Szeged Index of Symmetric Graphs

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Formulas for the Szeged index of several families of graphs are derived using symmetry.

1. INTRODUCTION

A topological index is a numerical quantity derived in an unambigous manner from the structural graph of a molecule. These indices are graph invariants, which usually reflect molecular size and shape.

The first nontrivial topological index in chemistry was introduced by H. Wiener[1] in 1947 to study boiling points of paraffins (for historical data see, for instance, ref 2). Since then, the Wiener index has been used to explain various chemical and physical properties of molecules and to correlate the structure of molecules to their biological activity.[3] The research interest in Wiener index and related indices is still considerable.[4,5]

Wiener originally defined his index on trees and studied its use for correlations of physicochemical properties of alkanes, alcohols, amines, and other analogous compounds.

The original definition was given in terms of edge weights. In an arbitrary tree, every edge is a bridge, that is, after deletion of the edge, the graph is no more connected. The weight of an edge is taken to be the product of the numbers of vertices in the two connected components. This number also equals the number of all shortest paths in the tree which go through the edge.[6] Therefore the usual generalization of the Wiener index on arbitrary graphs is defined to be the sum of all distances in a graph.

Another natural generalization was previously put forward and called the Szeged index, *Sz*.[7] Now the weights of edges are taken to be the product of the numbers of vertices closer to the two endpoints of the edge. For reasons to introduce the Szeged index and for basic properties of *Sz*, see refs 7 and 8. Formulas or special algorithms for the Szeged index of several families of graphs were proposed recently.[9−11]

Here we consider computation of the Szeged index on symmetric graphs. We show by several examples that the symmetry can be used to obtain formulas for the Szeged index of several families of graphs. Edge contributions to the Szeged index are considered, which already proved to be useful when computing the Wiener index of symmetric graphs.[12−14] The approach is analogous to one used in ref 14 where the Wiener index of symmetric graphs was treated.

We remark that the idea of using symmetry of graphs to simplify the computation of a graph invariant is more general. An analogouos approach can be used for any graph invariant that is defined in terms of edge weights.

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2. PRELIMINARIES

We use usual graph theoretical terminology (as for instance in ref 15). 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 *simple path* from x to y is a sequence of distinct vertices $P = x_0, x_1, ..., x_l$ such that each pair x_i, x_{i+1} is connected by an edge and $x_0 = x$ and $x_l = y$. The *length* of the path is the number of edges, $l(P) = l$. For any pair of vertices x, y we define the *distance* $d(x,y)$ to be the length of a shortest path between x and y. If there is no (finite) path, we define $d(x,y) = \infty$. We will also write $d(u,v) = d_u(v) = d_v(u)$. A graph G is *connected* if $d(x, y) < \infty$ for any pair of vertices x, y. Here we will consider only connected graphs.

Let us recall the definition of the Szeged index

$$Sz(G) = \sum_{e \in E(G)} n_1(e|G)\, n_2(e|G)$$

where the sum runs over all edges of G and the numbers $n_1(e|G)$ and $n_2(e|G)$ are cardinalities of the sets $N_1(e|G)$ and $N_2(e|G)$. $N_1(e|G)$ is the set of vertices of G that are closer to u than to v, where u and v are the endpoints of e.

From its very definition the Szeged index is a sum of edge contributions. The contribution of edge $e = uv$ will be denoted by

$$sz_G(e) = n_1(e|G)\, n_2(e|G)$$

The index G will be omitted if no confusion can occur.

$$Sz(G) = \sum_{e \in E(G)} sz_G(e) = \sum_{e \in E(G)} sz(e)$$

If G is a graph with the automorphism group Γ, then Γ acts as a permutation group on the vertex set $V(G)$. At the same time we may view it to act on the edge set $E(G)$. We can make a distinction by writing $[\Gamma, V(G)]$ in the first case and $[\Gamma, E(G)]$ in the second one. Each permutation group (Γ, X) partitions the set X into orbits. If there is only one orbit, we say that Γ is *transitive* on X. If Γ acts transitively on $V(G)$ the graph is said to be *vertex-transitive*; if the action of Γ on $E(G)$ is transitive, then the graph is said to be *edge-transitive*. For more information about graphs and permutation groups, the reader is referred to ref 16.

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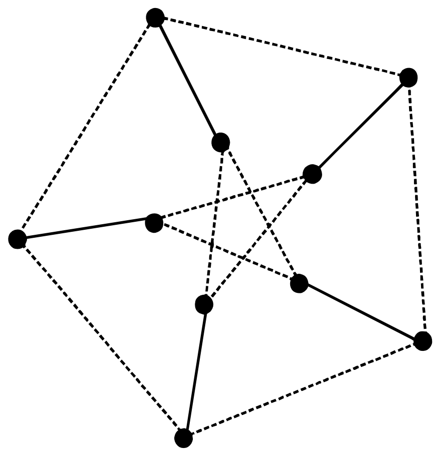

Figure 1. Petersen graph.

In general, the weights at each edge orbit are constant. To compute the Szeged index it suffices to compute the weights only once for each orbit. In the case of edge-transitive graphs, this means only one weight has to be determined. If E_1, E_2, ..., E_s are the edge orbits for the automorphism group of G, then for each orbit E_k the weights of edges in it are equal and the weight value will be denoted by $sz(E_k)$. Then the Szeged index can be expressed as:

$$Sz(G) = \sum_{k=1}^{s} |E_k| sz(E_k) \tag{1}$$

In the case of edge-transitive graph we have only one orbit and hence:

$$Sz(G) = |E(G)| sz(e) \tag{2}$$

Example (a). As a first example consider the Petersen graph. It has two edge orbits, one with 5 and the second with 10 edges (see Figure 1). In both cases, the edge contributions are $sz(e) = 3{\cdot}3 = 9$. Hence

$$Sz(P) = \sum_{E} sz(e) = 15{\cdot}9 = 135$$

Recall that the Wiener index of the Petersen graph is

$$W(P) = 10{\cdot}(3{\cdot}1 + 6{\cdot}2)/2 = 75$$

The Petersen graph is thus vertex-transitive and not edge-transitive. (All permutations that form the automorphism group for the Petersen graph are given in ref 17). Another example of a vertex-transitive graph with two edge orbits is the Heawood graph. There are also numerous examples of cubic vertex-transitive graphs with three edge orbits, called zero-symmetric graphs.[18]

Before giving more examples, we recall the definition and some basic facts on Cartesian product graphs and prove a formula for the Szeged index of Cartesian product of arbitrary graphs.

3. CARTESIAN PRODUCT GRAPHS

The *Cartesian product* of graphs G and H is the graph $K = G\Box H$ whose vertex set $V(K)$ is the Cartesian product $V(G) \times V(H)$, that is, each vertex of K is an ordered pair (u, v) of vertices $u \in V(G)$, $v \in V(H)$ and (u, v) is adjacent to (u', v') if and only if either u is adjacent to u' in G and $v = v'$ or $u = u'$ and v is adjacent to v' in H.

An example, the Cartesian product of a path, P_2, and a cycle, C_4, is depicted on Figure 2.

Here are some useful facts that can be found in graph-theoretical literature (see for instance ref 19).

Proposition 1. *For any vertex-transitive graphs* G *and* H, *the Cartesian product* G□H *is vertex-transitive.*

Note that G and H may be both vertex- and edge-transitive and $G\Box H$ need not be edge-transitive. For instance, let $G = K_2$, $H = K_3$. The Cartesian product $K_2\Box K_3$ is vertex-transitive but has six edges in one orbit and three edges in the other.

Proposition 2. *For any vertex and edge-transitive graph* G, *the* n*th Cartesian power* G^n *is vertex- and edge-transitive.*

In the above theorem both vertex- and edge-transitivity are needed. Note that the path on three vertices P_3 is edge-transitive but $P_3\Box P_3$ is not. Also, $K_2\Box K_3$ is vertex- transitive but $K_2\Box K_3\Box K_2\Box K_3$ is not edge-transitive.

We now consider a Cartesian product of arbitrary k graphs, G_1, G_2, ..., G_k.

In the Cartesian product, each edge of each factor appears in every copy of the factor. For example, if we have only two factors, then edges $e = \{(u, v), (u', v)\}$ and $f = \{(u, v'), (u', v')\}$ both appear in the product because of the edge $\{u, u'\}$ of G_1 and are therefore parallel. It is also well known that the distance in Cartesian product graphs is always the sum of distances of the projections to the factors.

Therefore for any pair of parallel edges

$$sz_G(e) = sz_G(f)$$

The above property of the distances in the Cartesian product also implies

$$sz_G(e) = sz_{G_i}(e) \times |V(G)|/|V(G_i)|$$

Now the Szeged index of the product can be written as

$$Sz(\Box_{i=1}^{k} G_i) = \sum_{e\in E(G)} sz_G(e) \tag{3}$$

$$= \sum_{i=1}^{k} |V(G)|/|V(G_i)| \sum_{e\in E(G_i)} sz_G(e) \tag{4}$$

$$= \sum_{i=1}^{k} |V(G)|/|V(G_i)| \sum_{e\in E(G_i)} sz_{G_i}(e)|V(G)|/|V(G_i)| \tag{5}$$

$$= \sum_{i=1}^{k} |V(G)|^2/|V(G_i)|^2 \sum_{e\in E(G_i)} sz_{G_i}(e) \tag{6}$$

$$= |V(G)|^2 \sum_{i=1}^{k} Sz(G_i)/|V(G_i)|^2 \tag{7}$$

Therefore the Szeged index of the product can be expressed as a simple function of the values of $Sz(G_i)$ of the factors.

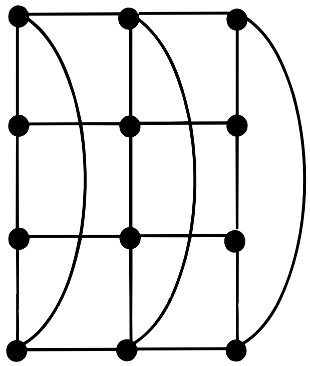

Figure 2. $G = P_2\square C_4$.

Theorem 1. *Let G_i, $i = 1, 2, ..., k$, be arbitrary graphs. Then*

$$Sz(\square_{i=1}^{k} G_i) = |V(G)|^2 \sum_{i=1}^{k} Sz(G_i)/|V(G_i)|^2$$

In particular, for a product of two factors

$$Sz(H\square K) = Sz(H)|V(K)|^2 + Sz(K)|V(H)|^2$$

It may be interesting to compare this with a similar expression for the Wiener index (see theorem 5.9. of ref 20):

$$W(H\square K) = W(H)|V(K)|^2 + W(K)|V(H)|^2$$

For a product of k copies of the same graphs we get

$$Sz(G^k) = k|V(G)|^{2(k-1)} Sz(G)$$

If G is a vertex- and edge-transitive graph then:

Theorem 2. *For any vertex and edge-transitive graph* G *of degree* d, *for any edge* e *of* G *and or any edge* $e^{(k)}$ *of the* k*th Cartesian power* G^k *we have:*

$$Sz(G^k) = |E(G^k)| sz_{G^k}(e) = k|E(G)||V(G)|^{2(k-1)} sz_G(e)$$

Proof. Recall that $|E(G^k)| = k|E(G)||V(G)|^{k-1}$ and $sz_{G^k}(e) = |V(G)|^{k-1} sz_G(e)$.

4. MORE EXAMPLES

The simplest examples of graphs that are vertex and edge-transitive are K_2 and complete graphs K_n, cycles C_n, and regular complete r-partite graphs $K_{n,n,...,n}$. We will consider these examples and their Cartesian powers.

Example (b). The kth Cartesian power of the K_2 is the k-cube graph Q_k. Obviously we have $Sz(K_2) = 1$. Therefore by the above theorem:

$$Sz(Q_k) = k|V(G)|^{2(k-1)} Sz(K_2) = k2^{2(k-1)}$$

Note that the Wiener index of the Q_k is $W(Q_k) = k2^{2k-2}$ (see, for example, ref 20).

This can be readily generalized to the kth Cartesian power of the complete graph on n vertices, K_n. Obviously we have $Sz(K_n) = 1$. Therefore $Sz(K_n^k) = kn^{2(k-1)}$ while $W(K_n^k) = k(n - 1)n^{2k-1}/2$.

The next example is the Cartesian power of cycles.

Example (c). Clearly,

$$Sz(C_n) = nsz(e) = n\left[\frac{n}{2}\right]^2 = \begin{cases} n(n-1)^2/4, & n \text{ odd} \\ n^3/4, & n \text{ even} \end{cases}$$

$$Sz(C_n^k) = \begin{cases} kn^{2k-1}(n-1)^2/4, & n \text{ odd} \\ kn^{2k+1}/4, & n \text{ even} \end{cases}$$

For comparison (see refs 13, 21, 22, and 14),

$$W(C_n) = \begin{cases} (n^2-1)n/8, & n \text{ odd} \\ n^3/8, & n \text{ even} \end{cases}$$

$$W(C_n^k) = \begin{cases} k(n^2-1)n^{2k-1}/8, & n \text{ odd} \\ kn^{2k+1}/8, & n \text{ even} \end{cases}$$

Example (c). The complete regular r-partite graph $K_{n,n,...,n}$. The graph has rn vertices and has degree $d = (r - 1)n$. It is vertex and edge-transitive. A straightforward calculation using $Sz_{K_{n,n,...,n}}(e) = (n - 1)^2$ and $|E(K_{n,n,...,n})| = \binom{r}{2}n^2$ shows that

$$Sz(K_{n,n,...,n}) = |E(G)|sz(e) = \binom{r}{2} n^2 (n-1)^2 = r(r-1)n^2(n-1)^2/2$$

and, using $|V(K_{n,n,...,n})| = nr$,

$$Sz(K_{n,n,...,n}^k) = k|V|^{2(k-1)} Sz(K_{n,n,...,n}) = k(nr)^{2(k-1)} r(r-1)n^2(n-1)^2/2 = \frac{1}{2}kr^{2k-1}(r-1)n^{2k}(n-1)^2$$

Recall that for the Wiener index we have[14]

$$W(K_{n,n,...,n}) = \binom{nr}{2} + r\binom{n}{2}$$

and

$$W(K_{n,n,...,n}^k) = k(nr + n - 2)(nr)^{2k-1}/2$$

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NOTE ADDED IN PROOF

For a recent survey on the Szeged index see ref 23.

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