Edge-contributions of some topological indices and arboreality of molecular graphs

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Abstract

Some graph invariants can be computed by summing certain values, called *edge-contributions* over all edges of graphs. In this note we use edge-contributions to study relationships among three graph invariants, also known as topological indices in mathematical chemistry: Wiener index, Szeged index and recently introduced revised Szeged index. We also use the quotient between the Wiener index and the revised Szeged index to study arboreality (tree-likeness) of graphs.

1 Introduction and Motivation

In mathematical chemistry some graph invariants are being studied intensively since they correlate well, when applied to molecular graphs, with certain properties of the corresponding molecules. In this note we explore three such invariants, all based on the Wiener index [24], that was initially defined for trees and admits several non-equivalent generalizations to general graphs.

Traditionally, the Wiener index for general graphs is defined as the sum of all distances in a graph. Ivan Gutman [9] introduced another generalization that is known under the name of *Szeged index.* Recently Milan Randić modified the definition of the Szeged index. The new index was named *revised Szeged index* by Pisanski and Randić [16].

Let G be any connected graph. Then one can define the usual distance function on its vertex set $V(G)$. Namely, $d(u, v)$ is the number of edges on

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any of the shortest paths joining vertex u to vertex v. The Wiener index is defined as:

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

where the sum runs over all ordered pairs of vertices. The factor (1/2) is needed in order to count each pair exactly once. If we want to avoid extra work, it is more convenient to consider unordered pairs. For example, if the vertex set is linearly ordered, we can write

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

Define

$$W(u,v) = \{x \in V(G) | d(u,x) < d(v,x)\}.$$

Let $w(u,v)$ denote the number of vertices that are closer to u than to v, i.e. $w(u,v) := |W(u,v)|$. Hence, $w(v,u)$ is the number of vertices that are closer to v than to u: $w(v,u) := |W(v,u)|$.

Proposition 1. *For any connected graph G and any pair of distinct vertices u and v the sets $W(u,v)$ and $W(v,u)$ are non-empty and disjoint.*

We may define : $O(u,v) := V(G) - W(u,v) - W(v,u)$. Clearly, $O(u,v) = O(v,u)$ and the sets $O(u,v), W(u,v), W(v,u)$ form the so-called *fundamental partition* of the vertex set $V(G)$. Note that sometimes these three sets are denoted by ${}_uW_v, W_{uv}, W_{vu}$, respectively; see, for instance [11].

Let T be a tree. Let $e = u \sim v$ be any of its edges joining adjacent vertices u and v. The Wiener index $W(T)$ of T can be computed as

$$W(T) = \sum_{u\sim v\in E(G)} w(u,v)w(v,u)$$

based on the following theorem (that was known already to Wiener [24]).

Theorem 2. *For any tree T*

$$W(T) = \sum_{u\sim v\in E(G)} w(u,v)w(v,u) = \sum_{u<v,u,v\in V(T)} d(u,v)$$

For instance, this theorem was the basis for efficient computation of the Wiener index for trees [14]. Wiener never applied his index to connected graphs that are not trees. So one can extend his definition to graphs arbitrarily, the only restriction is that it should behave as the Wiener index on trees.

The invariant:

$$Sz(G) = \sum_{u \sim v \in E(G)} w(u,v)w(v,u)$$

is called the *Szeged index* of a graph [9]. In [20] M. Randić proposed a modification of the Szeged index and called the resulting index the *revised Wiener index*. However, we feel the newly described index arises from the Szeged index and therefore should be called *the revised Szeged index* $Sz^*(G)$. Let $o(u,v) = o(v,u)$ denote the number of vertices of the same distance from u and from v:

$$o(u,v) = |\{x \in V(G) | d(u,x) = d(v,x)\}| = |O(u,v)|$$

The revised Szeged index is defined as follows:

$$Sz^*(G) = \sum_{u \sim v \in E(G)} (w(u,v) + (1/2)o(u,v))(w(v,u) + (1/2)o(u,v))$$

In this note we study relationships among the Wiener index, the Szeged index and the revised Szeged index. Independent proofs of some of the results that were obtained by Dobrynin and Gutman [3] are presented.

2 Edge Contributions

If we compare the three indices: $W(G), Sz(G)$ and $Sz^*(G)$ we see that the Szeged and the revised Szeged index can be naturally described as a sum over the corresponding *edge contributions*. For an edge $e = u \sim v$ define:

$$s(e) = w(u,v)w(v,u)$$

and

$$s^*(e) = (w(u,v) + (1/2)o(u,v))(w(v,u) + (1/2)o(u,v))$$

Then

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

and

$$Sz^*(G) = \sum_{e \in E(G)} s^*(e)$$

In what follows here we try to mimic the edge-contribution for the Wiener index. Let a and b be two vertices of graph G and let $p(a,b)$ denote the number of shortest paths in G between a and b and let $k(a,b,e)$ be the number of shortest paths between a and b passing through the edge e. Define the *edge contribution* $w(e)$ as

$$w(e) := \sum_{a<b, a,b \in V(G)} k(a,b,e)/p(a,b)$$

Lemma 3.

$$d(a,b) = \sum_{e \in E(G)} k(a,b,e)/p(a,b)$$

Theorem 4.

$$\sum_{e \in E(G)} w(e) = W(G)$$

Proof

$$\begin{aligned}
\sum_{e \in E(G)} w(e) &= \sum_{e \in E(G)} \sum_{a<b, a,b \in V(G)} k(a,b,e)/p(a,b) = \\
&= \sum_{a<b, a,b \in V(G)} \sum_{e \in E(G)} k(a,b,e)/p(a,b) = \sum_{a<b, a,b \in V(G)} d(a,b) = \\
&= W(G)
\end{aligned}$$

□

3 Results

Let us present the results from [16].

Theorem 5. *For a connected graph G we have*

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

The equality holds if and only if G is bipartite.

The proof obviously follows from the fact the $s(e) \leq s^*(e)$ for each edge e.

Theorem 6. *For a tree T the three indices are the same:*

$$W(T) = Sz(T) = Sz^*(T)$$

For general graphs the difference between the revised Szeged index and the original Szeged index may be quite large. Take for instance the complete graph K_n. The revised Szeged index is in this case equal to $Sz^*(K_n) = n^3(n-1)/8$ while $W(G) = Sz(G) = n(n-1)/2$. The quotient between the revised Szeged index and the original index is hence n^2.

This example shows that the leftmost equality may hold even for graphs that are not trees. However, it would be interesting to investigate the graphs, for which $W(G) = Sz^*(G)$. This equality clearly holds for trees. It would be interesting to know if such an equality may hold for any other graphs.

In a similar way one can compute the Szeged and the revised Szeged index for a cycle graph C_n: $Sz(C_n) = n(\lfloor(n/2)\rfloor)^2$ and $Sz^*(C_n) = n^3/4$. The Wiener index for cycles is $W(C_n) = n^3/8$ for even n and $W(C_n) = (n^2-1)n/8$ for odd values of n; see [26].

In [6] the authors have used symmetry of graphs in order to simplify the calculation of the Wiener index of a graph. In [26], the process has been repeated for the Szeged index, see also [16] for corrections of some errors.

Now we explore the relationship between $w(e)$ and $s(e)$.

Lemma 7. *For every connected graph G and for every edge $e = u \sim v$ it follows that*

$$w(e) \leq s(e).$$

The equality holds if and only if e is the only edge between $W(u,v)$ and $W(v,u)$ and each vertex $w \in O(u,v)$ adjacent to some vertex from $W(u,v) \cup W(v,u)$ determines a triangle K_3 on $\{u,v,w\}$.

Proof

$$w(e) := \sum_{a \in V(G), b \in V(G)} k(a,b,e)/p(a,b)$$

$$\leq \sum_{a \in W(u,v), b \in W(v,u)} k(a,b,e)/p(a,b) \leq \sum_{a \in W(u,v), b \in W(v,u)} 1 = w(u,v)w(v,u) = s(e)$$

The tricky part is to determine when

$$w(e) = s(e).$$

The leftmost inequality becomes equality if and only if the existence of a shortest path between a and b passing through e implies that all shortest paths from a to b pass through e. The second inequality turning into equality implies that for each vertex a from $W(u,v)$ and for each vertex b from $W(v,u)$ at least one shortest path between them passes through e. This implies that e is the only edge joining $W(u,v)$ with $W(v,u)$. If $O(u,v)$ is non-empty, it must have a vertex w that is connected both to $W(u,v)$ and $W(v,u)$ and forms an odd cycle including the edge e. Let $u' \in W(u,v)$ be adjacent to w and let $v' \in W(v,u)$ be adjacent to w. The distance between u' and v' is 2 and the shortest path does not involve e. This means the equality cannot hold if $O(u,v)$ is nonempty. □

Using the above Lemma one can prove the following inequality that was proven already in [12], see also [3].

Theorem 8. *For any connected graph G we have*

$$W(G) \leq Sz(G)$$

The equality holds for graphs with the following property. G is obtained from complete graphs by vertex identifications. Two maximal complete graphs have at most one vertex in common. Each cycle lies in a complete graph.

Corollary 9. *For any connected graph G we have*

$$W(G) = Sz^*(G)$$

if and only if G is a tree.

4 Arboreality of a graph

In [16] the quotient $\beta(G) = Sz(G)/Sz^*(G)$ is considered as a measure of bipartivity of a graph. Since $0 \leq Sz(G)/Sz^*(G) \leq 1$ and $Sz(G)/Sz^*(G) = 1$ only for bipartite graphs, it measures how close to a bipartite graph a given graph is. The question can be asked what is the minimum value of $\beta(G)$ for some classes of graphs.

There are two quotients that we may consider in a similar way:

$$\alpha(G) = W(G)/Sz(G)$$

and

$$\tau(G) = W(G)/Sz^*(G)$$

While $\alpha(G)$ measures how far from a tree composed of complete graphs is G, $\tau(G)$ measures the departure of G from a tree. Let us call it *arboreality* of G. We may say that low $\alpha(G)$ means that G is hollow, while large values mean it is dense. Obviously, $\alpha(G)\beta(G) = \tau(G)$ for any graph G.

The following tables lists some values of these parameters for certain graphs. First we look at the complete graphs K_n.

G	$W(G)$	$Sz(G)$	$Sz^*(G)$	$\alpha(G)$	$\beta(G)$	$\tau(G)$
K_n	$n(n-1)/2$	$n(n-1)/2$	$n^3(n-1)/8$	1	$8/n^2$	$8/n^2$
K_2	1	1	1	1	1	1
K_3	3	3	6.75	1	0.444444	0.444444
K_4	6	6	24	1	0.25	0.25
K_5	10	10	62.5	1	0.16	0.16
K_6	15	15	135	1	0.111111	0.111111
K_7	21	21	257.25	1	0.0816327	0.0816327
K_8	28	28	448	1	0.0625	0.0625
K_9	36	36	729	1	0.0493827	0.0493827

Next we consider complete bipartite graphs $K_{n,n}$

G	$W(G)$	$Sz(G)$	$Sz^*(G)$	$\alpha(G)$	$\beta(G)$	$\tau(G)$
$K_{n,n}$	$n(3n-2)$	n^4	n^4	$(3n-2)/n^3$	1	$(3n-2)/n^3$
$K_{1,1}$	1	1	1	1.	1.	1.
$K_{2,2}$	8	16	16	0.5	1.	0.5
$K_{3,3}$	21	81	81	0.259259	1.	0.259259
$K_{4,4}$	40	256	256	0.15625	1.	0.15625
$K_{5,5}$	65	625	625	0.104	1.	0.104
$K_{6,6}$	96	1296	1296	0.0740741	1.	0.0740741
$K_{7,7}$	133	2401	2401	0.0553936	1.	0.0553936
$K_{8,8}$	176	4096	4096	0.0429688	1.	0.0429688
$K_{9,9}$	225	6561	6561	0.0342936	1.	0.0342936
$K_{10,10}$	280	10000	10000	0.028	1.	0.028

In the next table are the hypercube graphs.

G	$W(G)$	$Sz(G)$	$Sz^*(G)$	$\alpha(G)$	$\beta(G)$	$\tau(G)$
Q_n						
Q_1	1.	1.	1.	1.	1.	1.
Q_2	8.	16.	16.	0.5	1.	0.5
Q_3	48.	192.	192.	0.25	1.	0.25
Q_4	256.	2048.	2048.	0.125	1.	0.125
Q_5	1280.	20480.	20480.	0.0625	1.	0.0625
Q_6	6144.	196608.	196608.	0.03125	1.	0.03125

In the next table with paths, only 1's appear in the columns $\alpha(G)$, $\beta(G)$, and $\tau(G)$ because all paths are trees.

G	$W(G)$	$Sz(G)$	$Sz^*(G)$	$\alpha(G)$	$\beta(G)$	$\tau(G)$
P_n						
P_2	1.	1.	1.	1.	1.	1.
P_3	4.	4.	4.	1.	1.	1.
P_4	10.	10.	10.	1.	1.	1.
P_5	20.	20.	20.	1.	1.	1.
P_6	35.	35.	35.	1.	1.	1.
P_7	56.	56.	56.	1.	1.	1.
P_8	84.	84.	84.	1.	1.	1.
P_9	120.	120.	120.	1.	1.	1.
P_10	165.	165.	165.	1.	1.	1.

Cycles:

G	$W(G)$	$Sz(G)$	$Sz^*(G)$	$\alpha(G)$	$\beta(G)$	$\tau(G)$
C_n						
C_3	3.	3.	6.75	1.	0.444444	0.444444
C_4	8.	16.	16.	0.5	1.	0.5
C_5	15.	20.	31.25	0.75	0.64	0.48
C_6	27.	54.	54.	0.5	1.	0.5
C_7	42.	63.	85.75	0.666667	0.734694	0.489796
C_8	64.	128.	128.	0.5	1.	0.5
C_9	90.	144.	182.25	0.625	0.790123	0.493827
C_{10}	125.	250.	250.	0.5	1.	0.5
C_{11}	165.	275.	332.75	0.6	0.826446	0.495868
C_{12}	216.	432.	432.	0.5	1.	0.5
C_{13}	273.	468.	549.25	0.583333	0.852071	0.497041
C_{14}	343.	686.	686.	0.5	1.	0.5
C_{15}	420.	735.	843.75	0.571429	0.871111	0.497778

Some generalized Petersen graphs.

graph	$W(G)$	$Sz(G)$	$Sz^*(G)$	$\alpha(G)$	$\beta(G)$	$\tau(G)$
$P(3,1)$	21.	51.	81.	0.411765	0.62963	0.259259
$P(4,1)$	48.	192.	192.	0.25	1.	0.25
$P(5,1)$	85.	285.	375.	0.298246	0.76	0.226667
$P(5,2)$	75.	135.	375.	0.555556	0.36	0.2
$P(6,1)$	144.	648.	648.	0.222222	1.	0.222222
$P(6,2)$	135.	354.	634.5	0.381356	0.55792	0.212766
$P(7,1)$	217.	847.	1029.	0.256198	0.823129	0.210884
$P(7,2)$	189.	602.	1029.	0.313953	0.585034	0.183673
$P(8,1)$	320.	1536.	1536.	0.208333	1.	0.208333
$P(8,2)$	280.	856.	1528.	0.327103	0.560209	0.183246
$P(8,3)$	272.	1536.	1536.	0.177083	1.	0.177083

The following comparison of the three indices is taken from Pisanski and Randić [16].

	Wiener index	Szeged Index	Revised Szeged index
source	[24]	[9]	[20]
notation	$W(G)$	$Sz(G)$	$Sz^*(G)$
$G = P_n$	$(n^3 - n)/6$	$(n^3 - n)/6$	$(n^3 - n)/6$
$G = C_n$, n even	$n^3/8$	$n^3/4$	$n^3/4$
$G = C_n$, n odd	$(n^3 - n)/8$	$n(n-1)^2/4$	$n^3/4$
$G = K_n$	$n(n-1)/2$	$n(n-1)/2$	$n^3(n-1)/8$
$G = H\square K$	$W(K)\|V(H)\|^2+$ $+W(H)\|V(K)\|^2$	$W(K)\|V(H)\|^3+$ $+W(H)\|V(K)\|^3$	$W(K)\|V(H)\|^3+$ $+W(H)\|V(K)\|^3$
G^k	$kW(G)\|V(G)\|^{2(k-1)}$	$kSz(G)\|V(G)\|^{3(k-1)}$	$kSz^*(G)\|V(G)\|^{3(k-1)}$
$G = Q_n$	$n2^{2(n-1)}$	$n2^{3(n-1)}$	$n2^{3(n-1)}$
$G = K_{n,n,\ldots,n}$	$nr(nr+n-2)/2$	$r(r-1)n^4/2$	$r^3(r-1)n^4/8$
G bipartite		$Sz(G)$	$Sz(G)$
T tree	$W(T)$	$W(T)$	$W(T)$

5 Conclusion

There is a natural difference between the Wiener index and the other indices described above. For the Wiener index one may usually compute the contribution of each vertex and then sum the contributions. In the Szeged index one may compute an edge contribution and then sum the obtained edge contributions. The same is true for the revised Szeged index. However, this distinction is not absolute. The latter approach may be used for the Wiener index as shown in [18] however, the computations are more involved. We hope we can use this approach to study more closely the relationship between the indices $W(G), Sz(G)$ and $Sz^*(G)$.

In [2] the authors have computed the Wiener index and the Szeged index for benzenoid graphs in linear time. It is clear that their methods give also the revised Szeged index since all benzenoids are bipartite. It is well-known that on trees, the Wiener index can be computed in linear time [14], and, consequently, the Szeged indices on trees can be computed in linear time. In general, the Wiener and Szeged indices can be computed in time $O(mn)$ [25]. The revised Szeged index can be computed within the same time complexity by a straightforward method using the distance matrix. The question is whether the computation of the revised Szeged index can be done faster for some classes of graphs.

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