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Bounds of the Hosoya index in graphs

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Abstract

A subset M of the edge set $E(G)$ of a graph G is a matching if no two edges of M are adjacent in G. In this paper we study the number of matchings in graphs, that is the Hosoya index. We study the problem of maximizing and minimizing the Hosoya index in a graph. For specific graphs this topological index is maximized by the Fibonacci number or the Lucas number. Next we give the generalizations of the Fibonacci number and the Lucas number which give the number of matchings in special multigraphs.

Keywords: Hosoya index, matching, Fibonacci number, Lucas number.

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1. Introduction

Let G be an undirected graph of order $n = |V(G)|$ and size $m = |E(G)|$. For a vertex $x \in V(G)$ let $deg_G(x)$ denote its *degree*. A *leaf* is the vertex of degree one. By *a path* from a vertex x_1 to a vertex x_n, $n \geq 2$, we mean a sequence of vertices $x_1, \ldots, x_n$ and edges $x_i x_{i+1} \in E(G)$, for $i = 1, \ldots, n-1$ and we denote it by $x_1 \ldots x_n$. *A cycle* is a path with $x_1 = x_n$. By P_n, $n \geq 2$, and C_n, $n \geq 3$ we mean graphs with the vertex set $V(P_n) = V(C_n) = \{x_1, \ldots, x_n\}$ and the edge set $E(P_n) = \{x_i x_{i+1}; i = 1, \ldots, n-1\}$ and $E(C_n) = E(P_n) \cup \{x_1 x_n\}$, respectively. Moreover P_1 is a graph which contains only one vertex. Let $X \subset V(G) \cup E(G)$. The notation $G \setminus X$ means the graph obtained from G by deleting the set X and all edges incident with vertices in X. Let $K_{1,n-1}$ denote the star consisting of one center vertex adjacent to $n-1$ leaves. A graph is said to be *claw-free* if it does not contain the star $K_{1,3}$ as an induced subgraph. For given integers n and k with $3 \le k \le n$ by $L_{n,k}$ we denote the graph of order n obtained from two vertex disjoint graphs C_k and P_{n-k} by adding an edge joining a vertex of C_k to an end vertex of P_{n-k}. For given integers n, $n \ge 2$, and m, $m \ge 1$, by $P_{n,m}$ we mean the graph of order n obtained from two vertex disjoint graphs P_m and $K_{1,n-m-1}$ by adding an edge joining an end vertex of P_m to the centre vertex of $K_{1,n-m-1}$. A subset $S \subseteq V(G)$ is *independent* if no two of its vertices are adjacent. Moreover the subset containing only one vertex and the empty set are independent. The number of all independent sets in G is denoted by $NI(G)$. For a graph G on $V(G) = \emptyset$ we put $NI(G) = 1$.

The parameter $NI(G)$ first appears in the mathematical literature in a paper of Prodinger and Tichy [8] in 1982 and this paper gave an impetus to the counting of independent sets in graphs. They called this parameter the *Fibonacci number of a graph* in view of the following facts:

(i) $NI(P_n) = F_{n+1}$, where F_n is the *n-th Fibonacci number* defined by $F_0 = F_1 = 1$ and $F_n = F_{n-1} + F_{n-2}$, for $n \ge 2$.

(ii) $NI(C_n) = L_n$, where L_n is the *n-th Lucas number* defined by $L_0 = 2$, $L_1 = 1$, and $L_n = L_{n-1} + L_{n-2}$, for $n \ge 2$.

The number L_n, for $n \ge 2$, has also another recurrence form $L_n = F_n + F_{n-2}$.

Independently, Merrifield and Simmons introduced the number of independent sets (which they called σ-index) to the chemical literature in 1989, see [6]. They showed the correlation between σ-index and some physicochemical properties such as boiling points. In the chemical literature $NI(G)$ is named as the Merrifield-Simmons index.

A subset $M \subseteq E(G)$ is a *matching* if no two of its edges are adjacent. Moreover the subset containing only one edge and the empty set also are matchings. The *edge independence number of G*, denoted by $\beta(G)$ is the cardinality of a largest matching in G. The number of all matchings in G is denoted by $NM(G)$. For a graph G on $E(G) = \emptyset$ we put $NM(G) = 1$. If $NM^{(k)}(G)$ denotes the number of k-element matching in G then $NM(G) = \sum_{k \ge 0} NM^{(k)}(G)$.

In the chemical literature the graph parameter $NM(G)$ is referred to as the Hosoya index which was introduced by Hosoya in [2]. This index has some applications in the design of combinatorial libraries for drug discovery, see [9] and in the study of Quantitative Structure Property Relationships models. An important direction is to determine the graphs with maximal or minimal Hosoya indices in a given class of graphs. The literature includes many papers dealing with the theory of counting of independent sets and matchings in graphs, see for instance [3], [4], [5], [7], [10], [11].

We list some obvious facts:

1. Let a graph G have components $G_1, \ldots, G_k$. Then

$$NM(G) = \prod_{i=1}^{k} NM(G_i).$$

2. Let $V = \{x_1, \ldots, x_p\}$ be the set of isolated vertices of a graph G. Then

$$NM(G) = NM(G \setminus V).$$

3. For an arbitrary graph G and its line graph $L(G)$,

$$NM(G) = NI(L(G)).$$

4. From (3) and by (i) and (ii) it immediately follows:

$$NM(P_n) = F_n \text{ and } NM(C_n) = L_n.$$

5. For an arbitrary graph of size m, $m \geq 1$, $NM(G) \leq 2^m$. The equality occurs if and only if $G = mK_2$.

2. Lower and upper bounds for $NM(G)$

In this section we give several bounds for the Hosoya index of graphs in terms of order, size and edge independence number.

Theorem 2.1. *Let G be any connected, simple graph of size m, $m \geq 1$ with edge independence number $\beta = \beta(G)$. Then $NM(G) \geq 2^\beta + m - \beta$.*

Moreover equality holds if and only if $G = P_4$, C_3, $L_{4,3}$ or $K_{1,m}$.

Proof. Let M denote a maximum matching in G. Clearly every subset of M and every subset of $E(G) \setminus M$ containing exactly one edge are matchings in G. Hence $NM(G) \geq 2^{|M|} + |E(G) \setminus M| = 2^\beta + m - \beta$.

If $G = P_4$, C_3, $L_{4,3}$, $K_{1,m}$ then it is obvious that $NM(G) = 2^\beta + m - \beta$ in each case. Assume now that equality occurs. Then it is clear that

(a) any two edges from $E(G) \setminus M$ are adjacent in G and

(b) every edge from M is adjacent to every edge from $E(G) \setminus M$.

In view of (a) we deduce that $E(G) \setminus M$ induces a connected subgraph of G. Hence we distinguish the following possibilities:

1. $|E(G) \setminus M| = 1$.

   In this case the set $E(G) \setminus M$ induces a K_2, hence $G = K_{1,2}$ or $G = P_4$.

2. $|E(G) \setminus M| = 2$.

   In this case $E(G) \setminus M$ induces P_3 hence it is obvious that $G = C_3$ or $G = K_{1,3}$ or $G = L_{4,3}$.

3. $|E(G) \setminus M| \geq 3$.

Since in view of (a) every two edges from $E(G) \setminus M$ are adjacent so $E(G) \setminus M$ induces either C_3 or $K_{1,p}$, for $p \leq m-1$. Firstly we shall show that for every graph G such that $E(G) \setminus M$ induced C_3 holds $NM(G) > 2^\beta + m - \beta$. It suffices to show that there is $e \in M$ nonadjacent with any edge of C_3. Let $e \in M$ be an edge incident to a vertex $x \in V(C_3)$. Then for an edge $e' \in E(C_3)$ non incident with x we have that e and e' are not adjacent, what gives by (b) that $NM(G) > 2^\beta + m - \beta$.

If $E(G) \setminus M$ induces $K_{1,p}$, $p \leq m-1$, then the condition (b) implies $p = m-1$ and $G = K_{1,m}$.

All this together completes the proof. □

Theorem 2.2. *Let G be any connected simple graph of order n and e be an edge adjacent with t edges, $t \geq 1$. Then $NM(G) \leq 2NM(G-e) - t$. Moreover $NM(G) = 2NM(G-e) - t$ if and only if*

(i) $G = P_{n,3}$ *if e is adjacent with exactly one edge in G and*

(ii) $G = K_{1,n}$, *otherwise.*

Proof. Let $e_1, \ldots, e_t$, $t \geq 1$ denote the edges adjacent to the edge e. Let $\mathcal{M}_e(G)$ (respectively: $\mathcal{M}_{-e}(G)$) be the set of matchings of G containing the edge e (respectively: not containing the edge e). Then $NM(G) = |\mathcal{M}_e(G)| + |\mathcal{M}_{-e}(G)|$. Clearly $|\mathcal{M}_{-e}(G)| = NM(G-e)$. Let $M \in \mathcal{M}_e(G)$. Then $M \setminus e \in \mathcal{M}_{-e}(G)$ which implies that $|\mathcal{M}_e(G)| \leq |\mathcal{M}_{-e}(G)|$. But $\{e_i\} \in \mathcal{M}_{-e}(G)$ for $i = 1, \ldots, t$ and $\{e_i\}$ corresponds to no set $M \setminus \{e\}$, where $M \in \mathcal{M}_e(G)$. Thus $|\mathcal{M}_{-e}(G)| \geq |\mathcal{M}_e(G)| + t$ which implies that $NM(G) \leq 2|\mathcal{M}_{-e}(G)| - t$.

If $G = P_{n,3}$ and e is adjacent with exactly one edge or $G = K_{1,n}$ then equality is obvious. Assume that $NM(G) = 2NM(G-e) - t$, for some edge e. We shall show that $e' \cap e_i \neq \emptyset$ for each $e' \in E(G) \setminus \{e, e_i\}$ for every $i \in \{1, \ldots, t\}$. Suppose on the contrary that there is $1 \leq i \leq t$ such that $e' \cap e_i = \emptyset$. Then $\{e', e_i\} \in \mathcal{M}_{-e}(G)$ and $\{e', e_i, e\} \notin \mathcal{M}_e(G)$ which gives $|\mathcal{M}_e(G)| < |\mathcal{M}_{-e}(G)| - t$. Consequently $NM(G) < 2NM(G-e) - t$, a contradiction. In view of this fact it immediately follows that $G = P_{n,3}$ if e is adjacent with exactly one edge or $G = K_{1,n}$ otherwise.

Thus the Theorem is proved. □

3. Generalized Fibonacci numbers and Lucas numbers in multigraphs

The Fibonacci numbers and the Lucas numbers have the graph interpretations as the total number of matchings in simple graphs P_n and C_n, respectively. In this section we give the generalizations of the Fibonacci numbers and the Lucas numbers with respect to the number of matchings in multigraphs.

Let $P_n^{t_1,\ldots,t_{n-1}}$ be a multigraph with the vertex set $V(P_n^{t_1,\ldots,t_{n-1}}) = V(P_n)$ and the edge set $E(P_n^{t_1,\ldots,t_{n-1}}) = \{e_1^1,\ldots,e_1^{t_1},\ldots,e_{n-1}^1,\ldots,e_{n-1}^{t_{n-1}}\}$ where $e_i^j = x_i x_{i+1}$, for $i = 1,\ldots,n-1$ and $j = 1,\ldots,t_i$. In other words the graph $P_n^{t_1,\ldots,t_{n-1}}$ is obtained from P_n by replacing the i-th edge e_i by t_i parallel edges with the same end vertices as e_i. If $t_i = 1$ for $i = 1,\ldots,n-1$ then $P_n^{1,\ldots,1}$ is isomorphic to P_n and we will write P_n instead of $P_n^{1,\ldots,1}$.

Theorem 3.3. *Let $k \geq 0$, $n \geq 2$ and $t_i \geq 1$ for $i = 1,\ldots,n-1$ be integers. Then $NM^{(0)}(P_n^{t_1,\ldots,t_{n-1}}) = 1$, $NM^{(1)}(P_n^{t_1,\ldots,t_{n-1}}) = t_1 + \cdots + t_{n-1}$ and for $k \geq 2$ we have the formula $NM^{(k)}(P_n^{t_1,\ldots,t_{n-1}}) = NM^{(k)}(P_{n-1}^{t_1,\ldots,t_{n-2}}) + t_{n-1}NM^{(k-1)}(P_{n-2}^{t_1,\ldots,t_{n-3}})$.*

Proof. The statements $NM^{(0)}(P_n^{t_1,\ldots,t_{n-1}}) = 1$ and $NM^{(1)}(P_n^{t_1,\ldots,t_{n-1}}) = t_1 + \cdots + t_{n-1}$ are obvious. Assume that $k \geq 2$. Let the edges of P_n be $e_1, e_2, \ldots, e_{n-1}$ in order. Then for each i, $i = 1,\ldots,n-1$ there are in $P_n^{t_1,\ldots,t_{n-1}}$, $(t_i - 1)$ edges that are parallel to e_i. Now any matching of size k in $P_n^{t_1,\ldots,t_{n-1}}$ can

(i) neither contain e_{n-1} nor any of its parallel edges, and there are $NM^{(k)}(P_{n-1}^{t_1,\ldots,t_{n-2}})$ such matchings, or

(ii) contains either e_{n-1} or any one of its parallel edges, and in this case, no matching can contain either e_{n-2} or any of its parallels. And hence there are $t_{n-1}NM^{(k-1)}(P_{n-2}^{t_1,\ldots,t_{n-3}})$ matchings of size k.

Thus the Theorem is proved. □

Using the above Theorem we obtain:

Theorem 3.4. *Let $n \geq 1$ and $t_i \geq 1$ for $i = 1,\ldots,n-1$ be integers. Then $NM(P_1) = 1$, $NM(P_2^{t_1}) = t_1 + 1$ and for $n \geq 2$ we have the formula $NM(P_n^{t_1,\ldots,t_{n-1}}) = NM(P_{n-1}^{t_1,\ldots,t_{n-2}}) + t_{n-1}NM(P_{n-2}^{t_1,\ldots,t_{n-3}})$.*

If $t_i = 1$ for $i = 1,\ldots,n-1$ then $NM(P_n) = F_n$.

Let $C_n^{t_1,\ldots,t_n}$ be a multigraph with the vertex set $V(C_n^{t_1,\ldots,t_n}) = V(C_n)$ and the edge set $E(C_n^{t_1,\ldots,t_n}) = E(P_n^{t_1,\ldots,t_{n-1}}) \cup \{e_n^1,\ldots,e_n^{t_n}\}$ where $e_n^i = x_1 x_n$, for $i = 1,\ldots,t_n$. In other words the graph $C_n^{t_1,\ldots,t_n}$ is obtained from C_n by replacing the j-th edge by t_j

parallel edges with the same end vertices as e_j. If $t_j = 1$ for $j = 1, \ldots, n$ then $C_n^{1,\ldots,1}$ is isomorphic to C_n and we will write C_n instead of $C_n^{1,\ldots,1}$.

Using the same method as for graph $P_n^{t_1,\ldots,t_{n-1}}$ we can prove:

Theorem 3.5. *Let $n \geq 3$, $k \geq 0$ and $t_j \geq 1$ for $j = 1, \ldots, n$ be integers. Then $NM^{(0)}(C_n^{t_1,\ldots,t_n}) = 1$, $NM^{(1)}(C_n^{t_1,\ldots,t_n}) = t_1 + \cdots + t_n$ and for $k \geq 2$ we have the formula $NM^{(k)}(C_n^{t_1,\ldots,t_n}) = NM^{(k)}(P_n^{t_1,t_2,\ldots,t_{n-1}}) + t_n NM^{(k-1)}(P_{n-2}^{t_2,\ldots,t_{n-3}})$.*

Theorem 3.6. *Let $n \geq 1$ and $t_j \geq 1$ for $j = 1, \ldots, n$ be integers. Then $NM(C_1) = 1$, $NM(C_2) = t_1 + 1$ and $NM(C_n^{t_1,\ldots,t_n}) = NM(P_n^{t_1,\ldots,t_{n-1}}) + t_n NM(P_{n-2}^{t_2,\ldots,t_{n-3}})$.*

If $t_j = 1$ for $j = 1, \ldots, n-1$ then $NM(C_n) = L_n$.

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