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FINDING TRICYCLIC GRAPHS WITH A MAXIMAL NUMBER OF MATCHINGS – ANOTHER EXAMPLE OF COMPUTER AIDED RESEARCH IN GRAPH THEORY

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Abstract. Tricyclic graphs on n vertices with maximal number of matchings are determined by a computer search for small values of n and by an induction argument for the rest. The computer search is performed by the interactive programming system "GRAPH", implemented at the University of Belgrade, and represents a typical example of the usage of this system in scientific research.

1. Introduction and the Main Result. We consider finite graphs without loops or multiple edges. Let $p(G,k)$ be the number of k-matchings of the graph G. We assume $p(G,0) = 1$ and $p(G,k) = 0$ for $k < 0$.

Let G and H be two graphs. If $p(G,k) \geq p(H,k)$ for all $k = 1, 2, \dots,$ then we say that G is *m-greater than* H or H *is m-smaller than* G and denote it by $G \succ H$ or $H \prec G$.

If $G \succ H$ and $H \succ G$, the graphs G and H are said to be m-equivalent, $G \sim H$. If neither $G \succ H$ nor $H \succ G$, the two graphs G and H are said to be m-incomparable and we denote this by $G \# H$. If $G \succ H$, but the graphs G and H are not m-equivalent, we say that G is strictly *m-greater than* H.

The relation N is an equivalence relation in any set of graphs γ. The corresponding equivalence classes will be called matching equivalence classes (of the set γ). The relation $\succ$ induces a partial ordering of the set $\gamma/\sim$. An equivalence class is said to be the greatest if it is greater than any other class. A class is maximal if there is no other class greater than it.

The graphs belonging to greatest (resp. maximal) matching equivalence classes will be said to be *m-greatest* (resp. *m-maximal*) in the set considered.

The m-greatest and/or m-maximal graphs have been determined for several classes of graphs [5, 6, 7]. For example, the m-greatest element in the set of all graphs with n vertices is the complete graph K_n[6].

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0. The m-greatest forest with n vertices is the path P_n[5].

1. The m-greatest unicyclic graph with n vertices is the cycle C_n[6]. The bicyclic graphs with greatest number of matchings have also been considered in [6]. Unfortunately, the result reported in [6] and also in [7] is erroneous. The correct statement is the following.

2. In the set of all bicyclic graphs with n vertices $(n \leq 4)$ there exists a greatest matching equivalence class. For all values of n, except for $n = 9$, the m-greatest graph is unique. For $n = 9$ the greatest matching equivalence class possesses two elements. The m-greatest bicyclic graphs are presented on Fig. 1.

In the present paper we shall describe the analogous result for the case of tricyclic graphs. The search for m-maximal tricyclic graphs proved, however, to be a much more difficult task and the results obtained are significantly more complex than the statements $0°$, $1°$ and $2°$.

3. We shall prove the following result.

THEOREM 1. *In the set of all tricyclic graphs with n vertices* $(n \geq 4)$ *the greatest matching equivalence class exists only for* $n = 4, 5, 6, 7, 8,$ *and* 9. *For* $n \geq 10$ *there exist two maximal matching equivalence classes. All these equivalence classes possess a unique element, except for* $n = 9$, *when the number of m-greatest graphs is two.*

The corresponding graphs are presented in Fig. 2.

2. Preliminaries. To begin the proof we need some more definitions and auxiliary results.

If two graphs G and H are isomorphic, we write $G = H$. If the graph G is composed of two components G_1 and G_2, we write $G = G_1 \dot{+} G_2$.

The basic properties of the numbers $p(G,k)$ and of the ordering $\succ$ have been considered elsewhere [3, 4, 5, 6 7]. Some elementary results about the relation $\succ$ are summarized in the following lemmas.

LEMMA 1. *If* $G = H$, *then* $G \sim H$. *In addition,* $G \dot{+} K \sim G$. *If* L *is a subgraph of* G, *then* $G \succ L$. *If* $G_1 \succ G_2$, *then* $G_1 \dot{+} H \succ G_2 \dot{+} H$.

LEMMA 2. *If in the graph G the edge e connects the vertices* v, *and* v_s *then* $p(G,k) = p(G - e, k) + p(G - v_r - v_s, k - 1)$.

Let e be an edge of the graph G connecting the vertices v_r and v_s. Then by $G(e/j)$ we denote the graph obtained by inserting j new vertices (of degree two) on the edge e. Hence if G has n vertices, then $G(e/j)$ has $n + j$ vertices; if $j = 0$, then $G(e/j) = G$; if $j > 0$, then the vertices v_n and v_s are not adjacent in $G(e/j)$.

We will say that the graph $G(e/j)$ possesses an internal path of length $j + 1$ (between the vertices v_r and v_s).

LEMMA 3. *For all* $j \geq 0$, $p(G(e/j+2), k) = p(G(e/j+1), k) + p(G(e/j), k-1)$.

Proof. A k-matching of the graph $G(e/j+2)$ belongs to one of the classes μ_1 to $\mu 5$, as indicated in Fig. 3. A k-matching of the graph $G(e/j+1)$ is either of the type μ'_1 or μ'_2 or μ'_3. A $(k-1)$-matching of $G(e/j)$ belongs either to the class μ'_4a or μ'_5. There is an obvious one-to-one correspondence between the classes μ_i and μ'_i for all $i = 1, 2, 3, 4$, and 5. In Fig. 3 the ellipse symbolizes the same subgraph in each of the cases, μ_1 to μ_5 and μ'_1 to μ'_5. □

Let $\gamma(n) = \gamma(n, 0)$ be a set of graphs with n vertices. Let $\gamma(n, j)$, $j > 0$, be the set of graphs with $n + j$ vertices, defined recursively as follows. $\gamma(n, j + 1)$ for $j \neq 1$ is the set of graphs obtained by inserting a new vertex into an edge in the graphs of the set $\gamma(n, j)$. In addition, $\gamma(n, 2)$ contains only those graphs formed by the described procedure from $\gamma(n, 1)$ whish possess internal paths of length three. Then, of course, all graphs from $\gamma(n, j)$, $j \geq 2$, possess internal paths of length three.

Lemma 3 has following important consequence.

LEMMA 4. *If $G(e/0)$ and $G(e/1)$ are the m-greatest graphs in $\gamma(n)$ and $\gamma(n, 1)$, respectively, then $G(e/j)$ is the m-greatest graph in the set $\gamma(n, j)$, for all j.*

Proof. The conclusion of Lemma 4 is true for $j = 0$ and $j = 1$ by hypothesis. Suppose it is true for some $j = j_0$ and $j = j_0 + 1$. For $G(e/j_0 + 2)$, Lemm 3 gives $p(G(e/jo + 2), k) = p(G(e/j_0 + 1), k) + p(G(e/j_0), k - 1)$.

Since every element of $\gamma(n, j_0 + 2)$ can be presented in the form $H(f/2)$, with $H \in \gamma(n, j_0)$ and, since f is an edge of H, we have by lemma 3,

$$p(H(f/2), k) = p(H(f/1), k) + p(H(f/0, k - 1),$$

where $H(f/1) \in \gamma(n, j_0 + 1)$ and $H(f/0) = H \in \gamma(n, j_0)$. The inductive hypothesis implies that $p(G(e/j_0 + 1), k) \geq p(H(f/1), k)$ and $p(G(e/j_0), k - 1) \geq p(H(f/0), k - 1)$ for all values of k. Therefore also $p(G(e/j_0 + 2), k) \geq p(H(f/2), k)$ and consequently $G(e/j_0 + 2) \succ H(f/2)$. □

We shall need the next two results previously obtained in [6].

LEMMA 5. *For every graph H with n vertices and cyclomatic number c there is a connected graph G with n vertices and cyclomcttic number c, such that G is m-greater than H. If H is disconnected then G is strictly m-greater than H.*

LEMMA 6. *For every graph H with n vertices and cyclomatic number c $(c > 0)$ there is a graph G with n vertices, cyclomatic number c and without vertices of degree one, such that G is m-greater than H. If H has vertices of degree 1, then G is strictly m-greater than H.*

3. Proof of Theorem 1. According to Lemmas 5 and 6 an m-greatest or m-maximal tricyclic graph must be connected and must not possess vertices of degree one. One can easily check by inspection that connected tricyclic graphs without vertices of degree one can be classified into 15 different types, which are presented in Fig. 4. Vertices of degree two are not indicated in Fig. 4.

We shall denote by $\gamma_i (i = 1, \ldots, 15)$ the classes of those tricyclic graphs which are indicated in Fig. 4. All graphs which are homeomorphic (i.e. differ only in the number and position of vertices of degree two) belong to the same class.

By $\gamma_i\{n\}$ we denote the set of the graphs from the class γ_i, having exactly n vertices.

Note that for every class γ_i, $i = 1, \ldots, 15$, there exists an integer n_i, such that for $n > n_i$, all graphs from $\gamma_i(n)$ possess internal paths od length three. For example, $n_1 = 10$, $n_8 = 9$, $n_1 5 = 12$, etc.

LEMMA 7. *For each set of graphs* $\gamma_i(n)$ $(i = 1, \ldots, 14)$ *there exists an integer* $n_0(i)$ *such that for* $n \geq n_0(i)$ *a greatest matching equivalence class exists in* $\gamma_i(n)$. *For* $i = 1, 2, 3, 4, 5, 7, 8, 9, 12, 13$, *and* 14 *the m-greatest graph in* $\gamma_i(n)$ *is unique whereas for* $i = 6$, 10 *and* 11 *there are two m-greatest graphs in* $\gamma_i(n)$.

The m-greatest graphs in $\gamma_i(n)$ will be denoted by G_n^i and (for $i = 6, 10$ and 11 only) $\overline{G}_n^i$. Of course, $G_n^i \sim \overline{G}_n^i$ $(i = 6, 10, 11)$. These graphs are presented in Fig. 5 together with the smallest value for $n_0(i)$. The dotted lines in Fig. 5 symbolize internal paths.

Proof. For each $i = 1, \ldots, 14$ Lemma 7 has been verified for $n = n_0(i)$ and $n = n_(i) + 1$ by computer search. Since for any $i = 1, \ldots, 14$ and for any $j > 0$ there exists an edge e in $G_{n_0(i)}^i$, such that $G_{n_0(i)+j}^i = G_{n_0(i)}^i(e/j)$, Lemma 7 can be proved by induction using Lemma 4. □

The set γ_{15} is very likely an exception. For $n \leq 16$ there is no greatest matching equivalence class in $\gamma_{15}(n)$. Moreover, we established that for $n \leq 16$ any two graphs from $\gamma_{15}(n)$ are m-incomparable. However, this does not disturb our search for maximal graphs since the following lemma is valid.

LEMMA 8. *Any graph from* $\gamma_{15}(n)$ *is strictly m-smaller than* G_n^8.

Proof. An arbitrary element of $\gamma_{15}(n)$ can be represented by the graph G, as displayed in Fig. 6. Deleting from G the edge e_{rs} joining vertices v_r and v_s and introducing a new edge e_{rt} joining vertices v_r and v_t we obtain a graph $H \in \gamma_8(n)$ (see Fig. 6). It is sufficient to prove that H is strictly m-greater than G.

By applying Lemma 2 to the edge e_{rs} of G and to the edge e_{rt} of H we immediately obtain $p(H, k) - p(G, k) = p(H - v_r - v_t, k - 1) - p(G - v_r - v_s, k - 1)$ since $H - e_{rt}$ and $G - e_{rs}$ are isomorphic. The graph $G - v_r - v_s$ is a subgraph of $H - v_r - v_t$ and therefore $p(H, k)$ is not smaller than $p(G, k)$ for all values of k and is greater than $p(G, k)$ for at least $k = 2$. □

In order to prove Theorem 1 it remains to compare the m-greatest graphs from particular classes.

LEMMA 9.

1. $G_n^1 \prec G_n^2$,	$n \geq n_1^* = 10$;	6. $G_n^8 \prec G_n^6$,	$n \geq n_6^* = 8$;
2. $G_n^4 \prec G_n^3 \prec G_n^2$,	$n \geq n_2^* = 7$;	7. $G_n^{11} \prec G_n^{10} \prec G_n^9$,	$n \geq n_7^* = 11$;
3. $G_n^5 \prec G_n^9$,	$n \geq n_3^* = 14$;	8. $G_n^{12} \prec G_n^9$,	$n \geq n_8^* = 14$;

4. $G_n^6 \prec G_n^5$, $n \geq n_4^* = 9$; 9. $G_n^{13} \prec G_n^9$, $n \geq n_9^* = 11$;
5. $G_n^7 \prec G_n^5$, $n \geq n_5^* = 9$; 10. $G_n^{14} \prec G_n^{10}$, $n \geq n_{10}^* = 10$.

All the relations 1.– 10. *are strict.*

Proof. Each relation can easily be verified for $n = n_i^*$ and $n = n_i^* + 1$. According to Lemma 4, the relations 1. – 10. hold then for any $n \geq n_i^*$, $i = 1, \ldots, 10$. □

Lemma 10. *For $n \geq 12$, the graphs G_n^2 and G_n^9 are m-incomparable.*

Proof. (a) It is easy to see that $p(G_n^2, 2) = p(G_n^9, 2)$. In addition, $p(G_n^2, 3) = p(G_n^9, 3) + 1$. For $n = 12$ and 13 this latter relation can be verified by direct calculation. Its general validity follows by induction using Lemma 3, $p(G_n^i, 3) = p(G_{n-1}^i, 3) + p(G_{n-2}, 2)$ for both $i = 2$ and 9. Hence, we have $p(G_n^2, k) > p(G_n^9, k)$ for $k = 3$. (b) By a fully analogous inductive argument one can verify that for $n \geq 12$, $p(G_n^2, n/2) = p(G_n^9, n/2) - 3$ if n is even, whereas $P(G_n^2, (n-1)/2) = p(G_n^9, (n-1)/2) - (3n - 35)/2$ if n is odd. Hence we have $p(G_n^2, k) < p(G_n^9, k)$ for $k = [n/2]$.

Therefore $G_n^2 \# G_n^9$ for $n \geq 12$. □

By Lemmas 7 – 10, Theorem 1 is proved for $n \geq 14$. The parts of Theorem 1 related to smaller values of n have been established by a computer search which will be described in the subsequent section.

This completes the proof of Theorem 1.

4. Computer Search. The computer search has been performed by the interactive programming system "GRAPH" for the classification and extension of knowledge in the field of graph theory [1, 2]. In order to find maximal graphs for the classes γ_1 to γ_{14} we had to determine the numbers $p(G, k)$, $k = 1, 2, \ldots$ for a few hundred graphs with at most 15 vertices. It was not clear at the beginning how many graphs we have to consider and how many vertices they have. It was not even clear whether m-greatest graphs exist at all in the classes considered.

The graphs were introduced into the system "GRAPH" via a graphical display and a light pen. The graphs were ordered so that the next graph was always a slight modification of the previous one (inserting or deleting few edges and/or vertices) and this modification was also performed by the light pen. By a special command the numbers $p(G, k)$ are obtained for obtained for the graph defined previously.

The search was organized in a few sessions of one hour, each session being sufficient to elaborate several dozens of graphs. The results of one session were the basis for defining a set of graphs for the next session. Each time we used several auxiliary results on the numbers $p(G, k)$ (some of which are included in this paper) in order to eliminate some graphs and therefore shorten the computer search.

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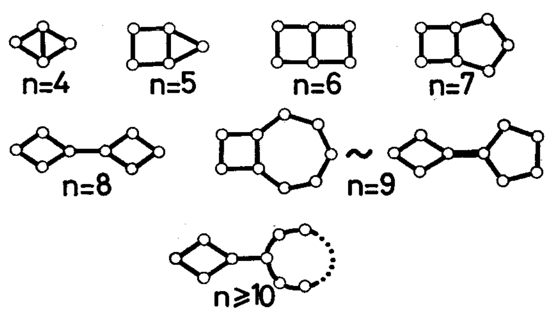

Fig. 1

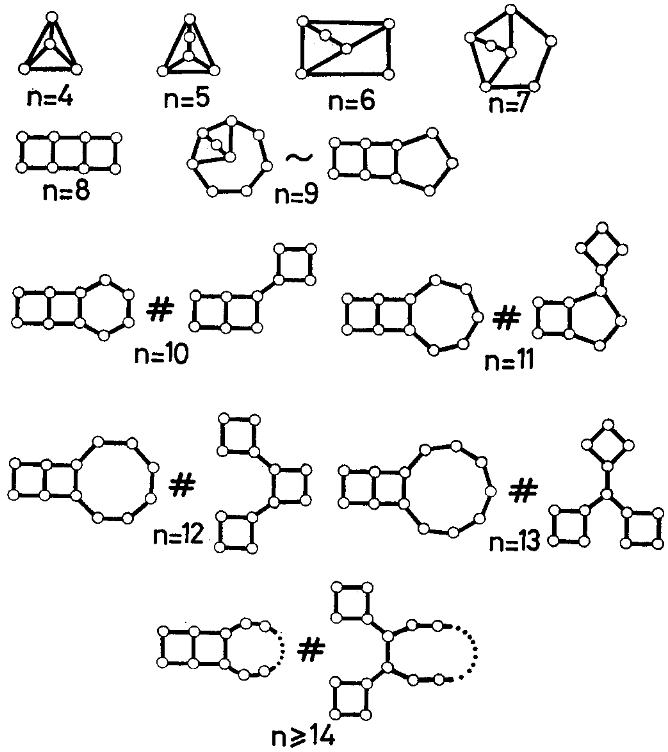

Fig. 2

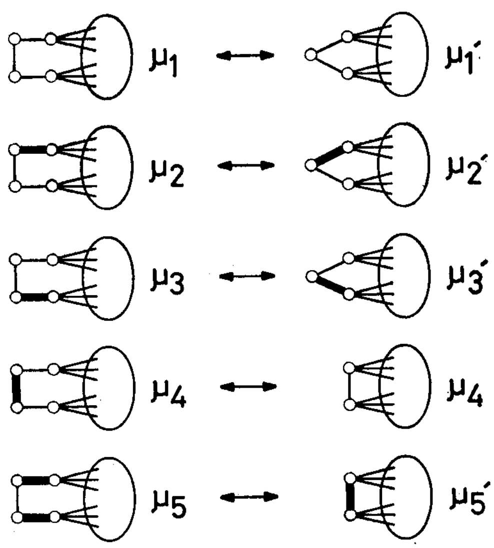

Fig. 3

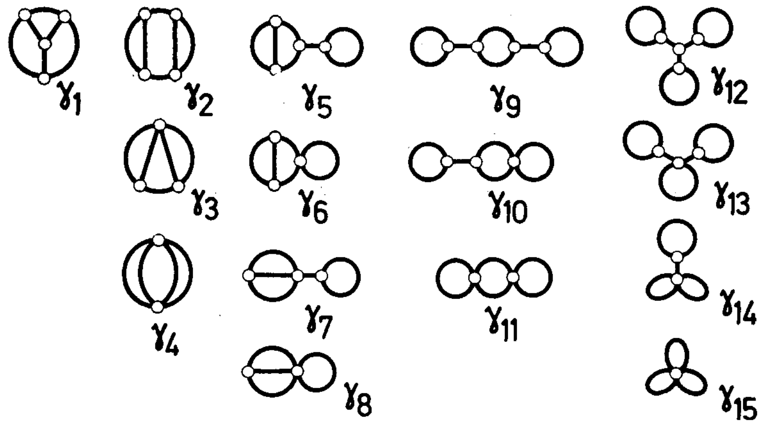

Fig. 4

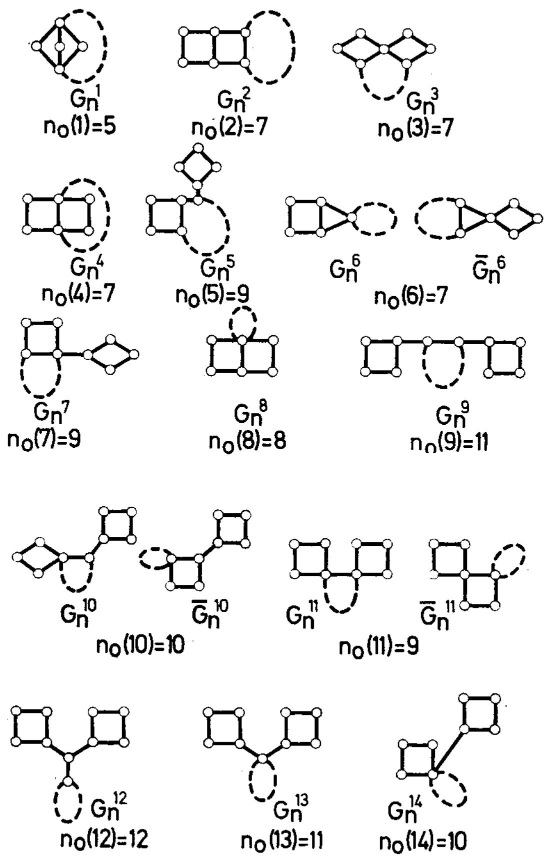

Fig. 5

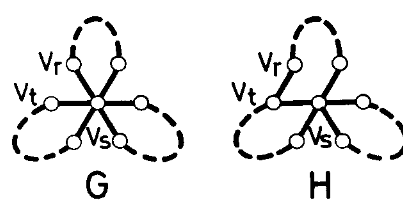

Fig. 6