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Use of the Szeged index and the revised Szeged index for measuring network bipartivity

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ABSTRACT

We have revisited the Szeged index (Sz) and the revised Szeged index (Sz^*), both of which represent a generalization of the Wiener number to cyclic structures. Unexpectedly we found that the quotient of the two indices offers a novel measure for characterization of the degree of bipartivity of networks, that is, offers a measure of the departure of a network, or a graph, from bipartite networks or bipartite graphs, respectively. This is because the two indices assume the same values for bipartite graphs and different values for non-bipartite graphs. We have proposed therefore the quotient Sz/Sz^* as a measure of bipartivity. In this note we report on some properties of the revised Szeged index and the quotient Sz/Sz^* illustrated on a number of smaller graphs as models of networks.

1. Motivation

Graph invariants, widely studied in mathematical chemistry, are of interest in structural, physical, organic and medicinal chemistry because they offer useful molecular descriptors for structure–property and structure–activity studies. Often they are derived from molecular graphs by considering various structural elements, often in an *ad hoc* manner. Interestingly many conceptually simple and computationally straightforward molecular descriptors, among the oldest so constructed, continue to offer satisfactory structure–property–activity correlations. Such are the path numbers of Platt [30], the Wiener number W [50,13,34], the "topological" index Z of Hosoya [18] the connectivity index of Randić [35], and the path/walks shape indices of Randić [36]. The Wiener number appears to be the first non-trivial molecular descriptor to be used in structure–property correlations, a clear structural interpretation of which is still somewhat elusive. The Wiener number W, which has attracted considerable attention, particularly during the last two decades, continues to be investigated [24,12,53,15]. Wiener has defined it only for acyclic structures. It can be simply calculated, as outlined by Wiener, by summing the bond contributions obtained by multiplying the number of atoms on each side of each bond.

Interestingly, Hosoya [18] noticed that W can be obtained simply from the distance matrix of a graph by summing all entries in the matrix above the main diagonal. The distance matrix of a graph has been introduced in graph theory by Harary [16]. The (i, j) matrix element of the distance matrix D of a graph has been defined as the length of the shortest path between vertices i and j, that is the number of edges between vertices i and j. In view of the Wiener number not being defined for cyclic graphs, the use of distance matrices offers alternative routes to its generalization to cyclic structures. A straightforward approach is to follow the Hosoya relationship of the Wiener number and distance matrix, valid strictly for acyclic graphs, and construct the distance matrix of cyclic graphs and add the entries of the distance matrix above the main diagonal. However, there are other possibilities for generalizing Wiener number to cyclic graphs, including the use of an alternative metric, for example, the distance–resistance matrix [22,9,20].

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In this contribution we will re-examine a particular generalization of W of Gutman [13], who starts from the definition of W as described by H. Wiener in his seminal work obtained it as a bond additive quantity, from contributions obtained by multiplying the number of atoms on each side of each bond. The same approach, again restricted to acyclic structures, has been used for the construction of the so called hyper-Wiener number WW [37,42,43,21]. There, the element (i, j) is given as the product of the number of atoms on one side of the path between vertices i and j. This particular generalization can also be applied to the Szeged index of Gutman [13], and the revised Szeged index [34].

Gutman has generalized the Wiener number for cyclic graphs by replacing the original wording of Wiener "*as a bond additive quantity, by adding contributions obtained by multiplying the number of atoms on each side of each bond*" by "*adding contributions obtained by multiplying the number of atoms closer to each of the atoms forming a bond*". The modified definition, which in the case of acyclic graphs is equivalent to the original definition of Wiener, has the advantage that it can be applied to cyclic graphs. It partitions vertices into those closer to one or the other terminal atoms of a bond, and those at an equal distance. The novel generalization of W when applied to cyclic structures has been known as the Szeged index. Observe that in the construction of the Szeged index, atoms that are at equal distance from both ends of a bond make no contribution to the Szeged index.

The Szeged index attracted attention not only in chemical graph theory but also in selected mathematical circles [14,51,3,52]. In applications to structure–property correlations, however, it did not produce satisfactory results [19]. This may have been disappointing in view of its mathematical elegance, but the modification that followed visibly improved its performance and did not disturb its elegance. The basic criterion for acceptance of mathematical descriptors for structure–property–activity studies is their performance. What saved the Szeged index from oblivion is a recent modification of the Szeged index, in which atoms that are at equal distances from the both ends of a bond are taken into account, rather than being ignored. This produced better correlation with boiling points in cyclo-alkanes than the original index [34], because of the preservation of size consistency, which is reflected in the fact that the magnitudes of the index are similar for molecules having the same number of atoms whether they have even or odd rings. This modification has been referred to as the revised Szeged index, here denoted as Sz^*.

2. The revised Szeged index

In this contribution we will report on some properties of the revised Szeged index. Let us start with the Wiener index and let T be a tree. Let $e = u \sim v$ be any of its edges joining adjacent vertices u and v. Let $n(u; v)$ denote the number of vertices that are closer to u than to v and similarly, let $n(v; u)$ denote the number of vertices that are closer to v than to u. The Wiener index $W(T)$ of T can be computed as follows:

$$W(T) = \sum_{u \sim v \in E(T)} n(u; v) n(v; u).$$

Hosoya has already shown that for any tree this definition is equivalent to the following [13]:

$$W(T) = \sum_{u,v \in V(T)} d(u, v)$$

where $d(u; v)$ is the usual distance in connected graphs and the summation is taken over all unordered pairs of vertices of T. Because Wiener never applied his index to connected graphs that are not trees, one can extend his definition to graphs in different ways, the only restriction being that it should behave as the Wiener index on trees. Usually, one defines the Wiener index of a graph G as

$$W(T) = \sum_{u,v \in V(T)} d(u, v).$$

The index

$$Sz(G) = \sum_{u \sim v \in E(T)} n(u; v) n(v; u)$$

is called the Szeged index of a graph [13]. In [34] Randić proposed a modification of the Szeged index and called the resulting index the revised Wiener index. However, we feel that the newly described index arises from the Szeged index and therefore should be called *the revised Szeged index* $Sz^*(G)$. Let $o(u; v) = o(v; u)$, the number of vertices of the same distance from u and from v. Then

$$Sz^*(G) = \sum_{u \sim v \in E(T)} (n(u; v) + (1/2)o(u; v))(n(v; u) + (1/2)o(v; u)).$$

3. Results

Theorem 1. *For a connected graph G we have*

$$Sz(G) \leq Sz^*(G).$$

The equality holds if and only if G is bipartite.