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Topological Indices of Hypercubes

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ABSTRACT

Wiener index of a graph is defined to be the sum of the distances of each pair of vertices. Schultz index of a graph is sum of *di(aij+dij)*, where *aij* and *dij* are the *ij*th entry of the adjacency and distance matrices of the graph and *di* is degree of vertex *i* for all $1 \le i, j \le |V(G)|$. Definition of Padmakar-Ivan (PI) and Szeged indices is based on the number of vertices and edges which are nearer to one end of a given edge than the other end. Topological indices of many molecules with structures near to cube has been widely studied in chemistry. In this paper we give explicit formulas for four topological indices(Wiener, Schultz, PI and Szeged) of hypercubes and their corresponding Euclidean graph, a weighted graph with weight of an edge is equal to Euclidean distance between its endpoints. Also some bounds have been deduced.
KEYWORDS: Topological indices, Hypercubes, Euclidean graphs.

1 INTRODUCTION

Graph theory is a useful tool in many areas in mathematical chemistry. Topological indices are graph theoretical concepts which has a lot of applications in chemistry [9]. These indices are parameters over graphs of molecules which has been usually based on the concept of distance between vertices (or edges) of the graph [10]. The first index of this type has been introduced in 1947 by H.Wiener [1]. Several other indices have been defined later [10]. A lot of work has been done on the indices either from a chemical point of view or through purely mathematical approaches. Some relations has been found between indices [3], indices of some classes of graphs has been detected[8], some complexity concepts has been studied on chemical graphs [5] and purely mathematical work has been done on relations of Wiener index and matching of a graph[4].

Our work aims to find out explicit mathematical formulas for four important indices of hypercubes. In this context $G=(V,E)$ is a graph with vertex set $V(G)=\{v_1,\dots,v_n\}$ and edge set $E(G)=\{e_1,\dots,e_m\}$. For simplicity we use *V* and *E* for vertex and edge set of *G* respectively. The adjacency matrix of *G*, written *A(G)*, is the *n*-by-*n* matrix in which entry a_{ij}, is the number of edges in *G* with endpoints $\{v_i, v_j\}$ [12]. Also *D(G)*, distance matrix of *G* has d_{ij} as its *ij*th entry, where d_{ij} is the distance between vertices *i* and *j* [11]. All over this paper our graphs are simple and connected so entries of adjacency matrix are *0* or *1*. In next section, we begin by the definition of four of these indices.

2 Definitions

The first topological index which introduced by Wiener was defined as follows due to the notations which are mentioned in last section.

Definition 2.1 [9] The Wiener index of a graph *G* is

$$W(G)=\frac{1}{2}\sum_{u,v\in V} d(u,v)$$

where *d(u, v)* is the distance between vertices *u* and *v* on the shortest path between them and sum is taken over all pairs of vertices of *G*.

Definition 2.2 [7] The Schultz index of a graph *G* is

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$$MTI(G) = \sum_i \sum_j d_i (a_{ij} + d_{ij})$$

where d_i is degree of *i*th vertex in *G* and a_{ij} and d_{ij} are entries in row *i* and column *j* of adjacency matrix *A(G)* and distance matrix *D(G)* of *G*.

Definition 2.3 [14] Let $e = uv$ be an edge of *G* with endpoints *u* and *v* and $m_e(u|G)$ be the number of vertices in *G* which are closer to *u* than *v*. Then the Szeged index of a graph *G* is $S_Z(G) = P_{e2E} m_e(u|G) m_e(v|G)$, where sum is taken over all edges of *G*.

The distance from a vertex to an edge in a graph is the minimum of the distances of the vertex from the end-points of the edge. With respect to this we have the following definition.

Definition 2.4 [13] Let $e = uv$ be an edge of *G* with endpoints *u* and *v* and $n_e(u|G)$ be the number of edges in *G* which are closer to *u* than *v*. Then, the PI index of *G* is $PI(G) = P_{e2E}(n_e(u|G) + n_e(v|G))$, where sum is taken over all edges of *G*.

Structure of many of molecules for which the indices has been studied is similar to a cube. In addition Euclidean distances in chemical structures are as important as lengths of paths in their graphs [6]. This motivates us to look for indices of hypercubes. To prepare mathematical background we need the following definitions.

Definition 2.5 [12] An *n*-dimensional cube or hypercube Q_n is the simple graph whose vertices are the *n*-tuples with entries in *{0, 1}* and whose edges are the pairs of *n*-tuples that differ in exactly one position.

Definition 2.6 [2] Euclidean graph is a weighted graph in which the weights are equal to the Euclidean lengths of the edges in a specified embedding.

In this context Euclidean graph of a graph G is a new graph, denoted by E_G, with vertex set $V(E_G) = V(G)$ and edge set $E(E_G) = V(G) \times V(G)$ such that weight of each edge is equal to its Euclidean length. (Corresponding to the above definition) For simplicity we use notation E_n instead of E_{Q_n}.

In what follows, we find the explicit mathematical formulas for Wiener, Shultz, PI and Szeged indices of hypercubes and Euclidean graphs.

3 Indices of hypercubes

At first, the Wiener index of hypercube Q_n is computed and the result expressed as an explicit mathematical formula.

Theorem 3.1 Let Q_n be an *n*-dimensional cube. Then Wiener index of Q_n is $W(Q_n) = n4^{n-1}$.

Proof. Note that Q_n is vertex transitive, so for each pair *u* and *v* of vertices of Q_n, sum of the distances of *v* from other vertices is equal to that of *u*. Now for every *i*, $1 \le i \le n$, if a vertex is at distance *i* from $v = (0, \ldots, 0)$ then it must have *1* in exactly *i* positions. The number of such vertices is $\binom{n}{i}$. So sum of distances of all vertices of Q_n from *v* is $\sum_{i=1}^{n} i \binom{n}{i}$. Now consider that $(1+x)^n = \sum_{i=1}^{n} \binom{n}{i} x^i$. Taking derivations from both sides of the equality we have $n(1+x)^{n-1}=\sum_{i=1}^{n} i\binom{n}{i}x^{i-1}$. If we put $x=1$ then $\sum_{i=1}^{n} i\binom{n}{i}=n2^{n-1}$. Q_n has 2^n vertices, therefore $W(Q_n)=\frac{1}{2}\times 2^n\times n2^{n-1}=n4^{n-1}$.

In the next theorem the Szeged index of hypercube Q_n is computed.

Theorem 3.2 Szeged index of *n*-dimensional cube Q_n of order n is 2^{3n-2}.

Proof. Let $e=uv$ be an arbitrary edge of Q_n and $m_e(u)$ the number of the vertices of Q_n nearer to *u* than *v*. Since Q_n is vertex transitive then $m_e(u)=m_e(v)$ for every edge $e=uv$. Again vertex transitivity allows us to suppose that $u=(0,\dots,0)$ and $v=(1,\dots,0)$ without loss of generality. If a vertex is at distance *i* from *u*, then its distance from *v* could not be more than $i+1$ ($1\le i\le n$). Such a vertex should have *1* in *i* coordinates other than the first one. The number of such vertices which are at distance *i* from *u* and at distance $i+1$ from *v* is $\binom{n-1}{i}$. So

$$\begin{aligned} Sz(Q_n) &= 2^n\sum_{i=0}^{n-1}\binom{n-1}{i}\sum_{i=0}^{n-1}\binom{n-1}{i} \\ &= 2^n(2^{n-1})^2 \\ &= 2^{3n-2}. \end{aligned}$$

An explicit formula is concluded for the PI index of Q_n in the following theorem.

Theorem 3.3 $PI(Q_n)=(n-1)2^{2n-1}$.

Proof. Let $e=uv$ be an edge of Q_n and $n_e(u)$ be the number of edges nearer to *u* than *v*. Because of vertex and edge transitivity of Q_n we just need to calculate $n_e(u)$ for $u=(0,\dots,0)$ and $v=(1,\dots,0)$. If an edge is at distance *i* ($1\le i\le n$) from *u* and distance $i+1$ from *v* then one of its endpoints should have *1* in *i* of its coordinates other than the first coordinate and the other endpoint should have exactly one extra *1* in a coordinate other than the former $i+1$ coordinates. So the number of such edges is $\binom{n-1}{i}(n-i-1)$. So

$$\begin{aligned} PI(Q_n) &= 2^n\times 2\times\sum_{i=0}^{n-1}\binom{n-1}{i}(n-i-1) \\ &= 2^{n+1}\sum_{i=0}^{n-1}\binom{n-1}{i}(n-i-1) \\ &= 2^{n+1}\sum_{i=0}^{n-1}\binom{n-1}{i} \\ &= 2^{n+1}\times(n-1)2^{n-2} \\ &= (n-1)2^{2n-1}. \end{aligned}$$

The forth index, Schultz index, is found for Q_n in next theorem.

Theorem 3.4 $MTI(Q_n) = 5n^2 2^{2n-1} - n2^n$.

Proof. We have $MTI(Q_n) = \sum_i \sum_j d_j (a_{ij} + d_{ij})$. Obviously $d_i = n$ for every vertex of Q_n. Also if two vertices are adjacent then $a_{ij} = 1$ and $d_{ij} = 1$, then $a_{ij} + d_{ij} = 2$, otherwise $a_{ij} + d_{ij} = d_{ij}$. The number of pair of adjacent vertices is $n \times 2 \times 2^{n-1}$ because each pair of adjacent vertices should have exactly one different coordinate (which is possible in *n* ways), this coordinate can be *0* or *1* (2 ways) and each of the other $n-1$ coordinates can be either 0 or 1(2^{n-1} ways). Similarly the number of pair of vertices in distance *i* is $\binom{n}{i} 2^i 2^{n-i}$ Therefore

$$\begin{aligned} MTI(Q_n) &= n\left[2(n2^{n}) + 2^n \sum_{i=2}^{n} i\binom{n}{i}\right] \\ &= n^2 2^{n+1} + n2^n(n2^{n-1} - n) \\ &= 5n^2 2^{2n-1} - n2^n. \end{aligned}$$

At the end of this section we just mention relations between some of these indices arisen easily from their formulas.

$$Sz(Q_n) = \frac{2^n}{n} W(Q_n)$$

and

$$PI(Q_n) = 8W(Q_{n-1}).$$

4 Indices of Euclidean graphs of *n*-dimensional cubes

For finding our desire indices for Euclidian graph of n-dimensional cube we need a lemma which is mentioned following.

Lemma 3.1 If two vertices in Q_n are at distance *i* from each other then their Euclidean distance is $\sqrt{i}$ and vice versa.

Proof. Two vertices in distance *i* have exactly *i* different coordinates, so their Euclidean distance is $\sqrt{i}$.

Now, by using the above lemma, we express the Wiener, Shultz, PI and Szeged indices of Euclidian graph of n-dimensional cube.

Theorem 4. 2 $W(E_n) = 2^{n-1} \sum_{i=1}^{n} \binom{n}{i} \sqrt{i}$.

Proof. From the above lemma we just need to replace *i* with $\sqrt{i}$ in theorem 1.0.1. Using Cauchy-Schwartz inequality we have

$$\left(\sum_{i=1}^{n} \sqrt{i}\binom{n}{i}\right)^2 \le \left(\sum_{i=1}^{n} i\right)\left(\sum_{i=1}^{n} \binom{n}{i}^2\right).$$

So

$$W(E_n) \le 2^{n-1} \sum_{i=1}^{n} \binom{n}{i} \sqrt{i}. \qquad \text{(I)}$$

Theorem 4. 3 $MTI(E_n) = 2nW(E_n) + n^2 2^{n+1}$.

Proof. From lemma 4.1 replace *i* with $\sqrt{i}$ in the proof of theorem 3.4 and use theorem 4.2.

Inequality I, gives the following bound

$$MTI(E_n) \le n2^n \left(\sqrt{\frac{n(n+1)}{2}\binom{2n}{n}} + 2n \right).$$

Theorem 4.4 PI and Szeged indices of Euclidean graph of an *n*-dimensional cube are equal to PI and Szeged indices of that *n*-dimensional cube respectively.

Proof. From lemma 4.1 it is obvious that for any edge *uv* in Q_n an arbitrary vertex *w* is nearer to *u* in Q_n if and only if it is nearer to *u* in E_n and hence PI and Szeged indices does not differ for Q_n and its Euclidean graph E_n.

5 Conclusion

We can compute and express completely the explicit mathematical formulas for four topological indices, Wiener, Schultz, PI and Szeged indices, for hypercubes and Euclidean graph of n-dimensional hypercubes that these indices have applications in mathematical chemistry, chemometrics and nano-computations.

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