ON THE SUM OF THE SQUARES OF ALL DISTANCES IN SOME GRAPHS

Xianya Geng
Zhixiang Yin
Xianwen Fang
Department of Mathematics and Physics
Anhui University of Science and Technology
Huainan 232001
P.R. China
gengxianya@sina.com

Abstract. Denote the sum of the squares of all distances between all pairs of vertices in G by $S(G)$. In this article, through the given vertices number of a graph and the chromatic, a lower bound of $S(G)$ is discussed. By giving the vertices number and the clique number of a graph, the upper and lower bounds of the $S(G)$ are discussed.

Keywords: chromatic number, clique number.

1. Introduction

In this paper, we only consider connected, simple and undirected graphs and assume that all graphs are connected, and refer to Bondy and Murty [2] for notation and terminologies used but not defined here.

Let $G = (V_G, E_G)$ be a graph with vertex set V_G and edge set E_G. $G-v, G-uv$ denote the graph obtained from G by deleting vertex $v \in V_G$ or edge $uv \in E_G$, respectively(this notation is naturally extended if more than one vertex or edge is deleted). Similarly, $G + uv$ is obtained from G by adding an edge $uv \notin E_G$. For $v \in V_G$, let $N_G(v)(N(v)$ for short) denote the set of all the adjacent vertices of v in G and $d(v) = |N_G(v)|$, the degree of v in G.

Recall that G is called *k-connected* if $|G| > k$ and $G - Z$ is connected for every set $Z \subseteq V_G$ with $|Z| < k$.The greatest integer k such that G is k-connected is the connectivity $k(G)$ of G. Thus, $k(G) = 0$ if and only if G is disconnected or H_1, and $k(H_1) = n - 1$ for all $n \geq 1$.

Analogously, if $|G| > 1$ and $G - N$ is connected for every set $N \subseteq E_G$ of fewer than l edges, then G is called *l-edge-connected*. The greatest integer l such that G is l-connected is the *edge-connectivity* $k'(G)$ of G. In particular, $k'(G) = 0$ if G is disconnected.

A bipartite graph G is a simple graph, whose vertex set V_G can be partitioned into two disjoint subsets V_1 and V_2 such that every edge of G joins a vertex of V_1 with a vertex of V_2. A bipartite graph in which every two vertices from different partition classes are adjacent is called complete, which is denoted by $H_{m,n}$, where $m = |V_1|, n = |V_2|$.

The distance $d(u, v)$ between vertices u and v in G is defined as the length of a shortest path between them. The diameter of G is the maximal distance between any two vertices of G. $L_G(u)$ denotes the sum of square of all distances from u in G.

Let $\mathscr{C}_n^s$ (resp.$\mathscr{D}_n^t$)be the class of all n-vertex bipartite graphs with connectivity s (resp.edge-connectivity t).

Let $S = S(G)$ be the sum of square of distances between all pairs of vertices of G, which is denoted by

$$S = S(G) = \sum_{u,v \in V_G} d_G^2(u, v) = \frac{1}{2} \sum_{v \in V_G} L_G(v).$$

This quantity was introduced by Mustapha Aouchich and Pierre Hansen in [1] and has been extensively studied in the monograph. Recently, $S(G)$ is applied to the research of distance spectral radius. Zhou and Trinajstić [17] proved an upper bound using the order n in addition to the sum of the squares of the distances $S(G)$, see [16, 18]. They also proved a lower bound on the distance spectral radius of a graph using only $S(G)$. As a continuance of it, in this paper, we determine sharp bounds on $S(G)$ for several classes of connected bipartite graphs. For surveys and some up-to-date papers related to Wiener index of trees and line graphs, see [5, 7, 9, 10, 11, 12, 13, 15] and [3, 4, 6, 8, 14], respectively.

In this paper we study the quantity S in the case of n-vertex bipartite graphs, which is an important class of graphs in graph theory. Based on the structure of bipartite graphs, sharp bounds on S among $\mathscr{C}_n^s$ (resp.$\mathscr{D}_n^t$) are determined. The corresponding extremal graphs are identified, respectively.

Further on we need the following lemma, which is the direct consequence of the definition of S.

Lemma 1.1. *Let G be a connected graph of order n and not isomorphic to S_n. Then for each edge $e \in \overline{G}, S(G) > S(G + e)$.*

In this article we only consider the simple, connected graphs. Let G be a graph with n vertices and $e(G)$ edges. The sum of distance between a vertex v and all other vertices is denoted by $d_G(v)$. The number of vertex pairs at distance k in G is denoted by $d(G, k)$. We use $\chi(G)$ and $C(G)$ to represent the chromatic number and clique number, respectively. K_n and P_n will denote the complement graph and the path on n vertices. Let $K_r \cdot P_n$ be the graph obtained from K_r and P_n by joining a vertex of K_r to one end vertex of P_n. We use the symbol $K_k(r_1, r_2, \cdots r_k)$ to denote the k-partite graph whose ith class contain exactly r_i vertices. The Turaán graph, $T_{m,n}$, is a complete m-partite graph on n vertices in which each part has either $\lceil n/k \rceil$ or $\lfloor n/k \rfloor$ vertices.

$S(G)$ is defined as the sum of square of distances between all pairs of vertices of G, which is denoted by

$$S(G) = \sum_{u,v \in V_G} d_G^2(u,v).$$

The upper and lower bound of a tree T_n, is given by the following lemma.

Lemma 1.2. *Let T_n be a tree on n vertices, then*

$$2n^2 - 5n + 3 \leq S(T_n) \leq \frac{n^4 - n^2}{12},$$

the upper bound is achieved if and only if $T_n \cong P_n$ and the lower bound is achieved if and only if $T_n \cong K_{1,n-1}$.

Proof. Let T^* be a graph with minimum $S(T)$ in the class of graphs with n vertices. It is obvious that T^* has a pendent vertex, say u. Let v be the pendent vertex of $K_{1,n-1}$. Then

$$\begin{aligned} S(T^*) &= S(T^* - u) + \sum_{p \in V_{T^*}} d^2(u,p) \\ S(K_{1,n-1}) &= S(K_{1,n-1} - v) + \sum_{p \in V_{K_{1,n-1}}} d^2(v,p). \end{aligned}$$

By the induction hypothesis,

$$S(T^* - u) \geq S(K_{1,n-1} - v).$$

It is easy to find that

$$\sum_{p \in V_{T^*}} d^2(u,p) \geq \sum_{p \in V_{K_{1,n-1}}} d^2(v,p)$$

thus,

$$S(T^*) \geq S(K_{1,n-1}).$$

Let $S(T')$ be the maximum value in the class of graphs. The pendent vertices of T' and P_n is u, v, repectively. Similar to the proof above, we can get that $S(T') \leq S(P_n)$. The computation of $K_{1,n-1}$ and P_n is following,

$$S(K_{1,n-1}) = \frac{[1 + 2^2(n-2)](n-1) + (n-1)}{2} = 2n^2 - 5n + 3.$$

Recall that

$$\begin{aligned} 1^2 + 2^2 + 3^2 + \cdots + n^2 &= \frac{n(n+1)(2n+1)}{6} \\ 1^3 + 2^3 + 3^3 + \cdots + n^2 &= \frac{n^2(n+1)^2}{4}. \end{aligned}$$

Then, we can compute the $S(P_n)$ by

$$\begin{aligned} S(P_n) &= \sum_{i-1}^{n-1} \frac{n(n+1)(2n+1)}{6} \\ &= \sum_{i=1}^{n-1} \frac{2i^3+3i^2+i}{6} \\ &= \frac{1}{6}\left(\sum_{i=1}^{n-1} 2i^3 + \sum_{i=1}^{n-1} 3i^2 + \sum_{i=1}^{n-1} i\right) \\ &= \frac{n^4-n^2}{12}. \end{aligned}$$

Therefore,

$$2n^2 - 5n + 3 \le T_n \le \frac{n^4-n^2}{12}$$

and the proof above implies that the upper bound is achieved if and only if $T_n \cong P_n$ and the lower bound is achieved if and only if $T_n \cong K_{1,n-1}$. □

A upper bound of $S(G)$ with giving the chromatic number is shown in the second section. The upper and lower of $S(G)$ with giving the clique number are shown in the third section.

2. Chromatic number

Theorem 2.1. *Let G be a graph with $\chi(G) = k$ .Then*

$$S(G) \ge 2n(n-1) - 3\binom{n-t}{2} - 3(k-1)\binom{t+1}{2}, \tag{2.1}$$

where $t = \lfloor n/k \rfloor$, and the equality holds if and only if $G \cong T_{k,n}$.

Proof. Assume G^* is a graph whose chromatic number is k and $S(G^*)$ is the minimum value in the class of graphs with n vertices. Then $V(G^*)$ can be partitioned into k classes such that no edges joins two vertices of the same class. Futhermore G^* contains all edges joining vertices in distinct classes. Otherwise, there exists two nonadiacent vertices, say x and y, in distinct class. Then the graph $G' + xy$ has chromatic number k and $S(G + xy) \le S(G^*)$, which is contradictory to the minimality of G^*. Thus G^* is a complete k-partite graph $K_k(r_1, r_2, \dots r_k)$ with $r_1 + r_2 + \dots r_k = n$.

We suppose that $G^* \cong T_{k,n}$. Otherwise, the class are not as equal as possible, that is to say the difference between the number of vertices in all classes are more than two, say $r_j \ge r_i + 2$, where $r_i(r_j)$ is the number of vertices in the ith(jth) class. Then by transferring one vertex from the jth class to the ith class, we would decrease the $S(G^*)$ by

$$[4(r_j - 1) + (n - r_j)] - [4r_i + (n - r_i - 1)] = 3[(r_j - r_i) - 1] \ge 1$$

which contradicts the minimality of G^*. Recall that

$$e(T_{k,n}) = \binom{n-t}{2} + (k-1)\binom{t+1}{2},$$

where $t = \lfloor n/k \rfloor$. so

$$\begin{aligned} S(G^*) &= S(T_{k,n}) \\ &= 4\binom{n}{2} - 3e(T_{k,n}) \\ &= 2n(n-1) - 3\binom{n-t}{2} - 3\binom{t+1}{2}. \quad \square \end{aligned}$$

The proof above implies that equality holds in (2.1) if and only if $G \cong T_{k,n}$.

3. Clique number

Theorem 3.1. *Let G be a graph on n vertices. If G contains no K_{m+1}, then $e(G) \le e(T_{m,n})$. Moreover, $e(G) = e(T_{m,n})$ only if $G \cong T_{m,n}$.*

The demonstrate about this well-known theorem can refer to [3].

In the following theorem, we only consider the graph G on n vertices with $C(G) < n-1$. since for $C(G) = n$ or $n-1$, it is easy to get the lower bound and upper bound on $S(G)$.

Theorem 3.2. *Let G be a graph on n vertices with $C(G) = k < n-1$. then*

$$\begin{aligned} 2n(n-1) &- \binom{n-t}{2} - 3(k-1)\binom{t+1}{2} \le S(G) \\ &\le \binom{k}{2} + \frac{n^4-n^2}{12} + (k-1)\frac{(n-k+1)(n-k+2)(2n-2k+3)}{6} \\ &+ \frac{(n-k+1)(n-k+2)(2n-2k+3)}{6}, \end{aligned}$$

where $t = \lfloor n/k \rfloor$. Moreover, the lower bound is achieved if and only if $G \cong T_{k,n}$ and the upper bound is achieved if and only if $G \cong K_k \cdot P_{n-k}$.

Proof. Let G be a graph on n vertices with $C(G) = k < n-1$. set $t = \lfloor n/k \rfloor$. suppose the diameter of G is l. then

$$\begin{aligned} S(G) = e(G) + \sum_{i=2}^{l} i^2 d(G,i) &\ge e(G) + 2^2 \sum_{i=2}^{l} d(G,i) \\ &\ge e(G) + 2^2 \sum_{i=2}^{l} d(G,i) \end{aligned}$$

$$(3.1) \qquad = e(G) + 4\left[\binom{n}{2} - e(G)\right] = 2n(n-1) - 3e(G)$$
$$\geq 2n(n-1) - 3T_{k,n} \ \text{(by Theorem 3.1)}$$
$$= 2n(n-1) - 3\binom{n-t}{2} - 3(k-1)\binom{t-1}{2}.$$

It is evident that equality in both (3.2) and (3.3) will hold if and only $G \cong T_{k,n}$. Note that the Turán graph $T_{k,n}$ has clique number k. So

$$S(G) \geq 2n(n-1) - 3\binom{n-t}{2} - 3\binom{t+1}{2},$$

and the equality holds if and only if $G \cong T_{k,n}$.

Assume G^* is a graph whose clique number is k and $S(G^*)$ is the minimum value in the class of graphs with n vertices. It is obvious that G^* has a pendent vertex, say u. Let v be the pendent vertex of $K_k \cdot P_{n-k}$. Then

$$S(G^*) = S(G^* - u) + \sum_{p \in V_G^*} d^2(u,p)$$
$$S(K_k \cdot P_{n-k}) = S(K_k \cdot P_{n-k} - v) + \sum_{p \in V_{K_k \cdot P_{n-k}}} d^2(v,p).$$

Since the graph $G^* - u$ has $n-1$ vertices and clique number k, by the induction hypothesis,

$$S(G^* - u) \leq S(K_k \cdot P_{n-k} - v).$$

It is easily checked that

$$\sum_{p \in V_G^*} d^2(u,p) \leq \sum_{p \in V_{K_k \cdot P_{n-k}}} d^2(v,p)$$

with the equality holding if and only if

$$G^* \cong K_k \cdot P_{n-k}.$$

So,

$$S(G^*) \leq S(K_k \cdot P_{n-k}).$$

A straightforward calculation gives that

$$S(K_k \cdot P_{n-k}) = \binom{k}{2} + \frac{n^4 - n^2}{12} + (k-1)$$
$$\cdot \left[\frac{(n-k+1)(n-k+2)(2n-2k+3)}{6} - 1\right]$$
$$+ \frac{(n-k)(n-k+1)}{2}.$$

Therefore,

$$S(G) \leq \binom{k}{2} + \frac{n^4 - n^2}{12} + (k-1) \cdot \left[\frac{(n-k+1)(n-k+2)(2n-2k+3)}{6} - 1 \right] + \frac{(n-k)(n-k+1)}{2}$$

and the proof above implies that the equality holds if and only if $G \cong K_k \cdot P_{n-k}$. □

Acknowledgements

The research is partially supported by National Science Foundation of China (11401008, 60873144, 61572035) and China Postdoctoral Science Foundation (2016M592030).

References

[1] Mustapha Aouchiche, Pierre Hansen, *Distance spectra of graphs: A survey*, Linear Algebra Appl., 458 (2014), 301386.

[2] J.A. Bondy, U.S.R. Murty, *Graph theory, in: GTM*, 224 (2008), Springer.

[3] B. Bollobás, *Extremal graph theory [M]*, Academic Press, London, New York, San Francisco, 1978.

[4] P. Dankelmann, I. Gutman, S. Mukwembi, H.C. Swart, *The edge-Wiener index of a graph*, Discrete Math., 309 (2009), 3452-3457.

[5] A. Dobrynin, R. Entringer, I. Gutman, *Wiener index of trees: theory and applications*, Acta Appl. Math., 66 (2001), 211-249.

[6] Y. Don, H. Bian, H. Gao, H. Yu, *The polyphenyl chains with extremal edge-Wiener indices*, MATCH Commun. Math. Comput. Chem., 64 (2010), 757-766.

[7] I. Gutman, S. Klavžar, B. Mohar (Eds.), *Fifty years of the Wiener index*, MATCH Commun. Math. Comput. Chem. 35 (1997), 1-259.

[8] A. Iranmanesh, A.S. Kafrani, *Computation of the first edge-Wiener index of $TUC_4C_8(S)$ nanotube*, MATCH Commun. Math. Comput. Chem., 62 (2009), 311-352.

[9] S.C. Li, Y.B. Song, *On the sum of all distances in bipartite graphs*, Discrete Applied Mathematics, 169 (2014), 176-185.

[10] M. Liu, B. Liu, *On the variable Wiener indices of trees with given maximum degree*, Math. Comput. Modelling, 52 (2010), 1651-1659.

[11] W. Luo, B. Zhou, *On ordinary and reverse Wiener indices of non-caterpillars*, Math. Comput. Modelling, 50 (2009), 188-193.

[12] R. Merris, *An edge version of the matrix-tree theorem and the Wiener index*, Linear Multilinear Algebra, 25 (1988), 291-296.

[13] T. Pisanski, J.Žerovnik, *Edge-contributions of some topological indices and arboreality of molecular graphs*, Ars Math. Contemp., 2 (2009), 49-58.65 (1976), 4111-4115.

[14] B. Wu, *Wiener index of line graphs*, MATCH Commun. Math. Comput. Chem., 64 (2010), 699-706.

[15] X.D. Zhang, Y. Liu, M.X. Han, *Maximum Wiener index of trees with given degree sequence*, MATCH Commun. Math. Comput. Chem., 64 (2010), 661-682.

[16] B. Zhou, N. Trinajstić, *Mathematical properties of molecular descriptors based on distances*, Croat. Chem. Acta, 83 (2010), 227-242.

[17] B. Zhou, N. Trinajstić, *On the largest eigenvalue of the distance matrix of a connected graph*, Chem. Phys. Lett., 447 (2007), 384-387.

[18] B. Zhou, N. Trinajstić, *Further results on the largest eigenvalues of the distance matrix and some distance based matrices of connected (molecular) graphs*, Internet Electron. J. Mol. Des., 6 (2007), 375-384.

[19] H.H. Zhang, S.C. Li, L.F. Zhao, *On the further relation between the (revised) Szeged index and the Wiener index of graphs*, Discrete Applied Mathematics, 206 (2016), 152-164.

Accepted: 16.11.2016