PUBLICATIONS DE L'INSTITUT MATHÉMATIQUE
Nouvelle série, tome 63 (77), 1998, 31–36

DISTANCE OF THORNY GRAPHS

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Communicated by Slobodan Simić

Abstract. Let G be a connected graph on n vertices. The thorn graph $G^\star$ of G is obtained from G by attaching to its i-th vertex p_i new vertices of degree one, $p_i \geq 0$, $i = 1, 2, \ldots, n$. Let $d(G)$ be the sum of distances of all pairs of vertices of G . We establish relations between $d(G)$ and $d(G^\star)$ and examine several special cases of this result. In particular, if $p_i = \gamma - \gamma_i$, where γ is a constant and γ_i the degree of the i-th vertex in G , and if G is a tree, then there is a linear relation between $d(G^\star)$ and $d(G)$, namely $d(G^\star) = (\gamma - 1)^2\, d(G) + [(\gamma - 1)n + 1]^2$.

Introduction

In this paper we consider connected finite graphs without loops and multiple edges. Let G be such a graph, $V = V(G)$ its vertex set, $E = E(G)$ its edge set, and let its vertices, whose number is n , be labeled by $u_1, u_2, \ldots, u_n$. The distance (= length of a shortest path) between the vertices u_i and u_j of G is denoted by $d(u_i, u_j|G)$. The sum of the distances between all pairs of vertices of G is *the distance of the graph* G and is denoted by $d(G)$.

In the mathematical literature the distance of a graph was first introduced by Entringer, Jackson and Snyder [**2**], although the chemical applications of this quantity are somewhat older [**8**]. For results concerning the distance of compound graphs as well as for additional references see [**3,6,9**].

Let $p_1, p_2, \ldots, p_n$ be non-negative integers.

Definition 1. The *thorn graph* of the graph G , with parameters $p_1, p_2, \ldots, p_n$, is obtained by attaching p_i new vertices of degree one to the vertex u_i of the graph G , $i = 1, 2, \ldots, n$.

The thorn graph of the graph G will be denoted by $G^\star$, or if the respective parameters need to be specified, by $G^\star(p_1, p_2, \ldots, p_n)$.

AMS Subject Classification (1991): Primary 05C12

Supported by Ministry of Science and Technology of Serbia, grant number 04M03/C

In this work we examine the relation between $d(G)$ and $d(G^\star)$. The motivation for this study comes from a particular special case, namely $G^\star(\gamma-\gamma_1, \gamma-\gamma_2, \ldots, \gamma-\gamma_n)$, where γ_i is the degree of the i-th vertex of G and γ is a constant ($\gamma \geq \gamma_i$ for all $i = 1, 2, \ldots, n$). Then the vertices of $G^\star$ are either of degree γ or of degree one. If, in addition, $\gamma = 4$, then the thorn graph is just what Cayley [**1**] calls a "plerogram" and Pólya [**7**] a "C–H graph". (The parent graph G would then be referred to as a "kenogram" [**1**] or a "C–graph" [**7**]. Clearly, these notions have their origins in the attempts to represent molecular structure by means of graphs [**4**].) It is also worth mentioning that the so–called "caterpillars" [**5**] are thorn graphs whose parent graph is a path.

Denote the vertex set of $G^\star$ by $V^\star$. Further, the set of degree–one vertices of $G^\star$, attached to the vertex u_i is V_i. Its cardinality is p_i and, clearly,

$$V^\star = V \cup V_1 \cup V_2 \cup \cdots \cup V_n \quad \text{and} \quad V_i \cap V_j = \emptyset \quad \text{for } i \neq j$$

The main results

Let $\{x,y\} \subseteq V^\star$. In order to compute $d(G^\star)$ we distinguish between four types of pairs of vertices of $G^\star$:
Type 1. $x \in V$, $y \in V$;
Type 2. $x \in V_i$, $y \in V$, for some i, $1 \leq i \leq n$;
Type 3. $x \in V_i$, $y \in V_j$, for some i,j, $1 \leq i < j \leq n$;
Type 4. $x \in V_i$, $y \in V_i$, for some i, $1 \leq i \leq n$.

Let the contributions of all such vertex pairs to $d(G^\star)$ be denoted by F_1, F_2, F_3 and F_4, respectively. Then,

$$d(G^\star) = F_1 + F_2 + F_3 + F_4 \tag{1}$$

If $\{x,y\}$ is a vertex pair of Type 1, then $d(x,y|G^\star) = d(x,y|G)$ and therefore

$$F_1 = d(G)$$

There are p_i vertex pairs $\{x,y\}$ of Type 2, and for each of them $d(x,y|G^\star) = d(u_i,y|G) + 1$. Therefore

$$F_2 = \sum_{i=1}^{n} \sum_{y \in V} p_i \, [d(u_i,y|G) + 1] = \sum_{1 \leq i < j \leq n} (p_i + p_j) \, d(u_i,u_j|G) + n \sum_{i=1}^{n} p_i$$

There are $p_i \cdot p_j$ vertex pairs $\{x,y\}$ of Type 3, and for each of them $d(x,y|G^\star) = d(u_i,u_j|G) + 2$. Therefore

$$F_3 = \sum_{1 \leq i < j \leq n} p_i \, p_j \, [d(u_i,u_j|G) + 2] = \sum_{1 \leq i < j \leq n} p_i \, p_j \, d(u_i,u_j|G) + \left(\sum_{i=1}^{n} p_i \right)^2 - \sum_{i=1}^{n} p_i^2$$

There are $\binom{p_i}{2}$ vertex pairs $\{x,y\}$ of Type 4, each of them at distance 2. Therefore

$$F_4 = \sum_{i=1}^{n} 2\binom{p_i}{2} = \sum_{i=1}^{n} p_i^2 - \sum_{i=1}^{n} p_i$$

Substituting the above relations back into Eq. (1) we arrive at the general expression for the distance of a thorn graph:

THEOREM 1. *If $G^\star$ is the thorn graph of the graph G, with parameters p_i , $p_i \geq 0$, $i = 1,2,\dots,n$, then*

$$d(G^\star) = d(G) + \sum_{1 \leq i < j \leq n} (p_i + p_j)\, d(u_i, u_j|G) + \sum_{1 \leq i < j \leq n} p_i\, p_j\, d(u_i, u_j|G) + \left(\sum_{i=1}^{n} p_i\right)^2 + (n-1)\sum_{i=1}^{n} p_i \tag{2}$$

i.e.,

$$d(G^\star) = \sum_{1 \leq i < j \leq n} (p_i+1)(p_j+1)\, d(u_i, u_j|G) + \left(\sum_{i=1}^{n} p_i\right)^2 + (n-1)\sum_{i=1}^{n} p_i \tag{3}$$

COROLLARY 1.1. *If $G^\star$ is the thorn graph of the graph G, with parameters $p_1 = p_2 = \cdots = p_n = p$, then $d(G^\star)$ and $d(G)$ are related as:*

$$d(G^\star) = (p+1)^2\, d(G) + np(np + n - 1)$$

Theorem 1 has been obtained by a routine combinatorial reasoning and the form of Eqs. (2) and (3) is neither appealing nor unexpected. Also, the existence of a simple linear connection between $d(G^\star(p,p,\dots,p))$ and $d(G)$, as specified in Corollary 1.1, is by no means a surprise. The following two special cases seem, however, to be somewhat less self–evident and hardly could have been anticipated.

Let T be an n-vertex tree and let γ_i be the degree of its i-th vertex. Recall that

$$\gamma_1 + \gamma_2 + \cdots + \gamma_n = 2n - 2$$

COROLLARY 1.2. *If $T^\star$ is the thorn graph of the tree T, with parameters $p_i = \gamma_i$, $i = 1,2,\dots,n$, then $d(T^\star)$ and $d(T)$ are related as:*

$$d(T^\star) = 9\, d(T) + (n-1)(3n-5)$$

COROLLARY 1.3. *Let γ be an integer with the property $\gamma \geq \gamma_i$, $i = 1,2,\dots,n$. If $T^\star$ is the thorn graph of the tree T, with parameters $p_i = \gamma - \gamma_i$, $i = 1,2,\dots,n$, then $d(T^\star)$ and $d(T)$ are related as:*

$$d(T^\star) = (\gamma-1)^2\, d(T) + [(\gamma-1)n + 1]^2$$

Proofs

Theorem 1 has already been verified, and Corollary 1.1 is immediate. What remains is to demonstrate the validity of Corollaries 1.2 and 1.3. For this we need:

LEMMA 1. *If T is a tree on n vertices $u_1, u_2, \dots, u_n$ and if the degree of u_i is γ_i , $i = 1, 2, \dots, n$, then*

$$\sum_{1 \le i < j \le n} (\gamma_i + \gamma_j)\, d(u_i, u_j|T) = 4\, d(T) - n(n-1) \tag{4}$$

and

$$\sum_{1 \le i < j \le n} \gamma_i\, \gamma_j\, d(u_i, u_j|T) = 4\, d(T) - (n-1)(2n-1) \tag{5}$$

Proof. Let $V(T)$ and $E(T)$ be the vertex and edge sets, respectively, of the tree T. Let $e \in E(T)$. Then the subgraph whose vertex set is $V(T)$ and whose edge set is $E(T) \setminus \{e\}$ consists of two components, $T_1 = T_1(e)$ and $T_2 = T_2(e)$, possessing $n_1 = n_1(e|T)$ and $n_2 = n_2(e|T)$ vertices, respectively. Recall that $n_1(e|T) + n_2(e|T) = n$ holds for all $e \in E(T)$.

It is long known [**8**] that the distance $d(T)$ of a tree T (in which the path between any two vertices is unique) may be calculated by counting the paths of T which contain the edge e, and summing this count over all edges of T. Now, the number of paths of T containing e is $n_1(e|T) \cdot n_2(e|T)$ and therefore,

$$d(T) = \sum_{e \in E(T)} n_1(e|T)\, n_2(e|T) \tag{6}$$

which may be rewritten as

$$d(T) = \sum_{e \in E(T)} \; \sum_{u_i \in V(T_1)} \; \sum_{u_j \in V(T_2)} 1 \tag{7}$$

Associate to each pair of vertices $u_i, u_j \in V(G)$ a weight ω_{ij} and define a generalized distance–sum $d_\omega(G)$ as

$$d_\omega(G) = \sum_{1 \le i < j \le n} \omega_{ij}\, d(u_i, u_j|G)$$

Clearly, if $\omega_{ij} = 1$ for all i, j , $1 \le i < j \le n$ then $d_\omega(G) = d(G)$.

Now, repeating the reasoning leading to Eq. (7), and bearing in mind that for T being a tree, in $d_\omega(T)$ the distance between the vertices u_i, u_j has to be counted with weight ω_{ij}, we obtain

$$d_\omega(T) = \sum_{e \in E(T)} \; \sum_{u_i \in V(T_1)} \; \sum_{u_j \in V(T_2)} \omega_{ij} \tag{8}$$

If we choose $\omega_{ij} = \gamma_i + \gamma_j$ then Eq. (8) yields

$$\sum_{1 \le i < j \le n} (\gamma_i + \gamma_j)\, d(u_i, u_j|T) = \sum_{e \in E(T)} \left[n_2 \sum_{u_i \in V(T_1)} \gamma_i + n_1 \sum_{u_j \in V(T_2)} \gamma_j \right] \tag{9}$$

Because T_1 and T_2 have $n_1 - 1$ and $n_2 - 1$ edges, respectively,

$$\sum_{u_i \in V(T_1)} \gamma_i = 2(n_1 - 1) + 1 \tag{10}$$

and

$$\sum_{u_j \in V(T_2)} \gamma_j = 2(n_2 - 1) + 1 \tag{11}$$

Recall that γ_i and γ_j in Eqs. (10) and (11) are the degrees of the vertices of the tree T; they coincide with the degrees of the vertices of the trees T_1 and T_2, respectively, except for one particular vertex of T_1 and for one particular vertex of T_2. These "exceptional" vertices of T_1 and T_2 have degrees by one less than in T. The terms $+1$ on the right–hand sides of Eqs. (10) and (11) occur because of this difference between the vertex degrees of T and the vertex degrees of T_1 and T_2.

Substituting (10) and (11) back into Eq. (9) results in

$$\sum_{1 \le i < j \le n} (\gamma_i + \gamma_j)\, d(u_i, u_j|T) = \sum_{e \in E(T)} [4\, n_1\, n_2 - (n_1 + n_2)] \tag{12}$$

Using the fact that T has $n - 1$ edges, that $n_1 + n_2 = n$ and that $d(T)$ obeys Eq. (6), Eq. (4) is directly obtained from Eq. (12).

This proves the first part of Lemma 1.

If, on the other hand, we choose $\omega_{ij} = \gamma_i \cdot \gamma_j$, then from Eq. (8),

$$\begin{aligned} \sum_{1 \le i < j \le n} \gamma_i\, \gamma_j\, d(u_i, u_j|T) &= \sum_{e \in E(T)} \left[\sum_{u_i \in V(T_1)} \gamma_i \right] \left[\sum_{u_j \in V(T_2)} \gamma_j \right] \\ &= \sum_{e \in E(T)} [2(n_1 - 1) + 1][2(n_2 - 1) + 1] \end{aligned}$$

Combining the above with Eq. (6) leads to Eq. (5).

This completes the proof of Lemma 1. $\square$

Proof of Corollary 1.2. Set $p_i = \gamma_i$ into Eq. (1) and use Eqs. (4) and (5) of Lemma 1. $\square$

Proof of Corollary 1.3. Set $p_i = \gamma - \gamma_i$ into Eq. (1) and use Lemma 1. The calculation is somewhat lengthier than, but fully analogous to the previous case. $\square$

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(Received 19 08 1997)