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A SIMPLE ALGORITHM FOR COMPUTING DETOUR INDEX OF NANOCLUSTERS

BEHZAD MANOOCHEHRIAN[1] AND ALI REZA ASHRAFI

ACADEMIC CENTER FOR EDUCATION, CULTURE AND RESEARCH, TEHRAN, IRAN
INSTITUTE OF NANOSCIENCE AND NANOTECNOLOGY, UNIVERSITY OF KASHAN, KASHAN 87317-51167, IRAN

E-MAIL: BEHZAD@KHAYAM.AC.IR
E-MAIL: ASHRAFI@KASHANU.AC.IR

Abstract. Let G be the chemical graph of a molecule. The matrix $D = [d_{ij}]$ is called the detour matrix of G, if d_{ij} is the length of longest path between atoms i and j. The sum of all entries above the main diagonal of D is called the detour index of G. In this paper, a new algorithm for computing the detour index of molecular graphs is presented. We apply our algorithm on copper and silver nanoclusters to find their detour index.

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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 $x, y = xy$ of distinct vertices of G called edges. A topological index is a real number related to a molecular graph. It must be a structural invariant, i.e., it does not depend on the labelling or the pictorial representation of a graph. There are several topological indices have been defined and many of them have found applications as means to model chemical, pharmaceutical and other properties of molecules. The first topological index was introduced by Harold Wiener in

[1]Corresponding author.

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1947, as the half-sum of distances between atoms in the H-suppressed molecule [8].

The detour index was introduced in graph theory some time ago by F. Harary for describing the connectivity in directed graphs [3]. The detour index, in contrast to the Wiener index that considers the length of the shortest path between vertices, considers the length of the longest distance between each pair of vertices. In other words, $DD(G)$ is the sum of all $dd(i,j)$, where $dd(i,j)$ is the length of the path that contains the largest number of edges between vertices i and j in graph G. This index has recently received some attention in the chemical literature, see [2,5] and references therein. The detour index certainly carries some interesting structural information for cyclic compounds. For acyclic structures the Wiener index and the detour index are the same, since there is only a single possible path connecting any pair of vertices [8].

The goal of this article is to obtain an algorithm for calculating the detour index of molecular graphs. Using this algorithm, we prepare a MATLAB program for computing the detour index of finite graphs, [1,4]. We encourage reader to consult [7] for another algorithm on detour index of arbitrary graphs. Our notation is standard and is taken mainly from [6]. A graph G is called connected if for every $x, y \in V(G)$ there exists a path connecting x and y.

2. Result and Discussion

There is no efficient method for computing the detour index of a graph G. This problem is closely related to several other long-standing algorithmic questions of graph theory, such as finding spanning cycles and solving salesman problems. The first algorithm for computing detour index of finite graphs was introduced by Trinajstic, Nikolic and Mihalic [7]. In this section, a new algorithm for computing the detour index of molecular graphs is presented. We first compute the detour index of some well-known graphs.

Example 2.1. Consider the complete graph K_n. Since every edge of this graph lies in a cycle of length n, $dd(i,j) = n-1$. Therefore, $DD(G) = 1/2n(n-1)^2$.

Example 2.2. Suppose C_n is a cycle of length n labeled by $1, 2, \ldots, n$. It is an easy fact that $dd(i,j) = Max(|i-j|, n(|i-j|))$. This shows that, $DD(G) = (n-1+\cdots+n-1)+(n-2+\cdots+n-2)+\cdots+([(n+1)/2]+\cdots+[(n+1)/2])$, in which $[x]$ denotes the integer part of x. Therefore,

$$DD(G) = \begin{cases} (n^2/8)(3n-2) & 2|n \\ (n/8)(n-1)(3n-1) & 2 \nmid n \end{cases}$$

Suppose G and H are graphs. H is called a subgraph of G, if $V(H) \subseteq V(G)$ and $E(H) \subseteq E(G)$. An acyclic and connected subgraph T of G is called an spanning tree of G, if $V(T) = V(G)$. We are now ready to prove our main result.

Theorem 2.3. *Let G be a graph and $T_1, \ldots, T_r$ be all of spanning trees of G. Then $dd_G(i,j) = \max\{d_{T_1}(i,j), \ldots, d_{T_r}(i,j)\}$, where for a subgraph H of G, $d_H(i,j)$ denotes the graph distance between vertices i and j in H.*

Proof. *Suppose u and v are arbitrary vertices of G and P is a maximum path between u and v. Since P is a tree, we can extend P to an spanning tree of G, named T. Thus $dd_G(u,v) = dd_T(u,v)$. On the other hand, $dd_T(u,v) \in \max\{d_{T_1}(u,v), \ldots, d_{T_r}(u,v)\}$ and T contains a maximum path between u and v, proving the theorem.*

As is well known, topological indices show degeneracy, that is, two or more non-isomorphic graphs may have identical numerical values for an index. Using the previous theorem we can prepare a MATLAB program to compute detour index of molecular graphs with a small number of vertices. We apply our program on graphs of Figures 1 and 2. The detour indices of these graphs are stored in Table 1. By this table, one can see that the non-isomorphic graphs G_7, G_8, G_9 have the same detour index, which is the same as detour index of K_5. Also, it remains an open problem to find an efficient algorithm for computing detour index of molecular graphs. We end this paper with the following question:

Question. *Under what condition the detour index of a graph is the same as the detour index of a complete graph?*

Table 1. The Detour Index of some Copper and Silver Clusters.

Graphs	*DD*	*Graphs*	*DD*
G_1	*352*	G_6	*40*
G_2	*1028*	G_7	*75*
G_3	*40*	G_8	*75*
G_4	*18*	G_9	*75*
G_5	*40*	G_{10}	*126*

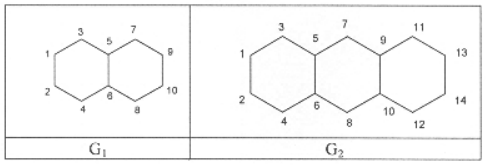

FIGURE 1. The Molecular Graph of Naphthalene and Antheracene.

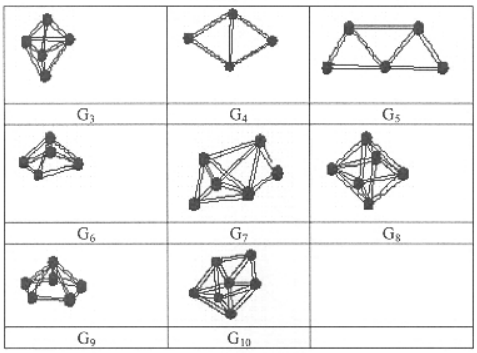

FIGURE 2. The 3D Graph of Naphthalene and Antheracene.

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