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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.

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 $\sigma : V \to V$ 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 can 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 theWiener 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 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 Weiner 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 $\{1',2',\ldots,6'\} \subseteq \{1,2,\cdots,6\}$ .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 $d(u,v) \le 2$ 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 $w = u$.

Case3. 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

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

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

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

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

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

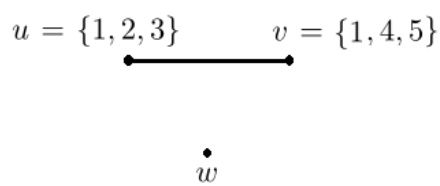
Proof. According to what we proved earlier $Sz(G_i) = |E_i|\, sz(e),$ where $e = uv$ is a fixed edge of $G_i, i = 0,1.$ But

$$sz(e) = n_u(e\,|\,G)\, n_v(e\,|\,G) = n_u(e\,|\,G)^2$$
$$= \left(1 + |\{v \neq w \in V \,|\, d(w,u) = 1\}|\right)^2$$

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

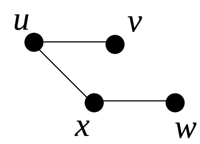
Case 1. $i = 0$. In this case we may take $u = \{1,2,3\}$ and $v = \{4,5,6\}$, the vertex w should be of distance 2 from v, hence should meet v and $w \cap u = \phi$. If w meets v in one element we have 3/2(n − 6)(n − 7) choices for it and if it meets v in 2 elements again we have $3(n-6)$ choices for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

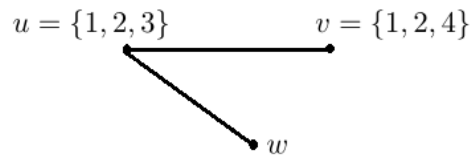


If $w \cap v = \phi,$ then we have $(n-5)(n-6)$ choices for W. If $|w \cap v| = 2,$ then if $1 \in w,$ we must have $w = \{1,4,x\}$ or $w = \{1,5,y\}$, hence the number of choices for w is $2(n-5)$ .For $1 \notin w$ we don't obtain a possibility for w. Therefore $Sz(G_1)$ is as above. ■

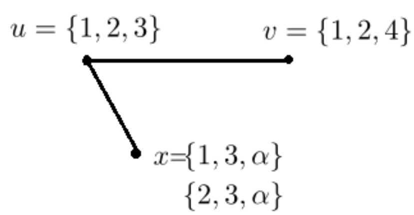
To calculate the Szeged index of G_2 we must calculate the size of the set $N_u(e|G) = \{w \in V \,|\, d(w,u) < d(w,v)\}$ .In this case $d(w,v) = 3$ may occur and $d(w,u) = 1$ or 2. If $d(w,u) = 1$, then $d(w,u) = 2$, a contradiction. Therefore $d(w,u) = 2$, i.e there is a vertex x such that $d(w,x)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



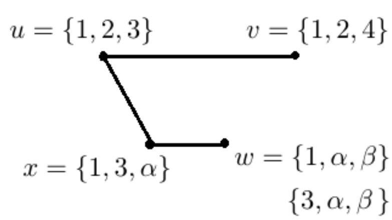
Let $u = \{1, 2, 3\}$, $v = \{1, 2, 4\}$ and find $|A_1|$.



In this case $d(w, v) = 2$, hence $|w \cap v| \neq 2$. If $w \cap v = \phi$, 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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