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Generalizations of Some Topological Indices

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Abstract

The Wiener index of a simple graph is defined as the sum of distances between all vertices of the graph. It is well known that the Wiener index of a tree can be obtained as an edge additive quantity where edge contributions are given as the product of the number of vertices closer to each of the two end points of each edge. Thus the distances between vertices are not used for computing the Wiener index of trees. In a similar manner we introduce new topological indices which yields the Wiener, hyper-Wiener, Schultz and modified Schultz indices as special cases for trees. One advantage of this method is that in computing Schultz and modified Schultz of trees we need not take in to account the distances between vertices.

1 Introduction

Throughout the paper all graphs are simple, graphs without loops and multiple edges. Our notations are standard and mainly taken from [1]. Let $G = (V, E)$ be a graph with vertex set $V = V(G)$ and edge set $E = E(G)$. We denote by $d(x, y)$, $N(x)$ and $d(x)$, the distance between vertices x and y, vertices of distance one with vertex x and the degree of x, respectively. Also for each $e = uv \in E(G)$ we use the notations $N_e(v)$, $n_e(v)$ and $\alpha_e(v)$ for the set of vertices $t \in V(G)$ with $d(v, t) < d(u, t)$, $|N_e(v)|$ and $\sum_{t\in N_e(v)} d(t)$, respectively.

A topological index is a number related to a graph which is structural invariant, i.e. it is fixed under graph automorphisms. The Wiener index, denoted by W, is defined as the sum of all distances between vertices of a graph [2]. Randić [3] introduced the

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hyper-Wiener index, denoted by WW, an extension of the Wiener index for trees. Klein et. al. [4] generalized this extension to cyclic structures as

$$WW(G) = \frac{1}{2} \sum_{\{u,v\} \subseteq V(G)} \left(d(u,v) + d(u,v)^2 \right).$$

The graph invariant hyper-Wiener is also a distance based graph invariant. In some recent papers Dobrynin and Kochetova [5] and Gutman [6] introduced a degree analogue of the Wiener index defined as

$$D(G) = \sum_{\{x,y\} \subseteq V(G)} (d(x) + d(y))d(x,y)$$

which is known as the Schultz index. Gutman [6] also defined

$$D^*(G) = \sum_{\{x,y\} \subseteq V(G)} [d(x)d(y)]d(x,y)$$

and later in [8] called it the modified Schultz index. The Szeged index, denoted by $Sz(G)$, is another topological index which is closely related to the Wiener index and is a vertex multiplicative type index, see [7], defined as

$$Sz(G) = \sum_{e=uv \in E(G)} n_e(u) n_e(v) \ .$$

In the case of trees, Wiener [2] showed that $Sz(G)$ coincides with the Wiener index $W(G)$. Hence for a tree T on n vertices, one can computes the Wiener index of T by the formula of $Sz(T)$ which is distance free and consists of just $n-1$ summands, but the usual formula for the Wiener index takes into the account the distance between vertices and has $\binom{n}{2}$ summands. More generally, Gutman [9] proved that if G satisfies the conditions

(a) The shortest path between any two vertices of G is unique;

(b) For each edge $e = uv \in E(G)$, if $x \in N_e(u)$ and $y \in N_e(v)$, then, and only then, the shortest path between x and y contains the edge e,

then $W(G) = Sz(G)$.

In a similar manner we want to find new formulae for the Schultz and modified Schultz indices in the graphs satisfying the above conditions (a) and (b), and then extend them for some topological indices.

2 New formulae for the Schultz and modified Schultz indices

A tree is an acyclic graph and so for each pair of vertices, there is exists a unique path between them. In the general case, for each graph G satisfying the condition (a) above, we can define $P(x,y)$ as the set of all edges in the shortest path between vertices x and y in G. In what follows, for a graph G satisfying the conditions (a) and (b), we obtain formulae for the Schultz and modified Schultz indices in terms of $n_e(v)$ and $\alpha_e(v)$'s for edges $e = uv \in E(G)$.

Theorem 1 If G is a graph satisfying the conditions (a) and (b), then

$$D(G) = \sum_{e=uv\in E(G)} \left(n_e(v)\alpha_e(u) + n_e(u)\alpha_e(v)\right) .$$

Proof. For each pair of vertices $x, y \in V(G)$ and each edge $e \in E(G)$ let

$$W_e(x,y) := \begin{cases} d(x) + d(y) & e \in P(x,y) \\ 0 & \text{otherwise} \end{cases}$$

and

$$W(e) := \sum_{\{x,y\}\subseteq V(G)} W_e(x,y) .$$

Using these notations we have

$$\sum_{e\in P(x,y)} W_e(x,y) = \sum_{e\in P(x,y)} (d(x) + d(y)) = (d(x) + d(y))d(x,y) .$$

Hence, by definition of $D(G)$, we obtain that

$$\begin{aligned}
D(G) &= \sum_{\{x,y\}\subseteq V(G)} (d(x) + d(y))d(x,y) \\
&= \sum_{\{x,y\}\subseteq V(G)} \sum_{e\in P(x,y)} W_e(x,y) \\
&= \sum_{\{x,y\}\subseteq V(G)} \sum_{e\in E(G)} W_e(x,y) \\
&= \sum_{e=uv\in E(G)} \sum_{x\in N_e(u)} \sum_{y\in N_e(v)} W_e(x,y) \\
&= \sum_{e=uv\in E(G)} \sum_{x\in N_e(u)} \sum_{y\in N_e(v)} [d(x) + d(y)] \\
&= \sum_{e=uv\in E(G)} \sum_{x\in N_e(u)} \left[n_e(v)d(x) + \sum_{y\in N_e(v)} d(y)\right]
\end{aligned}$$

$$= \sum_{e=uv\in E(G)} [n_e(v)\alpha_e(u) + n_e(u)\alpha_e(v)] \ . \qquad \blacksquare$$

In order to prove a similar result for the modified Schultz index, for each vertex pair (x, y) and each edge e of graph (G), we set

$$W_e^*(x,y) = \begin{cases} d(x)d(y) & e \in P(x,y) \\ 0 & \text{otherwise} \end{cases}$$

and

$$W^*(e) = \sum_{\{x,y\}\subseteq V(G)} W_e^*(x,y) \ .$$

Theorem 2 If G is a graph satisfying the conditions (a) and (b), then

$$D^*(G) = \sum_{e=uv\in E(G)} \alpha_e(u)\alpha_e(v) \ .$$

Proof. Using the above notations it is easy to see that

$$\sum_{e\in P(x,y)} W_e^*(x,y) = \sum_{e\in P(x,y)} d(x)d(y) = d(x)d(y)d(x,y) \ .$$

Therefore, by the definition of modified Schultz index, we get that

$$\begin{aligned}
D^*(G) &= \sum_{\{x,y\}\subseteq V(G)} [d(x)d(y)]d(x,y) \\
&= \sum_{\{x,y\}\subseteq V(G)} \sum_{e\in P(x,y)} W_e^*(x,y) \\
&= \sum_{\{x,y\}\subseteq V(G)} \sum_{e\in E(G)} W_e^*(x,y) \\
&= \sum_{e=uv\in E(G)} \sum_{x\in N_e(u)} \sum_{y\in N_e(v)} W_e^*(x,y) \\
&= \sum_{e=uv\in E(G)} \sum_{x\in N_e(u)} \sum_{y\in N_e(v)} d(x)d(y) \\
&= \sum_{e=uv\in E(G)} \sum_{x\in N_e(u)} d(x) \sum_{y\in N_e(v)} d(y) \\
&= \sum_{e=uv\in E(G)} \alpha_e(u)\alpha_e(v) \ . \qquad \blacksquare
\end{aligned}$$

It is easy to see that, for a graph $G = (V, E)$ satisfying the conditions (a) and (b), two formulae in Theorems 1 and 2 for the Schultz and modified Schultz are distance free and each of them consists of $|E|$ summands, but in the main formula for the Schultz and modified Schultz indices there are $\binom{|V|}{2}$ summands which each of them also contains the distance between some vertices of G.

Remark 3 If, for an arbitrary simple graph G, we define $D_1(G)$ and $D_1^*(G)$ as,

$$D_1(G) = \sum_{e=uv \in E(G)} [n_e(v)\alpha_e(u) + n_e(u)\alpha_e(v)]$$

and

$$D_1^*(G) = \sum_{e=uv \in E(G)} \alpha_e(u)\alpha_e(v) \ .$$

Then $D_1(G)$ (respectively $D_1^*(G)$) is a topological index which is equal to $D(G)$ (respectively $D^*(G)$) if and only if $W(G)$ is equal to $Sz(G)$.

3 The general case

Let Ω be the class of all the graphs and for each $G \in \Omega$ denote by $\sigma(G)$ the class of all complex valued functions $\psi : V(G) \times V(G) \longrightarrow \mathbb{C}$ with the property that $\psi(x, y) = \psi(\phi(x), \phi(y))$ for each automorphism ϕ of G and each pair of vertices $x, y \in V(G)$. Also, let $\Psi = \bigcup_{G\in\Omega} \sigma(G)$.

Definition 4 Let $f : \Omega \longrightarrow \Psi$ be a function with the property that $f(H) \in \sigma(H)$ for every $H \in \Omega$, and for each $G \in \Omega$ define the number $D_f(G)$ as

$$D_f(G) := \sum_{\alpha\in I} \sum_{\{x,y\}\subseteq V(G_\alpha)} [f(G)](x, y)d(x, y)$$

where G_α's, $\alpha \in I$, are all of the connected components of G.

Now by properties of the functions f and the elements of its image, it is easy to see that the function $D_f(.)$ is a graph invariant, i.e. a topological index.

Let $\Omega_{a,b}$ be the class of all the graphs which satisfy the conditions (a) and (b). Thus, in particular, $\Omega_{a,b}$ contains all the trees and $\Omega_{a,b} \subseteq \Omega$. Let $\Psi_{a,b} := \bigcup_{G\in\Omega_{a,b}} \sigma(G)$. Hence for each $G \in \Omega_{a,b}$, $\sigma(G)$ contains all constant functions on $V(G) \times V(G)$ and $\Psi_{a,b}$ is non-empty.

Remark 5 Every graph is a disjoint union of its connected components and evidently the graph invariant $D_f(.)$, for a suitable function f described in the above definition, can be obtained as the sum of its values on connected components of the graph. So in what follows we consider connected graphs.

Definition 6 Let $f : \Omega_{a,b} \longrightarrow \Psi_{a,b}$ be a function with the property that $f(G) \in \sigma(G)$ for every $G \in \Omega_{a,b}$. For each (connected) graph $G = (V, E) \in \Omega_{a,b}$, $x, y \in V$ and $e \in E$ define

$$f_G(e; x, y) := \begin{cases} [f(G)](x, y) & e \in P(x, y) \\ 0 & \text{otherwise} \end{cases}$$

and

$$f_G(e) := \sum_{\{x,y\}\subseteq V(T)} f_G(e;x,y) \ .$$

Using this notations, for graphs $G \in \Omega_{a,b}$, $D_f(G)$ can be computed by a simpler formula which is also distance free and has fewer summands than its usual formula. In fact, for each $G \in \Omega_{a,b}$ by a direct computation we see that

$$\begin{aligned}
D_f(G) &= \sum_{\{x,y\}\subseteq V(G)} [f(G)](x,y)d(x,y) \\
&= \sum_{\{x,y\}\subseteq V(G)} \sum_{e\in P(x,y)} [f(G)](x,y) \\
&= \sum_{\{x,y\}\subseteq V(G)} \sum_{e\in E(G)} f_G(e;x,y) \\
&= \sum_{e=uv\in E(G)} \sum_{x\in N_e(u)} \sum_{y\in N_e(v)} f_G(e;x,y) \\
&= \sum_{e\in E(G)} \sum_{\{x,y\}\subseteq V(G)} f_G(e;x,y) = \sum_{e\in E(G)} f_G(e) \ .
\end{aligned}$$

For every function f mentioned in the Definition 4, $D_f(.)$ is a topological index. But for some suitable choices of the function f we can obtain some well known indices as the following corollary shows.

Corollary 7 Let $f_i : \Omega \longrightarrow \Psi$, $1 \leq i \leq 4$, be functions defined by $[f_3(H)](x,y) = 1$ and

$$[f_1(H)](x,y) = d(x)+d(y),\ [f_2(H)](x,y) = d(x)d(y),\ [f_4(H)](x,y) = \frac{1+d(x,y)}{2}$$

for each $H \in \Omega$ and $x, y \in V(H)$. Then we have

$$D_{f_1}(G) = D(G),\ D_{f_2}(G) = D^*(G),\ D_{f_3}(G) = W(G),\ D_{f_4}(G) = WW(G)$$

for each $G \in \Omega$. ■

Using Corollary 7 we can easily deduce Theorems 1 and 2, and the distance free formula $Sz(T) = W(T)$ for trees T and more generally for graphs in $\Omega_{a,b}$. Let $G \in \Omega_{a,b}$. Since G satisfies the conditions (a) and (b), so for every $e = uv \in E(G)$ we have

$$(f_1)_G(e) = \sum_{\{x,y\}\subseteq V(G)} (f_1)_G(e;x,y) = \sum_{x\in N_e(u)} \sum_{y\in N_e(v)} [d(x)+d(y)] = n_e(u)\alpha_e(v) + n_e(v)\alpha_e(u)$$

and

$$(f_2)_G(e) = \sum_{\{x,y\}\subseteq V(G)} (f_2)_G(e;x,y) = \sum_{x\in N_e(u)} \sum_{y\in N_e(v)} d(x)d(y) = \alpha_e(u)\alpha_e(v)$$

and

$$\begin{aligned}(f_3)_G(e) &= \sum_{\{x,y\}\subseteq V(G)} (f_3)_G(e;x,y) = \sum_{x\in N_e(u)} \sum_{y\in N_e(v)} [f_1(G)](x,y)\\ &= \sum_{x\in N_e(u)} \sum_{y\in N_e(v)} 1 = n_e(u)n_e(v)\end{aligned}$$

which yield

$$D(G) = D_{f_1}(G) = \sum_{e\in E(G)} (f_1)_G(e) = \sum_{e\in E(G)} [n_e(u)\alpha_e(v) + n_e(v)\alpha_e(u)],$$

and

$$D^*(G) = D_{f_2}(G) = \sum_{e\in E(G)} (f_2)_G(e) = \sum_{e\in E(G)} \alpha_e(v)\alpha_e(u)$$

and

$$W(G) = D_{f_3}(G) = \sum_{e\in E(G)} (f_3)_G(e) = \sum_{e\in E(G)} n_e(u)n_e(v)\ .$$

For the hyper-Wiener index we have the following corollary, which extends a result of Gutman [10]

Corollary 8 If $G \in \Omega_{a,b}$, then

$$WW(G) = W(G) + \frac{1}{2} \sum_{e=uv\in E(G)} [n_e(u)\beta_e(v) + n_e(v)\beta_e(u)]$$

where $\beta_e(u) = \sum_{x\in N_e(u)} d(x,u)$ and $\beta_e(v) = \sum_{y\in N_e(v)} d(y,v)$.

Proof. Let $G \in \Omega_{a,b}$. Then for each $e = uv \in E(G)$ we have

$$\begin{aligned}(f_4)_G(e) &= \sum_{\{x,y\}\subseteq V(G)} (f_4)_G(e;x,y)\\ &= \sum_{x\in N_e(u)} \sum_{y\in N_e(v)} [f_4(G)](x,y)\\ &= \sum_{x\in N_e(u)} \sum_{y\in N_e(v)} \frac{1+d(x,y)}{2}\\ &= \frac{1}{2} \sum_{x\in N_e(u)} \sum_{y\in N_e(v)} [d(x,u) + 2 + d(v,y)]\\ &= \frac{1}{2}n_e(v)\beta_e(u) + n_e(u)n_e(v) + \frac{1}{2}n_e(u)\beta_e(v)\ .\end{aligned}$$

Above equation using Corollary 7 yields

$$\begin{aligned} WW(G) &= D_f(G) = \sum_{e\in E(G)} f_{G}(e) \\ &= \sum_{e\in E(G)} \left[\frac{1}{2}n_e(v)\beta_e(u) + n_e(u)n_e(v) + \frac{1}{2}n_e(u)\beta_e(v)\right] \\ &= W(G) + \frac{1}{2}\sum_{e\in E(G)} [n_e(u)\beta_e(v) + n_e(v)\beta_e(u)] \end{aligned}$$

which completes the proof. ■

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