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On the ordering of a class of graphs with respect to their matching numbers

Xiaoxia Wang and Xiaofeng Guo*
School of Mathematical Sciences, Xiamen University, Xiamen Fujian 361005, P.R. China
E-mail address: xfguo@xmu.edu.cn

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Based on the number of k-matching $m(G, k)$ of a graph G, Gutman and Zhang introduced an order relation $\succ$ of graphs: for graphs G_1 and G_2, $G_1 \succ G_2$ if $m(G_1, k) \geqslant m(G_2, k)$ for all k. The order relation has important applications in comparing Hosaya indices and energies of molecular graphs and has been widely studied. Especially, Gutman and Zhang gave complete orders of six classes of graphs with respect to the relation $\succ$. In this paper, we consider a class of graphs with special structure, which is a generalization of a class of graphs studied by Gutman and Zhang. Some order relations in the class of graphs are given, and the maximum and minimum elements with respect to the order relation are determined. The new results can be applied to order some classes of graphs by their matching numbers.

KEY WORDS: matching number, order relation

1. Introduction

In the present paper, we consider graphs without loops and multiple edges. Let $m(G, k)$ denote the number of k-matchings in a graph G, that is, the number of selections of k independent edges in G. It is both consistent and convenient to define $m(G, 0) = 1$ for any graph G.

Gutman and Zhang [1] introduced the relation $\succ$ as follows: If, for two graphs G_1 and G_2, $m(G, k) \geqslant m(G, k)$ for all k, then G_1 is m-greater than G_2, denoted by $G_1 \succ G_2$ or $G_2 \prec G_1$. If both $G_1 \succ G_2$ and $G_2 \succ G_1$ hold, then G_1 and G_2 are m-equivalent, denoted by $G_1 \sim G_2$. If neither $G_1 \succ G_2$ nor $G_2 \succ G_1$ holds, then G_1 and G_2 are m-incomparable.

The relation $\succ$ has important applications in comparing Hosaya indices and energies of molecular graphs [2].

Let a graph G represent the carbon-atom skeleton of a hydrocarbon molecule [2], the Hosoya index [3] of G, $Z(G)$, is defined as the total number of matchings in G, namely

*Corresponding author.

$$Z(G) = \sum_k m(G, k).$$

$Z(G)$ has been shown to be a monotone function of various thermodynamic properties of the corresponding hydrocarbon: boiling point, entropy, etc. Therefore, the ordering of molecular graphs according to $Z(G)$ is of certain interest in chemical thermodynamics. It is evident that $G_1 \succ G_2$ implies $Z(G_1) \geqslant Z(G_2)$ with equality if G_1 and G_2 are m-equivalent.

Within a certain model of chromaticity [4], the zeros $x_1, x_2, \ldots, x_n$ ($x_i \geqslant x_j$ for $i < j$) of the matching polynomial [5, 6, 7]

$$\alpha(G) = \sum_k (-1)^k m(G, k) x^{n-2k}$$

need to be calculated and then the sum $E(G)$,

$$E(G) = 2 \sum_{i=1}^{[n/2]} x_i$$

is interpreted as the energy of a certain reference structure. It was shown [8] that, for an acyclic graph G, $E(G)$ is a monotone increasing function of the numbers $m(G, k)$. Therefore, $G_1 \succ G_2$ implies $E(G_1) \geqslant E(G_2)$ with equality if G_1 and G_2 are m-equivalent.

This relation has been widely studied for various classes of graphs: acyclic [8, 9], unicyclic [10], bicyclic [10] and tricyclic [11] graphs with a given number of vertices. The maximal and minimal elements in these classes of graphs with respect to the relation $\succ$ were determined. In [1], Gutman and Zhang completely ordered six further classes of graphs.

Let $P_n = v_1 v_2, \ldots, v_n$ be a path with n vertices. Let G and H be two graphs whose vertex sets are disjoint. Then $G(v, w)H$ denotes the graph obtained from G and H by identifying vertex v of G and a vertex w of H. In particular, the graph $P_n(v_i, u)G$ is obtained from P_n and G by identifying the vertex v_i of P_n with a vertex u of G. Let u and v be two vertices of G. Then $G(u, v)(a, b)$ denotes the graph obtained from G by attaching a pendant edges to the vertex u and additional b pendant edges to the vertex v. Two vertices u and v of the graph G are called equivalent if the subgraphs $G - u$ and $G - v$ are isomorphic. With these notations, there are two well-known results as follows.

Theorem 1.1 [1]. If v is an arbitrary vertex of a graph G, then for $n = 4k + i$, $i \in \{-1, 0, 1, 2\}$, $k \geqslant 1$,

$$P_n(v_1, v)G \succ P_n(v_3, v)G \succ \cdots \succ P_n(v_{2k+1}, v)G \succ P_n(v_{2k}, v)G$$
$$\succ P_n(v_{2k-2}, v)G \succ \cdots \succ P_n(v_2, v)G.$$

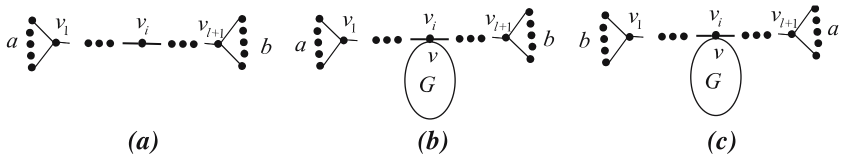

Figure 1. (a) $T_{l;\ a,b}$, (b) $T_{l;\ a,b}(v_i, v)G$, (c) $T_{l;\ b,a}(v_i, v)G$.

Theorem 1.2 [1]. If the vertices u and v of a graph G are equivalent, then

$$G(u, v)(0, n) \prec G(u, v)(1, n-1) \prec \cdots \prec G(u, v)(\lfloor n/2 \rfloor, n - \lfloor n/2 \rfloor).$$

In the present paper, we shall examine a further class of graphs with special structure.

Denote by $T_{l;\ a,b}$ the graph obtained from the path $P_{l+1} = v_1 v_2 \cdots v_{l+1}$ by attaching a pendant edges to v_1 and additional b pendant edges to v_{l+1}, by $T_{l;\ a,b}(v_i, v)G$ the graph obtained from $T_{l;\ a,b}$ and G by identifying the vertex v_i of $T_{l;\ a,b}$ with a vertex v of G (see figure 1), and by $\{T_{l;\ a,b}(v_i, v)G \mid a, b \geqslant 1,\ a+b = m\}$ the class of graphs with special structure. Obviously, when $a = b = 1$, $T_{l;\ a,b}(v_i, v)G \cong P_{l+3}(v_{i+1}, v)G$.

For the class of graphs, $\{T_{l;\ a,b}(v_i, v)G \mid a, b \geqslant 1,\ a+b = m\}$, we determine some order relations and the maximal and the minimal elements in the class of graphs with respect to the relation $\succ$.

Our main results are the following theorems.

Theorem 1.3 Let v be an arbitrary vertex of a graph G, and let $l = 4k + r,\ r \in \{0, 1, 2, 3\}$, $k \geqslant 1$, $a \geqslant b \geqslant 1$.

(1) If $r \in \{0, 1\}$, then

$$\begin{aligned}
&T_{l;\ a,b}(v_2, v)G \succ T_{l;\ b,a}(v_2, v)G \succ T_{l;\ a,b}(v_4, v)G \succ T_{l;\ b,a}(v_4, v)G \\
&\quad \succ \cdots \succ T_{l;\ a,b}(v_{2k}, v)G \succ T_{l;\ b,a}(v_{2k}, v)G \succ T_{l;\ b,a}(v_{2k+1}, v)G \\
&\succ T_{l;\ a,b}(v_{2k+1}, v)G \\
&\succ \cdots \succ T_{l;\ b,a}(v_3, v)G \succ T_{l;\ a,b}(v_3, v)G \succ T_{l;\ b,a}(v_1, v)G \succ T_{l;\ a,b}(v_1, v)G,
\end{aligned}$$

where $T_{l;\ b,a}(v_{2k+1}, v)G \sim T_{l;\ a,b}(v_{2k+1}, v)G$ when either $r = 0$ or $a = b$.

(2) If $r \in \{2, 3\}$, then

$$\begin{aligned}
&T_{l;\ a,b}(v_2, v)G \succ T_{l;\ b,a}(v_2, v)G \succ T_{l;\ a,b}(v_4, v)G \succ T_{l;\ b,a}(v_4, v)G \\
&\quad \succ \cdots \succ T_{l;\ a,b}(v_{2k+2}, v)G \succ T_{l;\ b,a}(v_{2k+2}, v)G \\
&\succ T_{l;\ b,a}(v_{2k+1}, v)G \succ T_{l;\ a,b}(v_{2k+1}, v)G \\
&\succ \cdots \succ T_{l;\ b,a}(v_3, v)G \succ T_{l;\ a,b}(v_3, v)G \succ T_{l;\ b,a}(v_1, v)G \succ T_{l;\ a,b}(v_1, v)G,
\end{aligned}$$

where $T_{l;\ a,b}(v_{2k+2}, v)G \sim T_{l;\ b,a}(v_{2k+2}, v)G$ when either $r = 2$ or $a = b$.

Theorem 1.4 Let v be an arbitrary vertex v of a graph G. Then, for $2 \leqslant i \leqslant l+1$,

$$T_{l;\ 1,m-1}(v_i, v)G \prec T_{l;\ 2,m-2}(v_i, v)G \prec \cdots \prec T_{l;\ \lfloor m/2\rfloor,\lceil m/2\rceil}(v_i, v)G. \qquad (1)$$

Theorem 1.5 For an arbitrary vertex v of a graph G and for any $l, m \geqslant 2$, the maximum and minimum elements in the class $\{T_{l;\ a,b}(v_i, v)G \mid a, b \geqslant 1,\ a+b = m\}$ with respect to the relation $\succ$ are $T_{l;\ \lceil m/2\rceil,\lfloor m/2\rfloor}(v_2, v)G$ and $T_{l;\ m-1,1}(v_1, v)G$, respectively.

Theorem 1.3 gives the complete order of all the graphs in $\{T_{l;\ a,b}(v_i, v)G\}$ with l, a, b given, and Theorem 1.4 gives the complete order of all the graphs in $\{T_{l;\ a,b}(v_i, v)G\}$ with $l, i, a+b$ given. It is easily seen that for $a=b$, $T_{l;\ a,b}(v_i, v)G \cong T_{l;\ b,a}(v_{l-i+2}, v)G$ and Theorem 1.3 is thus reduced to a simpler form, and especially to Theorem 1.1 when $a = b = 1$ (except for the first $\succ$, which can also be verified easily). Theorem 1.4 shows an order relation similar to that of Theorem 1.2. However, Theorem 1.2 holds only if u and v are equivalent, but v_1 and v_{l+1} in Theorem 1.4 might be not equivalent.

The above theorems can be applied to order some classes of graphs by their matching numbers. We will discuss their application in the end of the paper.

2. Proofs of the main results

In order to demonstrate the validity of the above theorems, we need a few auxiliary results.

Lemma 2.1 [1]. $m(G \cup H, k) = \sum_{h=0}^{k} m(G, h)m(H, k-h)$.

Lemma 2.2 [1]. If E_n is the graph with n vertices and without edges, then $G \cup E_n \sim G$.

Lemma 2.3 [1]. If H is a subgraph of G, then G is m-greater than H.

Lemma 2.4 [1]. If e is an edge of G, connecting the vertices u and v, then for all $k \geqslant 1$,

$$m(G, k) = m(G - e, k) + m(G - u - v, k - 1).$$

Lemma 2.5 [8]. Let G and H be two graphs. Denote by $G(u, v)H$ the graph obtained by fusing the vertex u of G and the vertex v of H. Suppose u and v are not singletons. Then

$$m(G \cup H, k) = m(G(u, v)H, k) + \sum_{uu_i \in G,\ vv_j \in H.} m((G - u - u_i) \cup (H - v - v_j), k - 2).$$

Lemma 2.6 Let G and H be two graphs. For $u \in V(G)$, $v \in V(H)$,

$$m(G(u,v)H,k) = m(G-u \cup H,k) + \sum_{uu_j \in G} m((G-u-u_j) \cup (H-v), k-1).$$

proof. Consider the edge set $E_G(u) = \{uu_j \in G\}$. The k-matchings of $G(u,w)H$ are partitioned into two parts: those including none of the elements of $E_G(u)$, and those including exactly one of them. Now, the conclusion of the lemma follows. □

Lemma 2.7 Let T_1 and T_2 be disjoint trees and G a graph. If $T_1 \succ T_2$, then $G \cup T_1 \succ G \cup T_2$.

This lemma is obvious according to the definition of the relation $\succ$. □

Lemma 2.8

(1) For $a, b \geqslant 1$, $1 \leqslant i \leqslant \lfloor l/2 \rfloor$,

$$T_{i;\ 0,a} \cup T_{l-i;\ 0,b} \prec T_{i-1;\ 0,a} \cup T_{l-i+1;\ 0,b}, \text{ if } i \text{ is odd},$$
$$T_{i;\ 0,a} \cup T_{l-i;\ 0,b} \succ T_{i-1;\ 0,a} \cup T_{l-i+1;\ 0,b}, \text{ if } i \text{ is even}.$$

(2) For $a \geqslant b \geqslant 1$, $2 \leqslant i \leqslant \lfloor l/2 \rfloor$,

$$T_{i;\ 0,a} \cup T_{l-i;0,b} \prec T_{i-2;\ 0,b} \cup T_{l-i+2;\ 0,a} \prec T_{i-2;\ 0,a} \cup T_{l-i+2;\ 0,b},$$
if i is even,
$$T_{i;\ 0,a} \cup T_{l-i;\ 0,b} \succ T_{i-2;\ 0,b} \cup T_{l-i+2;\ 0,a} \succ T_{i-2;0,a} \cup T_{l-i+2;\ 0,b},$$
if i is odd.

Proof. (1) Let $T_1 = T_{i;\ 0,a} \cup T_{l-i;\ 0,b}$ and $T_2 = T_{i-1;\ 0,a} \cup T_{l-i+1;\ 0,b}$. By lemma 2.5,

$$m(T_1,k) = m(T_{l;\ a,b},k) + m(T_{i-2;\ 0,a} \cup T_{l-i-2;\ 0,b}, k-2),$$
$$m(T_2,k) = m(T_{l;\ a,b},k) + m(T_{i-3;\ 0,a} \cup T_{l-i-1;\ 0,b}, k-2).$$

Then

$$\begin{aligned}
&m(T_1,k) - m(T_2,k)\\
&= m(T_{i-2;\ 0,a} \cup T_{l-i-2;\ 0,b}, k-2) - m(T_{i-3;\ 0,a} \cup T_{l-i-1;\ 0,b}, k-2)\\
&= \cdots = \begin{cases} m(T_{1;\ 0,a} \cup T_{l-2i+1;0,b}, k-i+1) \\ -m(T_{0;\ 0,a} \cup T_{l-2i+2;\ 0,b}, k-i+1), & \text{if } i \text{ is odd}, \\ m(T_{2;\ 0,a} \cup T_{l-2i+2;\ 0,b}, k-i+2) \\ -m(T_{1;\ 0,a} \cup T_{l-2i+3;\ 0,b}, k-i+2), & \text{if } i \text{ is even} \end{cases}\\
&= \begin{cases} m(T_{l-2i-1;\ 0,b}, k-i-1) - a \times m(T_{l-2i;\ 0,b}, k-i-1) \leqslant 0, & \text{if } i \text{ is odd}, \\ m(T_{0;\ 0,a} \cup T_{l-2i;\ 0,b}, k-i) - m(T_{l-2i+1;\ 0,b}, k-i) \geqslant 0. & \text{if } i \text{ is even}. \end{cases}
\end{aligned}$$

Thus (1) follows.

The proof of (2) is similar to that of (1). □

Proof of theorem 1.3. Applying Lemma 2.6 to $T_{l;\ a,b}(v_i, v)G$, we have

$$m(T_{l;\ a,b}(v_i, v)G, k) = \begin{cases} m((G-v)\cup T_{l;\ a,b}, k) \\ \quad + \sum_{vu_j \in G} m((G-v-u_j)\cup T_{i-2;\ 0,a} \cup T_{l-i;\ 0,b}, k-1), & \text{if } 2 \leqslant i \leqslant \lceil l/2 \rceil, \\ m((G-v)\cup T_{l;\ a,b}, k) \\ \quad + \sum_{vu_j \in G} m((G-v-u_j)\cup T_{l-1;\ 0,b}, k-1), & \text{if } i = 1. \end{cases}$$

It is easy to verify that $T_{l;\ a,b}(v_3, v)G \succ T_{l;\ b,a}(v_1, v)G$. Theorem 1.3 then follows from lemma 2.7 and lemma 2.8. □

Lemma 2.9 If $1 \leqslant a < b-1$ and $2 \leqslant i \leqslant l+1$, then $T_{l;\ a,b}(v_i, v)G \prec T_{l;\ a+1,b-1}(v_i, v)G$.

Proof. For $2 \leqslant i \leqslant l$, consider an edge of the graph $T_{l;\ a,b}(v_i, v)G$, which connects v_{l+1} with a pendant vertex. By Lemma 2.4, we have

$$m(T_{l;\ a,b}(v_i, v)G, k) = m(T_{l;\ a,b-1}(v_i, v)G, k) + m(T_{l-1;\ a,0}(v_i, v)G, k-1).$$

Similarly,

$$m(T_{l;\ a+1,b-1}(v_i, v)G, k) = m(T_{l;\ a,b-1}(v_i, v)G, k) + m(T_{l-1;\ 0,b-1}(v_{i-1}, v)G, k-1).$$

Then

$$\begin{aligned} & m(T_{l;\ a+1,b-1}(v_i, v)G, k) - m(T_{l;\ a,b}(v_i, v)G, k) \\ &= m(T_{l-1;\ 0,b-1}(v_{i-1}, v)G, k-1) - m(T_{l-1;\ a,0}(v_i, v)G, k-1) \\ &= (b-a-1) \times m(T_{l-2;\ 0,0}(v_{i-1}, v)G, k-2) + m(T_{l-1;\ 0,0}(v_{i-1}, v)G, k-1) \\ &\quad - m(T_{l-1;\ 0,0}(v_i, v)G, k-1) \\ &= \begin{cases} (b-a-1) \times m(T_{l-2;\ 0,0}(v_{i-1}, v)G, k-2) + m(T_{l-3;\ 0,0}(v_{i-1}, v)G, k-2) \\ -m(T_{l-3;\ 0,0}(v_{i-2}, v)G, k-2), \quad \text{if } i \geqslant 3, \\ (b-a-1) \times m(T_{l-2;\ 0,0}(v_1, v)G, k-2) + m(T_{l-3;\ 0,0}(v_1, v)G, k-2) \\ -m(G-v \cup T_{l-3;\ 0,0}, k-2), \quad \text{if } i = 2. \end{cases} \end{aligned}$$

Since $a < b-1$ and $T_{l-3;\ 0,0}(v_{i-2}, v)G$ (resp. $G - v \cup T_{l-3;\ 0,0}$) is a subgraph of $T_{l-2;\ 0,0}(v_{i-1}, v)G$ (resp. $T_{l-2;\ 0,0}(v_1, v)G$), by lemma 2.3, the values of the above equalities are no less than zero.

For $i = l + 1$, from lemma 2.6, we get

$$\begin{aligned}
&m(T_{l;\ a,b}(v_{l+1}, v)G, k) \\
&= m((G - v) \cup T_{l;\ a,b}, k) + \sum_{vu_j \in G} m((G - v - u_j) \cup T_{l-1;\ 0,a}, k - 1), \\
&m(T_{l;\ a+1,b-1}(v_{l+1}, v)G, k) \\
&= m((G - v) \cup T_{l;\ a+1,b-1}, k) + \sum_{vu_j \in G} m((G - v - u_j) \cup T_{l-1;\ 0,a+1}, k - 1).
\end{aligned}$$

Since $T_{l;\ a,b} \prec T_{l;\ a+1,b-1}$ for $a < b - 1$, and $T_{l-1;\ 0,a} \prec T_{l-1;\ 0,a+1}$, we get $T_{l;\ a,b}(v_{l+1}, v)G \prec T_{l;\ a+1,b-1}(v_{l+1}, v)G$.

The proof is complete. □

Proof of theorem 1.4. theorem 1.4 follows immediately from lemma 2.9. □

Remark. Since $T_{l;\ a,b}(v_i, v)G \cong T_{l;\ b,a}(v_{l-i+2}, v)G$ for $i \in \{2, \cdots, l + 1\}$,

$$T_{l;\ m-1,1}(v_j, v)G \prec T_{l;\ m-2,2}(v_j, v)G \prec \cdots \prec T_{l;\ \lceil m/2\rceil,\lfloor m/2\rfloor}(v_j, v)G, \quad j \in \{1, \cdots, , l\}. \tag{2}$$

Therefore, either $T_{l;\ \lceil m/2\rceil,\lfloor m/2\rfloor}(v_i, v)G$ or $T_{l;\ \lfloor m/2\rfloor,\lceil m/2\rceil}(v_i, v)G$ is the maximal element in $\{T_{l;\ a,b}(v_i, v)G \mid a, b \geqslant 1, \ a + b = m\}$ for a given i, $i \in \{2, \cdots, l\}$, depending on the parity of i. But for $i = 1$ and $i = l + 1$, formulae (1) and (2) can not hold simultaneously. For example, Let G be the Star S_3 and v be its non-pendant vertex, we have $T_{l;\ 3,1}(v_1, v)S_3 \prec T_{l;\ 2,2}(v_1, v)S_3$ while $T_{l;\ 1,3}(v_1, v)S_3 \succ T_{l;\ 2,2}(v_1, v)S_3$. Nevertheless, $T_{l;\ i,m-i}(v_1, v)G \succ T_{l;\ m-i,i}(v_1, v)G$ ($\cong T_{l;\ i,m-i}(v_{l+1}, v)G$) for any $i \in \{1, 2, \cdots, \lfloor m/2\rfloor\}$, and so we have $T_{l;\ m-1,1}(v_1, v)G \prec T_{l;\ a,b}(v_1, v)G$ by theorem 1.4.

Proof of theorem 1.5. By lemma 2.8, if $a \geqslant b$,

$$T_{l;\ a,b}(v_1, v)G \prec T_{l;\ b,a}(v_1, v)G, \quad T_{l;\ a,b}(v_2, v)G \succ T_{l;\ b,a}(v_2, v)G.$$

Then from theorem 1.3, for $a \geqslant b \geqslant 1$, $i \in \{1, 2, \cdots, l + 1\}$,

$$T_{l;\ a,b}(v_1, v)G \prec T_{l;\ a,b}(v_i, v)G \prec T_{l;\ a,b}(v_2, v)G.$$

By theorem 1.4 and the remark following it ,

$$T_{l;\ m-1,1}(v_1, v)G \prec T_{l;\ a,b}(v_1, v)G, \quad T_{l;\ a,b}(v_2, v)G \prec T_{l;\ \lceil m/2\rceil,\lfloor m/2\rfloor}(v_2, v)G.$$

Thus the theorem follows. □

3. Applications

The main results above can be applied to order some classes of graphs by their matching numbers, for example, the class of trees with n vertices and q non-pendant edges, denoted by $\Gamma(n, q)$. As mentioned in the Introduction, for a tree, its energy is an increasing function of its matching numbers, so we need only to order the trees by the order relation $\succ$ to determine the energy order of the trees. By Theorem 1.5, we know that the transformation from $T_{l;\ a,b}(v_i, v)G$ to $T_{l;\ a+b-1,1}(v_1, v)G$ keeps the number of non-pendant edges unchanged while $T_{l;\ a,b}(v_i, v)G \succ T_{l;\ a+b-1,1}(v_1, v)G$, that is, the resultant graph has smaller energy than the original one. The transformation has been used to determine the tree in $\Gamma(n, q)$ with the smallest energy. And by Theorem 1.3 and Theorem 1.4, we have that $T_{l;\ 1,1}(v_3, v)S_{p-2} \prec T_{l;\ a,b}(v_i, v)S_{p-a-b}$ for $a, b \geqslant 1$ and $i \in \{1, \ldots, l+1\}$, which is useful in determining the tree in $\Gamma(n, q)$ with the second smallest energy. For some cyclic graphs with special structure, Theorem 1.3–1.5 can also be used to compare their Hosoya indices and energies. We will further discuss them elsewhere.

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