^\lambda \ln 2 - 4^\lambda \ln 4) > 0.$$

Note that $h_1(\lambda)$ is increasing in $\lambda > 1$. We have $h_1(\lambda) > h(1) = 6 > 0$. Therefore $\forall \lambda_1 > 1$, ${}^{\lambda_1} M_2(G_1) - {}^{\lambda_1} M_1(G_1) > 0$.

Case 2

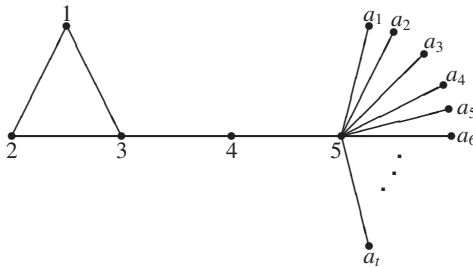


Figure 2. G_2

Since $G = G_2$ (see Fig.2),

$${}^\lambda M_2(G_2) - {}^\lambda M_1(G_2) = 6^\lambda + 6^\lambda + 6^\lambda + [2(t+1)]^\lambda + t(t+1)^\lambda - 4^\lambda - 4^\lambda - 9^\lambda - (t+1)^{2\lambda} - t.$$

Suppose $h_2(t) = 6^\lambda + 6^\lambda + 6^\lambda + [2(t+1)]^\lambda + t(t+1)^\lambda - 4^\lambda - 4^\lambda - 9^\lambda - (t+1)^{2\lambda} - t$, $(t \geq 1, \lambda > 1)$. Then

$$\begin{aligned} h'_2(t) &= 2\lambda[2(t+1)]^{\lambda-1} + (t+1)^\lambda + \lambda t(t+1)^{\lambda-1} - 2\lambda(t+1)^{2\lambda-1} - 1 \\ &= 2^\lambda \lambda(t+1)^{\lambda-1} + (t+1)^\lambda + \lambda t(t+1)^{\lambda-1} - 2\lambda(t+1)^{2\lambda-1} - 1. \end{aligned}$$

Moreover,

$$\begin{aligned} h''_2(t) &= 2^\lambda \lambda(\lambda-1)(t+1)^{\lambda-2} + \lambda(t+1)^{\lambda-1} + \lambda(t+1)^{\lambda-1} \\ &\quad + \lambda(\lambda-1)t(t+1)^{\lambda-2} - 2\lambda(2\lambda-1)(t+1)^{2\lambda-2} \\ &= [2^\lambda \lambda(\lambda-1) + 2\lambda t + 2\lambda + \lambda(\lambda-1)t - 2\lambda(2\lambda-1)(t+1)^\lambda](t+1)^{\lambda-2}. \end{aligned}$$

Suppose $l(t) = 2^\lambda \lambda(\lambda-1) + 2\lambda t + 2\lambda + \lambda(\lambda-1)t - 2\lambda(2\lambda-1)(t+1)^\lambda$, $(t \geq 1, \lambda > 1)$. Then

$$l'(t) = 2\lambda + \lambda(\lambda-1) - 2\lambda(2\lambda-1)\lambda(t+1)^{\lambda-1}$$

$$\begin{aligned}
 &< \lambda[2 + \lambda - 1 - 2\lambda(2\lambda - 1)] \\
 &= \lambda(1 + 4\lambda)(1 - \lambda) \\
 &< 0.
 \end{aligned}$$

Note that $l(t)$ is decreasing in $t \geq 1$, we have

$$\begin{aligned}
 l(t) \leq l(1) &= 2^\lambda \lambda^2 - 2^\lambda \lambda + 2\lambda + 2\lambda + \lambda^2 - \lambda - 2\lambda(2\lambda - 1)2^\lambda \\
 &= \lambda 2^\lambda + \lambda^2 + 3\lambda - 3\lambda^2 2^\lambda.
 \end{aligned}$$

Suppose $r(\lambda) = \lambda 2^\lambda + \lambda^2 + 3\lambda - 3\lambda^2 2^\lambda, (\lambda > 1)$. Then

$$\begin{aligned}
 r'(\lambda) &= 2^\lambda + \lambda 2^\lambda \ln 2 + 2\lambda + 3 - 6\lambda 2^\lambda - 3\lambda^2 2^\lambda \ln 2 \\
 &= (2^\lambda + 2\lambda + 3 - 6\lambda 2^\lambda) + (1 - 3\lambda)\lambda 2^\lambda \ln 2 \\
 &= [(2^\lambda - \lambda 2^\lambda) + (2\lambda - 2\lambda 2^\lambda) + (3 - 3\lambda 2^\lambda)] + (1 - 3\lambda)\lambda 2^\lambda \ln 2 \\
 &< 0.
 \end{aligned}$$

Note that $r(\lambda)$ is decreasing in $\lambda > 1$, we have $r(\lambda) < r(1) = 2 + 1 + 3 - 6 = 0$. It can be seen that $l(t) \leq l(1) = \lambda 2^\lambda + \lambda^2 + 3\lambda - 3\lambda^2 2^\lambda = r(\lambda) < r(1) = 0$. Therefore, $h_2'(t) = (t+1)^{t-2} \cdot l(t) < 0$, then $h_2(t)$ is a concave function, and $h_2'(t)$ is decreasing in $t \geq 1$. Hence we have

$$\begin{aligned}
 h_2'(t) \leq h_2'(1) &= 2^\lambda \lambda 2^{\lambda-1} + 2^\lambda + \lambda 2^{\lambda-1} - 2\lambda 2^{2\lambda-1} - 1 \\
 &= 2^\lambda + \lambda 2^{\lambda-1} - \lambda 2^{2\lambda-1} - 1.
 \end{aligned}$$

Suppose $s(\lambda) = 2^\lambda + \lambda 2^{\lambda-1} - \lambda 2^{2\lambda-1} - 1, (\lambda > 1)$. Then

$$\begin{aligned}
 s'(\lambda) &= 2^\lambda \ln 2 + 2^{\lambda-1} + \lambda 2^{\lambda-1} \ln 2 - 2^{2\lambda-1} - \lambda 2^{2\lambda} \ln 2 \\
 &= (2^{\lambda-1} - 2^{2\lambda-1}) + (2^\lambda + \lambda 2^{\lambda-1} - \lambda 2^{2\lambda}) \ln 2 \\
 &= (2^{\lambda-1} - 2^{2\lambda-1}) + [(2^\lambda - 2^\lambda \lambda 2^{\lambda-1}) + (\lambda 2^{\lambda-1} - 2^\lambda \lambda 2^{\lambda-1})] \ln 2 \\
 &< 0.
 \end{aligned}$$

Note that $s(\lambda)$ is decreasing in $\lambda > 1$, we have $s(\lambda) < s(1) = 2 + 1 - 2 - 1 = 0$. Therefore, $h_2'(t) \leq h_2'(1) = 2^\lambda + \lambda 2^{\lambda-1} - \lambda 2^{2\lambda-1} - 1 = s(\lambda) < s(1) = 0$. Then $h_2(t)$ is strictly decreasing in $t \geq 1$. By the discussion above, $h_2(t)$ is a strictly decreasing concave function. Therefore, $\forall \lambda_2 > 1$, we can find a positive integer T to cause ${}^{\lambda_2}M_2(G_2) - {}^{\lambda_2}M_1(G_2) < 0$ when $t \geq T$.

Combining Case 1 and Case 2, $\forall \lambda > 1$, we can find a suitable graph G_1^* to cause ${}^\lambda M_2(G_1^*) - {}^\lambda M_1(G_1^*) > 0$, or we can find a suitable graph G_2^* to cause ${}^\lambda M_2(G_2^*) - {}^\lambda M_1(G_2^*) < 0$. Therefore, when $\lambda > 1$, the relationship of numerical value between ${}^\lambda M_1(G)/n$ and ${}^\lambda M_2(G)/m$ is indefinite to the distinct unicyclic graphs.

4 Conclusion

With the foregoing discussion and the conclusion in [4], the relationship of ${}^{\lambda}M_1(G)/n$ and ${}^{\lambda}M_2(G)/m$ in unicyclic graphs for $\lambda \in R$ can be seen that:

- (i) ${}^{\lambda}M_1(G)/n \geq {}^{\lambda}M_2(G)/m, \lambda \in (-\infty, 0)$,
- (ii) ${}^{\lambda}M_1(G)/n \leq {}^{\lambda}M_2(G)/m, \lambda \in [0, 1]$,
- (iii) the relationship of numerical value between ${}^{\lambda}M_1(G)/n$ and ${}^{\lambda}M_2(G)/m$ is indefinite in the distinct unicyclic graphs when $\lambda \in (1, +\infty)$.

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