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An Algorithm for Computing the Merrifield–Simmons Index

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Abstract

The Merrifield–Simmons Index $i(G)$ of a molecular graph G is defined as the total number of the independent sets of the graph G, i.e., the total number of independent-vertex sets of G. it was shown that this index is correlated with the boiling points. In this paper, we present an algorithm for calculating the number of *k*-independent sets of graph G using its adjacency matrix and then we obtain the Merrifield–Simmons index of some graphs and some fullerene graphs by this algorithm.

1. Introduction

A graph $G = (V, E)$ is a combinatorial object consisting of an arbitrary set $V = V(G)$ of vertices and a set $E = E(G)$ of unordered pairs (i, j) of distinct vertices of G called edges. Suppose $|V| = n, |E| = m$, i.e., G has n vertices and m edges. The adjacency matrix of a simple graph (i.e. an unweighted, undirected graph containing no graph loops or multiple edges) is a matrix with n rows and n columns labeled by graph vertices, with a 1 or 0 in position (i, j) according to whether v_i and v_j are adjacent or not. Two vertices are adjacent if there is an edge between them.

A topological index is a real number related to a structural graph of a molecule. It does not depend on the labeling or pictorial representation of a graph. There are several topological indices have been defined.

The Merrifield-Simmons index [2-5] is one of the topological indices whose mathematical properties were studied in some detail [6-10]. We gave a recursive relation for computing this index for an infinite class of dendrimers [1]. In [4] it was shown that this index is correlated with the boiling points.

Let G be a simple graph on n vertices. A k-independent set of G is a set of k mutually independent vertices. Denote by $i(G,k)$ the number of the k-independent sets of G. By definition, the empty vertex set is an independent set. Then $i(G,0) = 1$ for any graph G. The Merrifield-Simmons index of G, denoted by (G) , is defined as

$$i(G) = \sum_{k=0}^{n} i(G,k),$$

where $i(G,0) = 1$ (by definition). If for some k, $i(G,k) = 0$ then $i(G,j) = 0$ for $j \geq k$. So $i(G)$ is equal to the total number of the independent sets of G.

This paper intends to present an algorithm for calculating the number of k-independent sets for a graph using its adjacency matrix and then we use that algorithm to compute The Merrifield-Simmons index of some graphs.

2. Main results

Suppose that $G(V,E)$ is given and let A be the adjacency matrix of graph G. A is an $n \times n$ matrix. The number of *1*-independent sets is equal to n, i.e., $i(G,1) \stackrel{\text{def}}{=} i_1 = n$. *2*-independent sets, $i(G,2) \stackrel{\text{def}}{=} i_2$ is the number of zeros above the main diagonal of A, because these zeros indicate the two independent vertices in G.

In A, we are looking for i such that there exists j,k and l, that we have

$$A(i,j) = A(j,k) = A(k,i) = 0, \quad i < j < k < l.$$

In that case we have found a *3*-independent set in graph G, because the vertices i,j and k are independent and form a *3*-independent set.

The above process should be repeated for $i = 1, \dots, n-2$, where n is the number of vertices of G.

Suppose we have a set of *3*-independent sets. For finding *4*-independent sets, let $\{i, j, k\}$ be a *3*-independent set, where $i < j < k$. We try to find vertex h such that

$$A(i,h) = A(j,h) = A(k,h) = 0,$$

for $k \le h \le n$. If there exists such h then $\{i, j, k, h\}$ is a *4*-independent set. The process should be repeated on all of *3*-independent sets to find all of *4*-independent sets.

In general, for finding *k*-independent sets ($k \le n$), we use all of (*k-1*)-independent sets. In this case we should find j_k such that

$$A(j_1, j_k) = A(j_2, j_k) = \cdots = A(j_{k-1}, j_k) = 0, \tag{1}$$

where $\{j_1, j_2, \dots, j_{k-1}\}$ forms a *(k-1)*-independent set and $j_1 < j_2 < \cdots < j_k$.

The number of sets $\{j_1, j_2, \dots, j_k\}$ that satisfy in (1) is i_k, where i_k is the number of *k*-independent sets.

The amount of Merrifield–Simmons index is equal to $1 + i_1 + i_2 + \cdots + i_n$.

3. Computational results

Using the above presented algorithm, the amount of Merrifield–Simmons index has been calculated for some graphs and the results are available in table 1. Also the index has been calculated for C_{20}, C_{24} , C_{26}, C_{28}, C_{30}, C_{34} and C_{36} (table 2).

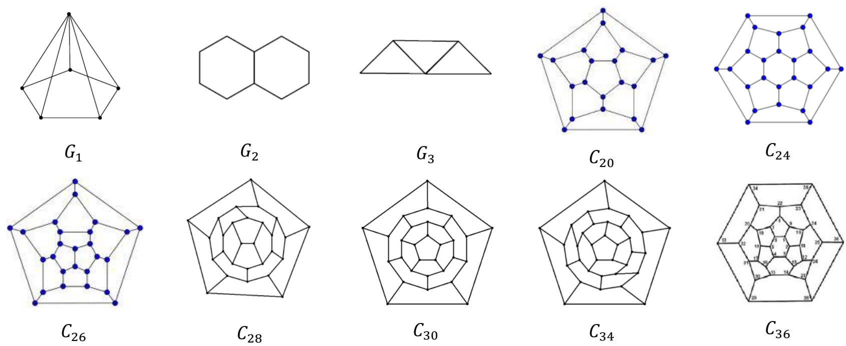

Figure 1. Graphs considered in this section

	i_0	i_1	i_2	i_3	i_4	i_5	i_6	$i(G)$
G_1	1	6	5	0	0	0	0	12
G_2	1	10	34	46	21	2	0	114
G_3	1	5	3	0	0	0	0	9

Table 1. The Merrifield–Simmons index for graphs G_1, G_2 and G_3.

	$\boldsymbol{C_{20}}$	$\boldsymbol{C_{24}}$	$\boldsymbol{C_{26}}$	$\boldsymbol{C_{28}}$	$\boldsymbol{C_{30}}$	$\boldsymbol{C_{34}}$	$\boldsymbol{C_{36}}$
i_0	1	1	1	1	1	1	1
i_1	20	24	26	28	30	34	36
i_2	160	240	286	336	390	510	576
i_3	660	1304	1742	2268	2890	4454	5412
i_4	1510	4212	6461	9506	13515	25177	33246
i_5	1912	8316	15120	25776	41724	96888	140712
i_6	1240	9918	22361	45684	86435	259981	421328
i_7	320	6756	20298	52200	119670	489986	902160
i_8	5	2292	10523	36903	108120	644745	1380057
i_9	0	264	2660	14840	60650	580930	1490514
i_{10}		0	218	2860	19263	345778	1109832
i_{11}			2	176	2910	128116	547776
i_{12}			0	0	150	26832	168525
i_{13}					0	2706	29328
i_{14}						94	2440
i_{15}						0	64
i_{16}							0
$i(G)$	5828	33327	79698	190578	455748	2606232	6232007

Table 2. The Merrifield–Simmons index for C_{20}, C_{24} , C_{26}, C_{28} , C_{30}, C_{34} and C_{36} shown in Figure 1.

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