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 \( \sigma(G) \), 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., \( i(G,1) \equiv i_1 = n \). 2-independent sets, \( i(G,2) \equiv i_2 \) 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 \( i = 1, \ldots, n-2 \), 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 $k \leq h \leq n$. 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 ($k \leq n$), we use all of $(k-1)$-independent sets. In this case we should find $j_k$ such that
\[ A(j_1,j_k) = A(j_2,j_k) = \cdots = A(j_{k-1},j_k) = 0, \quad (1) \]
where $\{j_1,j_2,\ldots,j_{k-1}\}$ forms a $(k-1)$-independent set and $j_1 < j_2 < \cdots < j_k$.

The number of sets $\{j_1,j_2,\ldots,j_k\}$ 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](image-url) Graphs considered in this section
Table 1. The Merrifield–Simmons index for graphs $G_1$, $G_2$ and $G_3$.

<table>
<thead>
<tr>
<th></th>
<th>$i_0$</th>
<th>$i_1$</th>
<th>$i_2$</th>
<th>$i_3$</th>
<th>$i_4$</th>
<th>$i_5$</th>
<th>$i_6$</th>
<th>$i(G)$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$G_1$</td>
<td>1</td>
<td>6</td>
<td>5</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>12</td>
</tr>
<tr>
<td>$G_2$</td>
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<td>10</td>
<td>34</td>
<td>46</td>
<td>21</td>
<td>2</td>
<td>0</td>
<td>114</td>
</tr>
<tr>
<td>$G_3$</td>
<td>1</td>
<td>5</td>
<td>3</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>9</td>
</tr>
</tbody>
</table>

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.
References


