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# ON A GRAPH INVARIANT RELATED TO THE SUM OF ALL DISTANCES IN A GRAPH

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**Abstract.** Let $\mathbf{W}(G)$ be the sum of distances between all pairs of vertices of a graph G. For an edge $e$ of $G$, connecting the vertices $u$ and $v$, the number $n_u(e)$ counts the vertices of $G$ that lie closer to $u$ than to $v$. In this paper we consider the graph invariant $\mathbf{W}^*(G) = \sum_e n_u(e) n_v(e)$, defined for any connected graph $G$. According to a long-known result in the theory of graph distances, if $G$ is a tree then $\mathbf{W}^*(G) = \mathbf{W}(G)$. We establish a number of properties of the graph invariant $\mathbf{W}^*$.

## 1. Introduction

In this paper we consider finite connected undirected graphs without loops or multiple edges. Let $G$ be such a graph, possessing $n$ vertices and $m$ edges. The vertex and edge sets of $G$ are denoted by $\mathbf{V}(G)$ and $\mathbf{E}(G)$, respectively.

The distance between the vertices of $G$ is defined in the usual manner [**1**], namely $d(x,y) = d(x,y\,|\,G)$ is equal to the number of edges in the shortest path connecting the vertices $x$ and $y$ of the graph $G$. If $G$ is connected, then $d(x,y)$ exists for all $x,y \in \mathbf{V}(G)$.

The distance of a vertex $v$ of $G$ is defined as

$$d(v) = d(v\,|\,G) = \sum_{x \in \mathbf{V}(G)} d(v,x\,|\,G)$$

whereas the distance of the graph $G$ is

$$\mathbf{W} = \mathbf{W}(G) = \frac{1}{2} \sum_{v \in \mathbf{V}(G)} d(v\,|\,G).$$

Clearly, $\mathbf{W}(G)$ is equal to the sum of distances between all pairs of vertices in $G$. This quantity is sometimes called the Wiener number (or Wiener index), because the American scientist Harold Wiener seems to be the first to study $\mathbf{W}$ and to

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*AMS Subject Classification* (1991): Primary 05 C 12 determine its properties [**7**]. The Wiener number has noteworthy applications in chemistry [**4**, **5**, **7**].

Let $u$ and $v$ be two adjacent vertices of the graph $G$ and $e$ be the edge between them. Throughout this paper it will be always assumed that the edge labeled by $e$ corresponds to a pair of vertices labeled by $u$ and $v, e = (u, v)$

Define the sets $\mathbf{B}_u(e)$ and $\mathbf{B}_v(e)$ of vertices of $G$:

$\mathbf{B}_u(e) = \{x \mid x \in \mathbf{V}(G), d(x, u) < d(x, v)\}$

$\mathbf{B}_v(e) = \{x \mid x \in \mathbf{V}(G), d(x, v) < d(x, u)\}$.

Observe that if $d(x, u) = d(x, v)$, then the vertex $x$ is neither in $\mathbf{B}_u(e)$ nor in $\mathbf{B}_v(e)$. Let further $n_u(e) = |\mathbf{B}_u(e)|$ ; $n_v(e) = |\mathbf{B}_v(e)|$.

The following result was both stated and proved in Wiener's first work [**7**] on the distance of graphs.

THEOREM 1. *If G is a tree then*

$$\mathbf{W}(G) = \sum_{e \in \mathbf{E}(G)} n_u(e) n_v(e) \tag{1}$$

The identity (1) motivated us to introduce [**2**] and examine a novel graph invariant $\mathbf{W}^* = \mathbf{W}^*(G)$:

*Definition* 1. If $G$ is a connected graph, then

$$\mathbf{W}^* = \mathbf{W}^*(G) = \sum_{e \in \mathbf{E}(G)} n_u(e) n_v(e). \tag{2}$$

From Theorem 1 and Definition 1 it is immediately seen that if $G$ is a tree, then $\mathbf{W}^*(G) = \mathbf{W}(G)$.

Furter details on the relation between the invariants $\mathbf{W}$ and $\mathbf{W}^*$ are given in the subsequent section.

## 1. Relations between W and W*

We first provide a proof of the long-known Theorem 1. The reason for this is that the arguments utilized in the proof will enable us to deduce a few additional results on the invariant $\mathbf{W}^*$.

*Proof of Theorem* 1. Let $G$ be a connected graph and $e = (u, v)$ an edge. Suppose that the following conditions are obeyed:

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

(b) if $x \in \mathbf{B}_u(e)$ and $y \in \mathbf{B}_v(e)$, then, and only then, the shortest path between $x$ and $y$ contains the edge $e$.

If both (a) and (b) hold, then the product $n_u(e)n_v(e)$ counts the number of times the edge $e$ belongs to the shortest path between pairs of vertices of $G$. The sum of $n_u(e)n_v(e)$ over all edges of $G$ is equal to the number of edges in the shortest paths between all pairs of vertices of $G$, i.e., equal to the sum of distances between all pairs of vertices of $G$, i.e. equal to $\mathbf{W}(G)$.

It is evident that the conditions (a) and (b) are fulfilled if $G$ is a tree. Consequently, the equation (1) hold for trees. □

COROLLARY 1. *The equality* $\mathbf{W}^* = \mathbf{W}$ *holds for all graphs that satisfy the conditions (a) and (b).*

COROLLARY 2. *If conditions (a) and (b) are not simultaneously satisfied, then* $\mathbf{W}^* > \mathbf{W}$.

*Proof.* If (a) is violated, then the right-hand side of (2) counts the edges of more than one shortest path between pairs of vertices of $G$. If (b) is violated, then the right-hand side of (2) counts some edges that do not belong to shortest paths between pairs of vertices. In both cases $\mathbf{W}^*$ will exceed $\mathbf{W}$. □

COROLLARY 3. *If $G$ is a connected cyclic bipartite graph, then* $\mathbf{W}^*(G) > \mathbf{W}(G)$.

*Proof.* Consider a circuit of $G$ having minimal size (say $2k$). Two vertices of this circuit, being at maximal distance ($= k$) are connected by two distinct shortest paths. Hence condition (b) from the proof of the Theorema 1 is violated. □

In the case of non-bipartite graphs it may happen that $\mathbf{W}^*(G) = \mathbf{W}(G)$. The simplest example for the equality between the two graph invariants is the complete graph $K_n,\ n \geq 1$ [**2**].

THEOREM 2. *Let $\mathcal{K}$ be the class of connected graphs in which every block is a complete graph. Then for $G \in \mathcal{K}$,* $\mathbf{W}^*(G) = \mathbf{W}(G)$.

*Proof of the Theorem* 2. It is sufficient to observe that the graphs from $\mathcal{K}$ satisfy the conditions (a) and (b) from the proof of the Theorem 1. □

Note that $\mathcal{K}$ contains the complete graphs (when the number of blocks is one) and the trees (when every block is a two-vertex complete graph).

*Conjecture.* $\mathbf{W}^*(G) = \mathbf{W}(G)$ holds if and only if $G \in \mathcal{K}$.

## 2. The Invariant $\mathbf{W}^*$ of Bipartite Graphs

LEMMA 1. *If $G$ is a connected bipartite graph on $n$ vertices, and $e$ its arbitrary edge, then $n_u(e) + n_v(e) = n$. If $G$ is non-bipartite, then for the edges lying on odd-membered circuits, $n_u(e) + n_v(e) < n$.*

Proof of the above Lemma is given in [**2**].

LEMMA 2. *If $G$ is a connected graph and $e$ an arbitrary edge, then*

$$n_u(e) - n_v(e) = d(v|G) - d(u|G) \tag{3}$$

*Proof.* Denote by $\mathbf{B}_0(e)$ the set of vertices of $G$ which are at equal distance to both $u$ and $v$. Then, of course, $\mathbf{B}_0(e) \cup \mathbf{B}_u(e) \cup \mathbf{B}_v(e) = \mathbf{V}(G)$.
Further,

$$d(u|G) = \sum_{x\in\mathbf{B}_u(e)} d(x,u) + \sum_{x\in\mathbf{B}_v(e)} d(x,u) + \sum_{x\in\mathbf{B}_0(e)} d(x,u) \tag{4}$$

$$d(v|G) = \sum_{x\in\mathbf{B}_u(e)} d(x,v) + \sum_{x\in\mathbf{B}_v(e)} d(x,v) + \sum_{x\in\mathbf{B}_0(e)} d(x,v) \tag{5}$$

Subtracting (4) from (5) and taking into account

$$\begin{aligned} d(x,v) &= d(x,u)+1 \quad \text{if } x \in \mathbf{B}_u(e) \\ d(x,v) &= d(x,u)-1 \quad \text{if } x \in \mathbf{B}_v(e) \\ d(x,v) &= d(x,u) \qquad\;\;\, \text{if } x \in \mathbf{B}_0(e) \end{aligned}$$

we straightforwardly arrive at (3). □

THEOREM 3. *If $G$ is a connected bipartite graph with $n$ vertices and $m$ edges, then*

$$\mathbf{W}^*(G) = \frac{1}{4}\left[n^2 m - \sum_{e\in\mathbf{E}(G)} [d(v|G) - d(u|G)]^2\right] \tag{6}$$

*Proof.* By Lemmas 1 and 2, $2n_u(e) = n + [d(v|G) - d(u|G)]$ and $2n_v(e) = n - [d(v|G) - d(u|G)]$. Substituting this back into (2) we arrive at (6). □

Denote by $\mathbf{N}(v) = \mathbf{N}(v|G)$ the set of all neighbors of the vertex $v$ of the graph $G$. Clearly, $|\mathbf{N}(v)| = \deg(v)$, where $\deg(v)$ is the degree of $v$.

COROLLARY 4. *Using the notation of Theorem 3,*

$$\mathbf{W}^*(G) = \frac{1}{4}\left[n^2 m - \sum_{v\in\mathbf{V}(G)} d(v|G)\left[d(v|G)\ deg(v) - \sum_{u\in\mathbf{N}(v)} d(u|G)\right]\right]. \tag{7}$$

*Proof.*

$$\begin{aligned} \sum_{e\in\mathbf{E}(G)} [d(v)-d(u)]^2 &= \frac{1}{2}\sum_{v\in\mathbf{V}(G)}\sum_{u\in\mathbf{N}(v)} [d(v)^2 + d(u)^2 - 2d(v)d(u)] \\ &= \sum_{v\in\mathbf{V}(G)} d(v)\left[d(v)\deg(v) - \sum_{u\in\mathbf{N}(v)} d(u)\right] \end{aligned} \tag{8}$$

because

$$\sum_{v\in\mathbf{V}(G)}\sum_{u\in\mathbf{N}(v)} d(v)^2 = \sum_{v\in\mathbf{V}(G)} d(v)^2 \deg(v)$$

and

$$\sum_{v\in\mathbf{V}(G)} \sum_{u\in\mathbf{N}(v)} d(u)^2 = \sum_{v\in\mathbf{V}(G)} d(v)^2 \deg(v).$$

Substituting (8) back into (6) we obtain (7). □

In the case of trees, equations (6) and (7) automatically become statements about the graph distance $\mathbf{W}$. In the case, however, we can say more because of the identity

$$\sum_{u\in\mathbf{N}(v)} d(u) = d(v)\deg(v) + n\deg(v) - 2(n-1). \tag{9}$$

Relation (9) follows immediately from Lemmas 1 and 2, and from the fact that for trees $\sum_{u\in\mathbf{N}(v)} n_u(e) = n-1$. By combining (7) and (9) we get

COROLLARY 5. *If $T$ is a tree with $n$ vertices, then*

$$\mathbf{W}(T) = \mathbf{W}^*(T) = \frac{1}{4}\left[n(n-1) + \sum_{v\in\mathbf{V}(T)} d(v|T)\, deg(v)\right] \tag{10}$$

A result equivalent to (10) was recently obtained by Klein et al. [**6**], using a completely different way of reasoning. Another approach leading to (10), also based on a completely different way of reasoning, was put forward by one of the authors [**3**].

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