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#### Steiner Degree Distance<sup>\*</sup>

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#### Abstract

The degree distance DD(G) of a connected graphs G was invented by Dobrynin and Kochetova in 1994. Recently, one of the present authors introduced the concept of k-center Steiner degree distance defined as

$$SDD_k(G) = \sum_{\substack{S \subseteq V(G) \\ |S| = k}} \left[ \sum_{v \in S} deg_G(v) \right] d_G(S)$$

where  $d_G(S)$  is the Steiner k-distance of S and  $deg_G(v)$  is the degree of the vertex v in G. Expressions for  $SDD_k$  for some special graphs are obtained, as well as sharp upper and lower bounds of  $SDD_k$  of a connected graph. Some properties of  $SDD_k$  of trees are established.

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## 1 Introduction

All graphs in this paper are assumed to be undirected, finite, and simple. Let G be such a graph with vertex set V(G) and edge set E(G). Then the order and size of G are n = n(G) = |V(G)| and m = m(G) = |E(G)|. In other words, G has n vertices and m edges.

The degree  $deg_G(u)$  of the vertex  $u \in V(G)$  is number of first neighbors of this vertex.

Distance is one of the basic concepts of graph theory [7]. If G is connected and  $u, v \in V(G)$ , then the distance  $d(u, v) = d_G(u, v)$  between u and v is the length of a shortest path connecting u and v. If v is a vertex of a connected graph G, then the eccentricity  $\varepsilon(v)$  of v is defined as  $\varepsilon(v) = \max\{d(u, v) | u \in V(G)\}$ . Furthermore, the radius rad(G) and diameter diam(G) of G are  $rad(G) = \min\{\varepsilon(v) | v \in V(G)\}$  and  $diam(G) = \max\{\varepsilon(v) | v \in V(G)\}$ . These latter two quantities are related by the inequalities  $rad(G) \leq diam(G) \leq 2rad(G)$ . More details on this subject can be found in [14].

We refer to [5] for graph theoretical notation and terminology not specified here.

\* \* \* \* \*

For a graph G with vertex set V(G), the *degree distance* is defined as [13]

$$DD = DD(G) = \sum_{\{u,v\} \in V(G)} [deg_G(u) + deg_G(v)] d_G(u,v)$$
(1)

For more details on degree–and–distance–based graph invariant, we refer to [2–4, 6, 16, 17, 22, 24, 27].

The Wiener index W(G) of the graph G is defined as

$$W(G) = \sum_{\{u,v\} \subseteq V(G)} d_G(u,v) \,. \tag{2}$$

Details on this oldest distance–based topological index can be found in numerous surveys, e.g., in [11, 12, 18, 19, 25, 26, 28].

The Steiner distance of a graph, introduced by Chartrand et al. in 1989 [9], is a natural and nice generalization of the concept of classical graph distance. For a subset S of the vertex set V(G), consisting of at least two vertices, the *Steiner distance* d(S) (or simply the distance of S) is the minimum size (number of edges) of a connected subgraphs whose vertex set contains S. This connected subgraph is necessarily a tree and is referred to as a *Steiner tree*.

Note that if  $S = \{u, v\}$ , then d(S) = d(u, v) is nothing new, but the classical distance between u and v. Clearly, if |S| = k, then  $d(S) \ge k - 1$ .

Let *n* and *k* be integers such that  $2 \le k \le n$ . The Steiner *k*-eccentricity  $\varepsilon_k(v)$  of a vertex *v* of *G* is  $\varepsilon_k(v) = \max\{d(S) | S \subseteq V(G), |S| = k, \text{ and } v \in S\}$ . The Steiner *k*-radius of *G* is  $srad_k(G) = \min\{\varepsilon_k(v) | v \in V(G)\}$ , whereas the Steiner *k*-diameter of *G* is  $sdiam_k(G) = \max\{\varepsilon_k(v) | v \in V(G)\}$ . Note that for every connected graph *G*,  $\varepsilon_2(v) = \varepsilon(v)$  for all vertices *v* of *G*,  $srad_2(G) = rad(G)$  and  $sdiam_2(G) = diam(G)$ . For more details on Steiner distance, we refer to [1, 8-10, 14, 23].

The following result is immediate.

**Observation 1.** If H is a connected spanning subgraph of G, then

$$sdiam_k(G) \leq sdiam_k(H)$$

holds for all  $k, 2 \leq k \leq n$ .

Li et al. [20] put forward a Steiner–distance–based generalization of the Wiener index concept. According to [20], the *k*-center Steiner Wiener index  $SW_k(G)$  of the graph G is defined by

$$SW_k(G) = \sum_{\substack{S \subseteq V(G) \\ |S| = k}} d(S) .$$
(3)

For k = 2, the above defined Steiner Wiener index coincides with the ordinary Wiener index, Eq. (2). It is usual to consider  $SW_k$  for  $2 \le k \le n - 1$ , but the above definition would be applicable also in the cases k = 1 and k = n, implying  $SW_1(G) = 0$  and  $SW_n(G) = n - 1$ .

In [20], Li et al. obtained the following results.

**Lemma 2.** [20] Let  $S_n$ ,  $P_n$ ,  $K_n$ , and  $K_{a,b}$  be the star, path, and complete graph of order n, and the complete bipartite graph of order a + b. Then for k being an integer such that  $2 \le k \le n-2$  or  $2 \le k \le a+b-2$ ,

$$SW_k(S_n) = (n-1)\binom{n-1}{k-1}$$
 (4)

$$SW_k(P_n) = (k-1)\binom{n+1}{k+1}$$
 (5)

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$$SW_k(K_n) = (k-1)\binom{n}{k}$$

$$SW_k(K_{a,b}) = \begin{cases} (k-1)\binom{a+b}{k} + \binom{a}{k} + \binom{b}{k} & \text{if } 1 \le k \le a \\ (k-1)\binom{a+b}{k} + \binom{b}{k} & \text{if } a < k \le b \\ (k-1)\binom{a+b}{k} & \text{if } b < k \le a+b. \end{cases}$$

$$(6)$$

Recently, one of the present authors [15] offered an analogous generalization of the concept of degree distance, Eq. (1). Thus, the *k*-center Steiner degree distance  $SDD_k(G)$  of G is defined as

$$SDD_k(G) = \sum_{\substack{S \subseteq V(G) \\ |S|=k}} \left[ \sum_{v \in S} deg_G(v) \right] d_G(S) \,. \tag{8}$$

In Section 2, we report expressions for the k-center Steiner degree distance of the star, path, as well as the complete and complete bipartite graphs. We also get general expressions for  $SDD_k(G)$  for k = n, n - 1. In Section 3, we obtain sharp lower and upper bounds for  $SDD_k$ .

## 2 Steiner degree distance of special graphs

Beginning this section, we note that in the special case k = 2, all formulas derived here for the k-center Steiner degree distance reduce to expressions for the ordinary degree distance.

**Theorem 1.** Let  $S_n$ ,  $P_n$ ,  $K_n$ , and  $K_{a,b}$  be the path, star, and complete graph of order n, and the complete bipartite graph of order a + b. Then for k being an integer such that  $2 \le k \le n-2$  or  $2 \le k \le a+b-2$ ,

$$SDD_k(S_n) = (2kn - n - 3k + 2) \binom{n-1}{k-1}$$
(9)

$$SDD_k(P_n) = \frac{2(k-1)(kn-1)}{k+1} \binom{n}{k}$$
 (10)

$$SDD_k(K_n) = n(n-1)^2 \binom{n-2}{k-2}$$
 (11)

$$SDD_{k}(K_{a,b}) = \begin{cases} 2ab(k-1)\binom{a+b-1}{k-1} + ka\binom{b}{k} + kb\binom{a}{k} & \text{if } 1 \le k \le a \\ 2ab(k-1)\binom{a+b-1}{k-1} + ka\binom{b}{k} & \text{if } a < k \le b \\ 2ab(k-1)\binom{a+b-1}{k-1} + k(k-1)a\binom{b}{k} & \text{if } b < k \le a+b . \end{cases}$$

*Proof.* We first verify the expression for  $SDD_k(S_n)$ .

Let w be the center of  $S_n$ . For any  $S \subseteq V(S_n)$  and |S| = k, if  $w \in S$ , then  $d_{S_n}(S) = k - 1$  and  $\sum_{v \in S} deg_{S_n}(v) = (n - 1) + (k - 1) = n + k - 2$ . If  $w \notin S$ , then  $d_{S_n}(S) = k$  and  $\sum_{v \in S} deg_{S_n}(v) = k$ . Therefore,

$$SDD_{k}(S_{n}) = \sum_{\substack{S \subseteq V(S_{n}) \\ |S|=k, w \in S}} \left[ \sum_{v \in S} deg_{S_{n}}(v) \right] d_{S_{n}}(S) + \sum_{\substack{S \subseteq V(S_{n}) \\ |S|=k, w \notin S}} \left[ \sum_{v \in S} deg_{S_{n}}(v) \right] d_{S_{n}}(S)$$
$$= \binom{n-1}{k-1} (n+k-2)(k-1) + \binom{n-1}{k} k^{2}$$
$$= \binom{n-1}{k-1} (n+k-2)(k-1) + \binom{n-1}{k-1} (n-k)k$$

from which Eq. (9) directly follows.

Next we consider the Steiner degree distance of  $K_n$ .

Let  $S \subseteq V(K_n)$  and |S| = k. Since  $K_n$  is a regular graph of degree n - 1,

$$\sum_{v \in S} deg_{K_n}(v) = k(n-1)$$

implying

$$SDD_{k}(K_{n}) = \sum_{\substack{S \subseteq V(K_{n}) \\ |S| = k}} \left[ \sum_{v \in S} deg_{K_{n}}(v) \right] d_{K_{n}}(S)$$
$$= k(n-1) \sum_{\substack{S \subseteq V(K_{n}) \\ |S| = k}} d_{K_{n}}(S) = k(n-1) SW_{k}(K_{n})$$

Eq. (11) follows now from Lemma 2.

The proofs of Eqs. (10) and (12) are similar, yet somewhat more complicated, and are omitted.  $\hfill \Box$ 

**Observation 3.** Let G be the connected graph of order n and size m. Then directly from the definition of  $SDD_n(G)$ , Eq. (8), it follows

$$SDD_n(G) = 2m(n-1).$$

In [21], Mao obtained the following result.

**Lemma 4.** [21] Let G be a connected graph of order n. Then  $sdiam_{n-1}(G) = n - 2$  if and only if G is 2-connected.

We now show how to compute  $SDD_{n-1}(G)$ . Denote the vertex-connectivity of the graph G by  $\kappa(G)$ .

**Theorem 2.** Let G be a connected graph of order n and size m.

(1) If  $\kappa(G) \geq 2$ , then

$$SDD_{n-1}(G) = 2m(n-2)(n-1).$$
 (13)

(2) If  $\kappa(G) = 1$ , then

$$SDD_{n-1}(G) = 2m(n^2 - 3n + 2 + p) - \sum_{i=1}^{p} deg_G(w_i)$$
 (14)

where  $w_i \ (1 \le i \le p)$  are the cut vertices of G.

*Proof.* (1) Since  $\kappa(G) \ge 2$ , all subgraphs of G with n-1 vertices have  $\kappa \ge 1$ , and therefore the Steiner distance of the respective n-1 vertices is n-2. Hence,

$$SDD_{n-1}(G) = (n-2)\sum_{\substack{S \subseteq V(G) \\ |S|=n-1}} \left[\sum_{v \in S} deg_G(v)\right]$$

For each  $v \in V(G)$ , there are (n-1) (n-1)-element subsets of V(G) such that each of these contains v. The contribution of vertex v to  $SDD_{n-1}(G)$  is exactly  $(n-1)deg_G(v)$ . From the arbitrariness of v, we get Eq. (13).

(2) Note that  $w_1, w_2, \ldots, w_p$  are the cut vertices of G. For any  $S \subseteq V(G)$  and |S| = n-1, if  $V(G) \setminus S = \{w_i\}$  for some i, then by Lemma 4,  $d_G(S) = n-1$ . If  $V(G) \setminus S \neq \{w_i\}$  for each i  $(1 \le i \le p)$ , then Lemma 4 implies  $d_G(S) = n-2$ . Then  $SDD_{n-1}(G)$  is equal to

$$(n-2)\sum_{\substack{S\subseteq V(G)\\|S|=n-1\\V(G)\setminus S\neq \{w_i\}}} \left[\sum_{v\in S} deg_G(v)\right] + (n-1)\sum_{\substack{S\subseteq V(G)\\|S|=n-1\\V(G)\setminus S=\{w_i\}}} \left[\sum_{v\in S} deg_G(v)\right]$$

$$= (n-2)\left[2(n-p)m - \sum_{i=p+1}^{n} deg_G(w_i)\right] + (n-1)\left[2pm - \sum_{i=1}^{p} deg_G(w_i)\right]$$

which is equal to the right-hand side of Eq. (14).

In [15], a result for  $SDD_3$  of a tree T was obtained. Here we calculate  $SW_{n-1}(T)$ .

**Theorem 3.** Let T be a tree of order n, possessing p pendent vertices. Then

$$SDD_{n-1}(T) = 2(n-1)^3 - p(2n-3)$$
 (15)

irrespective of any other structural detail of T.

Proof. Since k = n - 1, the respective subsets S contain all except one vertices of T. If the vertex missing from S is pendent, then the vertices contained in S form a tree of order n - 1. Therefore  $d_T(S) = n - 2$ , and  $\sum_{v \in S} deg_T(v) = 2m(T) - 1 = 2n - 3$ . There are p such subsets, contributing to  $SDD_{n-1}$  by  $p \times (2n - 4)(n - 2) = 2p(n - 2)^2$ .

If the vertex of T, not present in S, is non-pendent, then the vertices contained in S cannot form a tree, and the respective Steiner tree must contain all the n vertices of T. Therefore,  $d_T(S) = n - 1$ , and  $\sum_{v \in S} deg_T(v) = 2m(T) - d_T(w)$ , where  $w \in V(G) \setminus S$ . There are n - p such subsets, contributing to  $SDD_{n-1}$  by

$$2(n-1)(n-p)m(T) - (n-1)\sum_{d_T(w)\ge 2} d_T(w)$$
  
=  $2(n-1)(n-p)m(T) - 2(n-1)[2m(T) - 2p]$   
=  $2(n-1)^2(n-p) - (n-1)(2n-2-p)$   
=  $2(n-1)^3 - p(n-1)(2n-3)$ 

which straightforwardly leads to Eq. (15).

#### 3 Lower and upper bounds for general graphs

Denote by  $\delta(G)$  and  $\Delta(G)$  the smallest and greatest vertex degree of the graph G. The bounds stated as Proposition 5, follow immediately from the the definitions of the Steiner Wiener index, Eq. (3), and Steiner degree distance, Eq. (8).

**Proposition 5.** Let G be a connected graph of order n. Then

$$k\delta(G)SW_k(G) \le SDD_k(G) \le k\Delta(G)SW_k(G)$$

holds for all k,  $2 \le k \le n$ , with equality if and only if G is a regular graph.

**Theorem 4.** Let G be a connected graph of order n and size m. Then

$$2m\binom{n-1}{k-1}(k-1) \le SDD_k(G) \le 2m\binom{n-1}{k-1}(n-1)$$
(16)

holds for all k,  $2 \le k \le n$ .

*Proof.* For any  $S \subseteq V(G)$  and |S| = k, we have  $k - 1 \leq d_G(S) \leq n - 1$ , and hence

$$(k-1)\sum_{\substack{S\subseteq V(G)\\|S|=k}}\left[\sum_{v\in S} deg_G(v)\right] \le SDD_k(G) \le (n-1)\sum_{\substack{S\subseteq V(G)\\|S|=k}}\left[\sum_{v\in S} deg_G(v)\right].$$
 (17)

Let

$$M = \sum_{\substack{S \subseteq V(G) \\ |S| = k}} \left[ \sum_{v \in S} deg_G(v) \right].$$

For each  $v \in V(G)$ , there are  $\binom{n-1}{k-1}$  k-subsets in G containing the vertex v. The contribution of v to M is thus  $\binom{n-1}{k-1} deg_G(v)$ . From the arbitrariness of v, we have

$$M = \binom{n-1}{k-1} \sum_{v \in V(G)} \deg_G(v) = 2m \binom{n-1}{k-1}$$

which substituted back into (17) yields (16).

Li et al. [20] obtained the following sharp bounds for the Steiner Wiener index.

**Lemma 6.** [20] Let G be a connected graph of order n. Then

$$\binom{n}{k}(k-1) \le SW_k(G) \le (k-1)\binom{n+1}{k+1}$$

holds for all k,  $2 \le k \le n$ . Moreover, the lower bound is sharp.

**Proposition 7.** Let G be a connected graph of order n. Then

$$k\delta(G)\binom{n}{k}(k-1) \le SDD_k(G) \le k\Delta(G)(k-1)\binom{n+1}{k+1}$$

holds for all k,  $2 \le k \le n$ . Moreover, the lower bound is sharp.

Proof. From Proposition 5 and Lemma 6, we have

$$SDD_k(G) \ge k\delta(G) SW_k(G) \ge k\delta(G) \binom{n}{k} (k-1)$$

and

$$SDD_k(G) \le k\Delta(G) SW_k(G) \le k\Delta(G)(k-1)\binom{n+1}{k+1}.$$

In order to show the sharpness of the lower bound, consider the complete graph  $K_n$ . Since  $\Delta(K_n) = n - 1$ , it follows from Eqs. (6) and (11) that

$$SDD_k(K_n) = n(n-1)^2 \binom{n-2}{k-2} = \binom{n}{k} k(n-1)(k-1) = k\delta(K_n) SW_k(K_n).$$

To show the sharpness of the upper bound, we consider the path  $P_2$ . Since  $\delta(P_2) = 1$ , it follows from Eqs. (5) and (10) that

$$SDD_2(P_n) = DD(P_n) = 2 = 2\Delta(P_2) SW_2(P_2).$$

#### References

- P. Ali, P. Dankelmann, S. Mukwembi, Upper bounds on the Steiner diameter of a graph, *Discr. Appl. Math.* 160 (2012) 1845–1850.
- [2] P. Ali, S. Mukwembi, S. Munyira, Degree distance and vertex-connectivity, Discr. Appl. Math. 161 (2013) 2802–2811.
- [3] P. Ali, S. Mukwembi, S. Munyira, Degree distance and edge-connectivity, Australas. J. Comb. 60 (2014) 50–68.
- [4] M. An, L. Xiong, K.C. Das, Two upper bounds for the degree distances of four sums of graphs, *Filomat* 28 (2014) 579–590.
- [5] J. A. Bondy, U. S. R. Murty, Graph Theory, Springer, New York, 2008.
- [6] O. Bucicovschi, S. M. Cioabă, The minimum degree distance of graphs of given order and size, Discr. Appl. Math. 156 (2008) 3518–3521.
- [7] F. Buckley, F. Harary, *Distance in Graphs*, Addison–Wesley, Redwood, 1990.
- [8] J. Cáceresa, A. Márquezb, M. L. Puertasa, Steiner distance and convexity in graphs, *Eur. J. Comb.* 29 (2008) 726–736.
- G. Chartrand, O. R. Oellermann, S. Tian, H. B. Zou, Steiner distance in graphs, *Časopis Pest. Mat.* 114 (1989) 399–410.
- [10] P. Dankelmann, O. R. Oellermann, H. C. Swart, The average Steiner distance of a graph, J. Graph Theory 22 (1996) 15–22.

- [11] A. Dobrynin, R. Entringer, I. Gutman, Wiener index of trees: theory and application, Acta Appl. Math. 66 (2001) 211–249.
- [12] A. A. Dobrynin, I. Gutman, S. Klavžar, P. Žigert, Wiener index of hexagonal systems, Acta Appl. Math. 72 (2002) 247–294.
- [13] A. Dobrynin, A. Kochetova, Degree distance of a graph: A degree analogue of the Wiener index, J. Chem. Inf. Comput. Sci. 34 (1994) 1082–1086.
- [14] W. Goddard, O. R. Oellermann, Distance in graphs, in: M. Dehmer (Ed.), Structural Analysis of Complex Networks, Birkhäuser, Dordrecht, 2011, pp. 49–72.
- [15] I. Gutman, On Steiner degree distance of trees, Appl. Math. Comput. 283 (2016) 163–167.
- [16] I. Gutman, On two degree-and-distance-based graph invariants, Bull. Acad. Serbe Sci. Arts (Cl. Sci. Math. Natur.), in press.
- [17] I. Gutman, B. Furtula, K. C. Das, On some degree-and-distance-based graph invariants of trees, Appl. Math. Comput. 289 (2016) 1–6.
- [18] I. Gutman, Y. N. Yeh, S. L. Lee, Y. L. Luo, Some recent results in the theory of the Wiener number, *Indian J. Chem.* **32A** (1993) 651–661.
- [19] M. Knor, R. Škrekovski, A. Tepeh, Mathematical aspects of Wiener index, Ars Math. Contemp. 11 (2016) 327–352.
- [20] X. Li, Y. Mao, I. Gutman, The Steiner Wiener index of a graph, Discuss. Math. Graph Theory 36 (2016) 455–465.
- [21] Y. Mao, The Steiner diameter of a graph, Bull. Iran. Math. Soc., in press.
- [22] S. Mukwembi, S. Munyira, Degree distance and minimum degree, Bull. Austral. Math. Soc. 87 (2013) 255–271.
- [23] O. R. Oellermann, S. Tian, Steiner centers in graphs, J. Graph Theory 14 (1990) 585–597.
- [24] K. Pattabiraman, P. Kandan, Generalization of the degree distance of the tensor product of graphs, Australas. J. Comb. 62 (2015) 211–227.
- [25] D. H. Rouvray, Harry in the limelight: The life and times of Harry Wiener, in: D. H. Rouvray, R. B. King (Eds.), *Topology in Chemistry Discrete Mathematics of Molecules*, Horwood, Chichester, 2002, pp. 1–15.
- [26] D. H. Rouvray, The rich legacy of half century of the Wiener index, in: D. H. Rouvray, R. B. King (Eds.), *Topology in Chemistry – Discrete Mathematics of Molecules*, Horwood, Chichester, 2002, pp. 16–37.
- [27] V. Sheeba Agnes, Degree distance and Gutman index of corona product of graphs, Trans. Comb. 4(3) (2015) 11–23.
- [28] K. Xu, M. Liu, K. C. Das, I. Gutman, B. Furtula, A survey on graphs extremal with respect to distance–based topological indices, *MATCH Commun. Math. Comput. Chem.* **71** (2014) 461–508.