

Computing Szeged Index of Graphs on Triples

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ABSTRACT

Let $G=(V,E)$ be a simple connected graph with vertex set V and edge set E . The Szeged index of G is defined by $Sz(G) = \sum_{e=uv \in E} n_u(e|G)n_v(e|G)$, where $n_u(e|G)$ is the number of vertices of G closer to u than v and $n_v(e|G)$ can be defined in a similar way. Let S be a set of size $n \geq 8$ and V be the set of all subsets of S of size 3. We define three types of intersection graphs with vertex set V . These graphs are denoted by $G_i(n)$, $i=0,1,2$ and we will find their Szeged indices.

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1. INTRODUCTION

Let $G = (V,E)$ be a simple graph with vertex set V and edge set E . An automorphism of G is a one-to-one mapping $\sigma : V \rightarrow V$ that preserves adjacency of vertices in G . The distance between two vertices u and v is the length of a shortest path from u to v and is denoted by $d(u,v)$. A function f from the set of all graphs into real numbers is called a *graph invariant* if and only if $G \cong H$ implies that $f(G) = f(H)$. A graph invariant is said to be *distance-based* if it can be defined by distance function $d(-,-)$. A graph invariant applicable in chemistry is called a *topological index*.

In recent research in mathematical chemistry, distance-based graph invariants are of particular interest. One of the oldest descriptors concerned with the molecular graph is the *Wiener index*, which was proposed by Wiener [8]. The definition of the Wiener index in terms of distances between vertices of a graph is due to Hosoya [6].

The *Szeged index* [4,5,7] is a topological index closely related to the Wiener index and coincides with the Wiener index in the case when the graph is a tree. For the

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basic definition of the Szeged index of graph, let $G = (V, E)$ be a connected simple graph. Let $e = uv$ be an edge of G . We define two subsets of vertices of G as follows:

$$N_u(e|G) = \{w \in V \mid d(w, u) < d(w, v)\}$$

$$N_v(e|G) = \{w \in V \mid d(w, v) < d(w, u)\}$$

Let $n_u(e|G) = |N_u(e|G)|$ and $n_v(e|G) = |N_v(e|G)|$. The Szeged index of the graph G is defined by the following formula:

$$Sz(G) = \sum_{e=uv \in E} n_u(e|G)n_v(e|G)$$

We see that the Szeged index is a sum of edge-contribution for the edge $e = uv$ of the graph G , we set $sz(e) = n_u(e|G)n_v(e|G)$, hence $Sz(G) = \sum_{e \in E} sz(e)$.

Let Γ denote the automorphism group of the graph G . Then Γ acts as a permutation group on the vertex set V of G . If $e = uv$ is an edge of G and $\sigma \in \Gamma$, then by defining $e^\sigma = u^\sigma v^\sigma$, we observe that Γ acts on the set E of edges of G . If Γ acts transitively on V , then G is called a vertex-transitive graph and if it acts transitively on E , then G is called an edge-transitive graph. We refer the reader to the book [2] for further reading about permutation groups.

In [1], the case of edge-transitive graph is studied. In this case, the edge-distribution at each edge is the same, i.e., $sz(e) = sz(e')$ for all edges e and e' of G holds, hence $Sz(G) = |E|sz(e)$ for a single edge of G holds. The above situation is also studied in [9].

2. PRELIMINARY RESULTS

In this paper we are concerned with the graphs on triples. Let S be a set of size n where n is a suitable natural number. Let V be the set of all the 3-element subsets of S . The graph $G_i, i = 0, 1, 2$, called intersection graphs, are defined as $G = (V, E_i)$, where V is the set of vertices of G and two vertices are joined by an edge if and only if they intersect in i elements. It is clear that $|V| = \binom{n}{3}$ and the size of each $E_i; i = 0, 1, 2$, is $\binom{n-3}{3}, 3\binom{n-3}{2}$ and $3(n-3)$ respectively, it is worth mentioning that the Wiener indices of the graphs $G_i; i = 0, 1, 2$, were computed in [3].

Lemma 2.1. Each of the graphs $G_i; i = 0, 1, 2$, is edge-transitive.

Proof. By [3], the automorphism graph of each graph $G_i; i=0,1,2$, has a subgroup isomorphic to the symmetric group S_n . Let $e = uv$ and $e' = u'v'$ be two edges of $G_i; i=0,1,2$. Then $|u \cap v| = i = |u' \cap v'|$.

Case 1. $i=0$. In this case we may take $u = \{1,2,3\}, v = \{4,5,6\}, u' = \{1',2',3'\}, v' = \{4',5',6'\}$ where $\{1',2',\dots,6'\} \subseteq \{1,2,\dots,6\}$. The permutation $\sigma = \begin{pmatrix} 1 & 2 & 3 & 4 & 5 & 6 \\ 1' & 2' & 3' & 4' & 5' & 6' \end{pmatrix} \in S_n$ take e to e' .

Case 2. $i=1$. In this case we may take $u = \{1,2,3\}, v = \{1,4,5\}, u' = \{1', 2', 3'\}, v' = \{1', 4', 5'\}$ and choose $\sigma = \begin{pmatrix} 1 & 2 & 3 & 4 & 5 \\ 1' & 2' & 3' & 4' & 5' \end{pmatrix} \in S_n$ which takes e to e' .

Case 3. $i=2$. In this case we may choose $u = \{1,2,3\}, v = \{1,2,4\}, u' = \{1', 2', 3'\}, v' = \{1', 2', 4'\}$ and in this case $\sigma = \begin{pmatrix} 1 & 2 & 3 & 4 \\ 1' & 2' & 3' & 4' \end{pmatrix} \in S_n$ takes e to e' . ■

We have the following result from [3] that will be used.

Result 2.1. Let u and v be two vertices of $G_i; i=0,1,2$. Then $d(u,v) \leq 2$ unless $i=2$ where $d(u,v) = 3$ also occurs.

3. COMPUTATION OF THE SZEGED INDEX

Now because of Lemma 2.1, we have $Sz(G_i) = |E_i|sz(e), i = 0, 1, 2$, where $sz(e) = n_u(e|G_i)n_v(e|G_i)$. By definition we have $n_u(e|G_i) = |\{ w \in V \mid d(w,u) < d(w,v)\}|$. By the above result $d(w,v) = 0, 1, 2$ in the case G_1 and G_2 .

Case 1. $d(w,v) = 0$ is impossible.

Case 2. If $d(w,v) = 1$, then $d(w,v) = 0$ implying $w = u$.

Case 3. If $d(w,v) = 2$, then $d(w,v) = 0$ or 1 . If $w = u$, then $d(u,v) = 1$ a contradiction, hence $d(w,u) = 1$. We conclude that

$$n_u(e|G) = 1 + |\{v \neq w \in V \mid d(w,u) = 1\}|.$$

By symmetry we have $n_v(e|G) = n_u(e|G)$.

Corollary 3.1. The Szeged index of G_0 and G_1 are as follows:

$$Sz(G_0) = \binom{n-3}{3} \left(1 + 3 \binom{n-6}{2} + 3 \binom{n-6}{1} \right)^2$$

$$Sz(G_1) = 3 \binom{n-3}{2} \left(1 + 2 \binom{n-5}{2} + 2 \binom{n-5}{1} \right)^2$$

Proof. According to what we proved earlier $Sz(G_i) = |E_i| sz(e)$, where $e = uv$ is a fixed edge of $G_i, i = 0, 1$. But

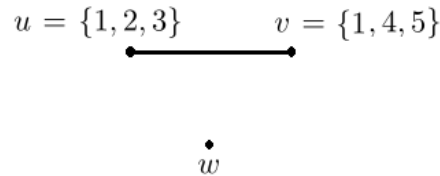
$$sz(e) = n_u(e|G) n_v(e|G) = n_u(e|G)^2$$

$$= (1 + |\{v \neq w \in V \mid d(w, u) = 1\}|)^2$$

Therefore we must find the number of vertices $w \neq v$ of V with distance 1 from u .

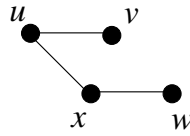
Case 1. $i = 0$. In this case we may take $u = \{1, 2, 3\}$ and $v = \{4, 5, 6\}$, the vertex w should be of distance 2 from v , hence should meet v and $w \cap u = \emptyset$. If w meets v in one element we have $3/2(n-6)(n-7)$ choices for it and if it meets v in 2 elements again we have $3(n-6)$ choices for it and the formula for $Sz(G_0)$ is obtained as above.

Case 2. $i = 1$. In this case we may choose $u = \{1, 2, 3\}, v = \{1, 4, 5\}$. we have $d(w, v) = 2$, hence $w \cap v = \emptyset$ or $|w \cap v| = 2$, but $|w \cap u| = 1$.

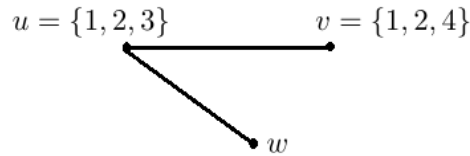


If $w \cap v = \emptyset$, then we have $(n-5)(n-6)$ choices for w . If $|w \cap v| = 2$, then if $1 \in w$, we must have $w = \{1, 4, x\}$ or $w = \{1, 5, y\}$, hence the number of choices for w is $2(n-5)$. For $1 \notin w$ we don't obtain a possibility for w . Therefore $Sz(G_1)$ is as above. ■

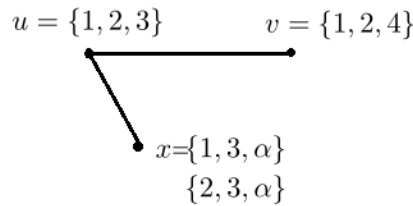
To calculate the Szeged index of G_2 we must calculate the size of the set $N_u(e|G) = \{w \in V \mid d(w, u) < d(w, v)\}$. In this case $d(w, v) = 3$ may occur and $d(w, u) = 1$ or 2. If $d(w, u) = 1$, then $d(w, v) = 2$, a contradiction. Therefore $d(w, u) = 2$, i.e. there is a vertex x such that $d(w, x) = 1$. If we set $A_1 = \{v \neq w \in V \mid d(w, u) = 1\}$ and $A_2 = \{w \in V \mid d(w, u) = 2\}$ then we must find the sizes of A_1 and A_2 .



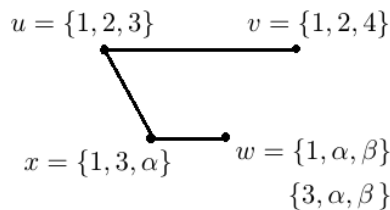
Let $u = \{1, 2, 3\}$, $v = \{1, 2, 4\}$ and find $|A_1|$.



In this case $d(w, v) = 2$, hence $|w \cap v| \neq 2$. If $w \cap v = \emptyset$, then there is no possibility for w . If $|w \cap v| = 1$, then $w = \{1, 3, x\}, \{2, 3, x\}$, and hence the following corollary is proved. There are $2(n - 4)$ possibilities for w and $|A_1| = 2(n - 4)$. To find $|A_2|$ we may assume again $u = \{1, 2, 3\}, v = \{1, 2, 4\}$.



The number of vertices x is $2(n - 4)$. Now having chosen x the number of w with distance 1 from x is $2(n - 5)$.



Corollary 3.2. For the Szeged index of G_2 we have

$$Sz(G_2) = 3(n - 3) \left(1 + 2 \binom{n - 4}{1} + 4 \binom{n - 4}{1} \binom{n - 5}{1} \right)^2.$$

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