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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

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

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*

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

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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