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On Sensitivity of Hamming Energy of a Graph

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Abstract: A novel graph quantity, named Hamming energy of a graph $HE(G)$, has been proposed. It is defined as a sum of the absolute values of the eigenvalues of the Hamming matrix. To be used in chemistry, graph quantity should be able to discriminate between different isomers, i.e., it should be sensitive. Therefore, in this paper, we investigate the sensitivity of $HE(G)$, using different sets of isomers. It was found that $HE(G)$ shows exceptional sensitivity compared to graph energy and other eigenvalue-based graph quantities.

Keywords: Hamming matrix, eigenvalues, graph spectrum, graph energy, degeneracy of graph quantity

1 Introduction

Let $G = (V,E)$ be a simple, undirected graph with n vertices and m edges, and $V(G)$ and $E(G)$ being its vertex and edge set, respectively. If the vertices $v_i, v_j \in V(G)$ are adjacent, then the edge connecting them is denoted by v_iv_j. For other graph-theoretical notions, the readers are referred to textbooks [1, 3]. The adjacency matrix $A(G) = [a_{ij}]$ of the graph G is symmetric matrix of order n, whose elements are defined as:

$$a_{ij} = \begin{cases} 1 & \text{if } v_iv_j \in E(G) \\ 0 & \text{if } v_iv_j \notin E(G) \\ 0 & \text{if } i = j. \end{cases}$$

The energy of a graph G, $E(G)$, is defined as the sum of the absolute values of the eigenvalues $\lambda_1, \lambda_2, \ldots, \lambda_n$ of adjacency matrix $A(G)$ [4], i.e.,

$$E(G) = \sum_{i=1}^{n} |\lambda_i|.$$

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This graph quantity found remarkable applications, especially in chemistry as a topological descriptor, and nowadays it is heavily studied, see for example [8, 9, 10, 13]. Namely, graph energy served as a model for the introduction of many other graph energies [5, 6].

Quite recently, a novel graph energy based on the Hamming matrix eigenvalues has been proposed [12]. The Hamming matrix of a graph G, $H(G) = [h_{ij}]$, is a square matrix whose elements are Hamming distances H_d:

$$h_{ij} = H_d[s(v_i), s(v_j)]$$

where $s(v_i)$ and $s(v_j)$ denote the row of the incidence matrix corresponding to the vertices v_i and v_j, respectively.

Note that the Hamming distance $H_d(x,y)$ between the strings $x = x_1x_2\ldots x_n$ and $y = y_1y_2\ldots y_n$ is the number of is such that $x_i \neq y_i$, $i = 1,2,\ldots,n$. Thus, $H_d(x,y)$ is a number of positions in which x and y differ. Therefore, $H(G)$ has zeros on its main diagonal, since

$$H_d[s(v_i), s(v_i)] = 0.$$

Let $\rho_1, \rho_2, \ldots, \rho_n$ be the eigenvalues of the Hamming matrix of a graph, then the Hamming energy of a graph $HE(G)$ is defined as [12]:

$$HE(G) = \sum_i^n |\rho_i|.$$

2 Sensitivity of Hamming energy of a graph

In order to be used for the quantification of molecular structure, a graph quantity should possess high discriminative potential among a set of isomers. In other words, it should be sensitive to the small structural differences between the isomeric molecules. A simple sensitivity measure was put by Konstantinova [7]. Namely, the sensitivity of topological descriptor TD is defined as:

$$S(TD) = \frac{N - N_{TD}}{N}$$

where N is the total number of isomers and N_{TD} is the number of isomers that cannot be distinguished by topological descriptor, i.e., by graph quantity. It is well-known that graph quantities based on adjacency matrix eigenvalues cannot fully discriminate among isomers due to the existence of isospectral graphs [2].

In this work, we say that graphs G and H have the same value of the Hamming energy if $|HE(G) - HE(H)| < 10^{-13}$. This threshold value is chosen because of the precision of the common Python computations, which is 15 decimal digits. The same applies to graph energy.

The sensitivity results for the Hamming energy of a graph are presented in Table 1 for the chemical graphs. Also, the sensitivity of the graph energy for the same set of graphs is presented.

Table 1. The percentage of sensitivity of $HE(G)$ and $E(G)$ for chemical trees with n vertices

n	# of isomers	$S[HE(G)]$	$S[E(G)]$
8	18	100 %	100 %
9	35	100 %	82.86 %
10	75	100 %	97.33 %
11	159	100 %	84.82 %
12	355	100 %	85.07 %
13	802	100 %	78.05 %
14	1858	100 %	83.58 %
15	4347	99.95 %	76.05 %
16	10359	99.99 %	79.37 %
17	24894	99.99 %	73.51 %
18	60523	99.99 %	79.26 %
19	148284	99.99 %	77.58 %
20	366319	99.99 %	82.23 %

As one may see, Table 1 shows exceptional sensitivity of the Hamming energy of a graph in the case of chemical trees with 8 up to 20 vertices. Namely, $HE(G)$ is able to completely distinguish isomers with $n = 8-14$, and for the really big datasets with $n = 15-20$ only a few chemical trees cannot be differentiated. On the other hand, the sensitivity of $E(G)$ is significantly lower, even in the case of a small set of isomers like $n = 9$. Such behavior of $E(G)$, as we mentioned earlier, may be attributed to the isospectrality of some chemical trees. These results indicate that $HE(G)$ may be used as a molecular descriptor, especially for the average-sized datasets, since it is capable of successfully discriminating among structurally similar acyclic molecules compared to other eigenvalue-based graph quantities [11].

Since molecules containing cycles are of high importance, in the Table 2 we present the sensitivity results of $HE(G)$ and $E(G)$ for the unicylic chemical graphs with $n = 6-15$.

Table 2. The percentage of sensitivity of $HE(G)$ and $E(G)$ for unicyclic chemical graphs with n vertices

n	# of isomers	$S[HE(G)]$	$S[E(G)]$
6	12	100 %	100 %
7	29	96.55 %	100 %
8	73	95.89 %	93.15 %
9	185	96.22 %	92.97 %
10	475	97.47 %	89.05 %
11	1231	96.99 %	88.63 %
12	3232	96.97 %	82.98 %
13	8506	97.67 %	83.60 %
14	22565	97.87 %	82.46 %
15	60077	97.97 %	83.40 %

The Table 2 shows that the Hamming energy of a graph exhibit better performance also on the unicyclic chemical graphs. Only for the graphs with $n = 7$ graph energy shows higher sensitivity. In large sets of isomers, the Hamming energy of a graph has very low degeneracy (less than 4 %), which is not the case with graph energy. These results indicate that the Hamming energy of a graph may be also used for the quantification of a molecular structure of unicyclic molecules.

3 Conclusion

The Hamming energy of a graph is a recently introduced graph quantity based on the Hamming matrix eigenvalues. One of the requirements for the graph quantity to fulfil to be used in chemistry is to properly distinguish among molecules. In this paper, we tested sensitivity of the Hamming energy on chemical trees and chemical unicyclic graphs. It was found that the Hamming energy of a graph shows high sensitivity, especially in the case of chemical trees. Previous studies show that other eigenvalue-based quantities operate with the significantly lower sensitivity.

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