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Steiner Gutman Index

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Abstract

The concept of *Gutman index* SGut(*G*) of a connected graph *G* was introduced in 1994. The Steiner distance in a graph, introduced by Chartrand et al. in 1989, is a natural generalization of the concept of classical graph distance. In this paper, we generalize the concept of Gutman index by Steiner distance. The *Steiner Gutman* k-index SGut_k(*G*) of *G* is defined by SGut_k(*G*) = $\sum_{\substack{S \subseteq V(G) \\ |S| = k}} [\prod_{v \in S} deg_G(v)] d_G(S)$, where $d_G(S)$ is the Steiner distance of *S* and $deg_G(v)$ is the degree of *v* in *G*. Expressions for SGut_k for some special graphs are obtained. We also give sharp upper and lower bounds of SGut_k of a connected graph, and get the expression of SGut_k(*G*) for k = n, n - 1. Finally, we compare between *k*-center Steiner degree distance *SDD_k* and SGut_k of graphs.

1 Introduction

In graph theory applied to chemical problems, a large number of molecular structure descriptors, so-called "topological indices", has been studied [27]. Many of these descriptors are defined in terms of vertex degrees; see [6, 16, 27]. Equally many of these descriptors are in terms of distance between vertices; see [27, 28]. There are also several degree-anddistance-based topological indices; see [11, 13, 14, 18].

Throughout this paper graph is connected. For a graph G, let V(G), E(G), and m = |E(G)| denote the set of vertices, the set of edges, and the size of G, respectively.

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The minimum vertex degree is denoted by δ and the maximum by Δ . Distance is one of the basic concepts of graph theory [4]. If G is a connected graph 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.

In [14], the *degree distance* of a graph G is defined as

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

where $deg_G(u)$ is the degree of the vertex $u \in V(G)$, and d(u, v) is the distance between the vertices $u, v \in V(G)$. For more details on degree distance, we refer to [2,3,12,25].

In [18], the *Gutman index* of a graph G is defined as

$$\mathrm{SGut}(G) = \sum_{\{u,v\}\subseteq V(G)} [deg_G(u)deg_G(v)]d_G(u,v),$$

where $deg_G(u)$ is the degree of the vertex $u \in V(G)$, and d(u, v) is the distance between the vertices $u, v \in V(G)$. For more details on Gutman index, we refer to [8, 12, 15, 27].

The Steiner distance of a graph, introduced by Chartrand et al. in 1989, is a natural and nice generalization of the concept of classical graph distance. For a graph G(V, E)and a set $S \subseteq V(G)$ of at least two vertices, an S-Steiner tree or a Steiner tree connecting S (or simply, an S-tree) is a such subgraph T(V', E') of G that is a tree with $S \subseteq V'$. Let G be a connected graph of order at least 2 and let S be a nonempty set of vertices of G. Then the Steiner distance d(S) among the vertices of S (or simply the distance of S) is the minimum size of a connected subgraph whose vertex set contain S. Note that if H is a connected subgraph of G such that $S \subseteq V(H)$ and $|E(H)| = d_G(S)$, then H is a tree. Clearly, $d_G(S) = \min\{|E(T)|, S \subseteq V(T)\}$, where T is subtree of G. Furthermore, if $S = \{u, v\}$, then $d_G(S) = d_G(u, v)$ is nothing new, but the classical distance between uand v. Clearly, if |S| = k, then $d_G(S) \ge k - 1$.

If v is a vertex of a connected graph G, then the eccentricity $\varepsilon(v)$ of v is defined by $\varepsilon(v) = \max\{d(u,v) \mid u \in V(G)\}$. Furthermore, the radius rad(G) and diameter diam(G) of G are defined by $rad(G) = \min\{\varepsilon(v) \mid v \in V(G)\}$ and $diam(G) = \max\{\varepsilon(v) \mid v \in V(G)\}$. 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 defined by $\varepsilon_k(v) = \max\{d_G(S) \mid S \subseteq V(G), |S| = k, \text{ and } v \in S\}$. The Steiner k-radius of G is $srad_k(G) = \min\{\varepsilon_k(v) \mid v \in V(G)\}$, while the Steiner k-diameter of G is $sdiam_k(G) = \max\{\varepsilon_k(v) \mid v \in V(G)\}$. 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, 5, 7, 9, 10, 26].

The following observation is easily seen.

Observation 1.1 Let k be an integer such that $2 \le k \le n$. If H is a spanning subgraph of G, then $sdiam_k(G) \le sdiam_k(H)$.

Li et al. [19] generalized the concept of Wiener index by Steiner distance. The Steiner Wiener k-index or k-center Steiner Wiener index $SW_k(G)$ of G is defined by

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

For k = 2, the above defined Steiner Wiener index coincides with the ordinary Wiener index. It is usual to consider SW_k for $2 \le k \le n-1$, but the above definition implies $SW_1(G) = 0$ and $SW_n(G) = n-1$. For more details on the Steiner Wiener index, we refer to [19, 20, 24].

Recently, Gutman [17] generalized the concept of degree distance by Steiner degree distance. The k-center Steiner degree distance $SDD_k(G)$ of G is defined by

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

For more details on the Steiner degree distance, we refer to [18,23].

We now generalize the concept of Gutman index by Steiner distance. The *Steiner* Gutman k-index $SGut_k(G)$ of G is defined by

$$\operatorname{SGut}_k(G) = \sum_{\substack{S \subseteq V(G) \\ |S|=k}} \left(\prod_{v \in S} \deg_G(v) \right) d_G(S)$$

The relations between the Steiner degree distance, Steiner Gutman index and Steiner Wiener index are shown in the following Table 1:

	*
Parameters	Definitions
Steiner Wiener k -index	$SW_k(G) = \sum_{\substack{S \subseteq V(G) \\ S =k}} d_G(S)$
k-center Steiner Degree distance	$SDD_k(G) = \sum_{\substack{S \subseteq V(G) \\ S =k}} \left[\sum_{v \in S} deg_G(v) \right] d_G(S)$
Steiner Gutman k -index	$\operatorname{SGut}_{k}(G) = \sum_{\substack{S \subseteq V(G) \\ S =k}} \left[\prod_{v \in S} \deg_{G}(v) \right] d_{G}(S)$

Table 1. Three Steiner distance parameters.

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In Section 2, we obtain the exact values of the Steiner Gutman k-index of the complete graph, complete bipartite graph, path and star. When G is a connected graph or tree, we also get the expression of $SGut_k(G)$ for k = n, n - 1. In Section 3, we obtain sharp lower and upper bounds for $SGut_k$ in terms of degree, or both order and size, or order. In Section 4, comparison between SDD_k and $SGut_k$ of graphs is given.

2 Results for some special graphs

Beginning this section, we note that the special case for k = 2 of all formulas derived here for the Steiner Gutman k-index, thus pertaining to the ordinary Gutman index, are well known and mentioned many times in the earlier literature. From the definition of Steiner Gutman k-index, one can easily obtain the following result:

Proposition 2.1 Let K_n be the complete graph of order n, and let k be an integer such that $2 \le k \le n$. Then

$$\operatorname{SGut}_k(K_n) = \binom{n}{k} (n-1)^k (k-1).$$

By the similar method in [22], we can derive the following result for complete bipartite graphs.

Theorem 2.1 Let $K_{a,b}$ be the complete bipartite graph of order a + b $(1 \le a \le b)$, and let k be an integer such that $2 \le k \le a + b$. Then

$$\operatorname{SGut}_{k}(K_{a,b}) = \begin{cases} ka^{k} {\binom{b}{k}} + kb^{k} {\binom{a}{k}} + (k-1) \sum_{x=1}^{k-1} {\binom{a}{x}} {\binom{b}{k-x}} b^{x} a^{k-x} & \text{if } 1 \le k \le a \\ ka^{k} {\binom{b}{k}} + (k-1) \sum_{x=1}^{a} {\binom{a}{x}} {\binom{b}{k-x}} b^{x} a^{k-x} & \text{if } a < k \le b \\ (k-1) \sum_{x=1}^{a} {\binom{a}{x}} {\binom{b}{k-x}} b^{x} a^{k-x} & \text{if } b < k \le a+b. \end{cases}$$

The following corollary is immediate from the above theorem.

Corollary 2.1 Let S_n be the star of order $n \ (n \ge 3)$, and let k be an integer such that $2 \le k \le n$. Then

$$\operatorname{SGut}_k(S_n) = (kn - 2k + 1) \binom{n-1}{k-1}.$$

For paths of order n, we have the following.

Proposition 2.2 Let P_n be the path of order n, and let k be an integer such that $2 \le k \le n-2$. Then

$$\operatorname{SGut}_k(P_n) = 2^k (k-1) \binom{n}{k+1} + 2^{k-2} (n-1) \binom{n-2}{k-2}.$$

Proof. Let $P_n = v_1 v_2 \dots v_n$, and $G = P_n$. Note that $d_G(v_1) = d_G(v_n) = 1$ and $d_G(v_i) = 2$ for each i $(2 \le i \le n-1)$. We first regard the degree of both v_1 and v_n as 2. In this way, all the degree of v_1, v_2, \dots, v_n are 2.

$$\sum_{\substack{S \subseteq V(G) \\ |S|=k}} \left(\prod_{v \in S} deg_G(v) \right) d_G(S) = 2^k \sum_{\substack{S \subseteq V(G) \\ |S|=k}} d_G(S) = 2^k SW_k(G) \,.$$

Next, let us compute how we add additional contributions for $2^k SW_k(G) - SGut_k(G)$ by assuming $d_G(v_1) = d_G(v_n) = 2$. It is clear that

 $2^k SW_k(G) - SGut_k(G)$

$$= 2^{k-1} \sum_{\substack{S \subseteq V(G), |S| = k \\ v_1 \in S, \ deg_G(v_n) = 2}} d_G(S) + 2^{k-1} \sum_{\substack{S \subseteq V(G), |S| = k \\ v_n \in S, \ deg_G(v_1) = 2}} d_G(S) - 2^{k-2} \sum_{\substack{S \subseteq V(G), |S| = k \\ v_1 \in S, \ v_n \in S}} d_G(S),$$

where $deg_G(v_1) = 2$ or $deg_G(v_n) = 2$ means that we regard the degree of v_1 or v_n as 2.

For symmetry, we only need to compute $\sum_{\substack{S \subseteq V(G), |S|=k \\ v_1 \in S, deg_G(v_1)=2}} d_G(S)$. Choose $S \subseteq V(G)$ and |S| = k. Without loss of generality, let $S = \{u_1, u_{i_2}, \ldots, u_{i_k}\}$ where $1 < i_2 < \cdots < i_k \le n$. Then $k \le i_k \le n$. Let $d_G(u_1, u_{i_k}) = j - 1$. Since $d_G(S) = d_G(u_1, u_{i_k}) = j - 1$, it follows that $k - 1 \le j - 1 \le n - 1$, and hence $k \le j \le n$. Once the vertex u_{i_k} is chosen, since $d_G(u_1, u_{i_k}) = j - 1$, we have $\binom{j-2}{k-2}$ ways to choose $u_{i_2}, u_{i_3}, \ldots, u_{i_k-1}$. Therefore, we have

$$2^{k-1} \sum_{\substack{S \subseteq V(G), |S|=k \\ v_1 \in S, \ deg_G(v_n)=2}} d_G(S) + 2^{k-1} \sum_{\substack{S \subseteq V(G), |S|=k \\ v_n \in S, \ deg_G(v_1)=2}} d_G(S)$$

$$= 2 \cdot 2^{k-1} \sum_{\substack{S \subseteq V(G_1), |S|=k \\ v_1 \in S}} d_G(S) = 2^k \sum_{k \le j \le n} (j-1) \binom{j-2}{k-2}$$

$$= 2^k (k-1) \sum_{k \le j \le n} \binom{j-1}{k-1} = 2^k (k-1) \binom{n}{k}.$$

We now turn our attention to compute $\sum_{\substack{S \subseteq V(G), |S|=k \\ v_1 \in S, v_n \in S}} d_G(S)$. Without loss of generality, let $S = \{u_1, u_{i_2}, \dots, u_{i_{k-1}}, u_n\}$ where $1 < i_2 < \dots < i_{k-1} < n$. Clearly, $d_G(S) = n - 1$,

and we have $\binom{n-2}{k-2}$ ways to choose $u_{i_2}, u_{i_3}, \ldots, u_{i_{k-1}}$. Therefore, we have

$$2^{k-2} \sum_{\substack{S \subseteq V(G), |S| = k \\ v_1 \in S, v_n \in S}} d_G(S) = 2^{k-2} (n-1) \binom{n-2}{k-2}.$$

Therefore, we have

$$SGut_k(G) = 2^k SW_k(G) - 2^k (k-1) \binom{n}{k} + 2^{k-2} (n-1) \binom{n-2}{k-2}$$
$$= 2^k (k-1) \binom{n+1}{k+1} - 2^k (k-1) \binom{n}{k} + 2^{k-2} (n-1) \binom{n-2}{k-2}$$
$$= 2^k (k-1) \binom{n}{k+1} + 2^{k-2} (n-1) \binom{n-2}{k-2}.$$

For k = n, the following result is immediate.

Observation 2.1 Let G be the connected graph of order n. Then

$$\operatorname{SGut}_n(G) = (n-1) \prod_{v \in V(G)} d_G(v).$$

In [21], Mao obtained the following result.

Lemma 2.1 [21] Let G be a graph. Then $sdiam_{n-1}(G) = n-2$ if and only if G is 2-connected.

We now give the expression of $SGut_{n-1}(G)$ for a graph G.

Proposition 2.3 Let G be a connected graph of order n.

(1) If G is 2-connected, then

$$\operatorname{SGut}_{n-1}(G) = (n-2) \left(\prod_{v \in V(G)} d_G(v)\right) \left(\sum_{v \in V(G)} \frac{1}{d_G(v)}\right).$$

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

$$\operatorname{SGut}_{n-1}(G) = \left(\prod_{v \in V(G)} d_G(v)\right) \left[(n-2) \left(\sum_{v \in V(G)} \frac{1}{\deg_G(v)}\right) + \left(\sum_{i=1}^p \frac{1}{\deg_G(v_i)}\right) \right]$$

where v_i $(1 \le i \le p)$ are all cut vertices of G.

Proof. (1) Since G is 2-connected, it follows from Lemma 2.1 that $d_G(S) = n - 2$ for any $S \subseteq V(G)$ and |S| = n - 1, and hence

$$\operatorname{SGut}_{n-1}(G) = (n-2) \sum_{\substack{S \subseteq V(G) \\ |S|=n-1}} \left(\prod_{v \in S} \deg_G(v) \right) = (n-2) \left(\prod_{v \in V(G)} d_G(v) \right) \left(\sum_{v \in V(G)} \frac{1}{d_G(v)} \right).$$

(2) Note that v_1, v_2, \ldots, v_p are all the cut vertices in G. For any $S \subseteq V(G)$ and |S| = n-1, if $V(G) - S = \{v_i\}$ for some i $(1 \leq i \leq p)$, then it follows from Lemma 2.1 that $d_G(S) = n-1$; if $V(G) - S \neq \{v_i\}$ for each i $(1 \leq i \leq p)$, then it follows from Lemma 2.1 that $d_G(S) = n-2$. Let $U = \{v_{p+1}, v_{p+2}, \ldots, v_n\}$ be the set of non-cut vertices. Then

$$\begin{aligned} & \text{SGut}_{n-1}(G) \\ &= (n-2) \sum_{\substack{S \subseteq V(G), |S|=n-1, \\ V(G)-S=\{v_i\}, \ p+1 \le i \le n}} \left(\prod_{v \in S} deg_G(v) \right) + (n-1) \sum_{\substack{S \subseteq V(G), |S|=n-1, \\ V(G)-S=\{v_i\}, \ 1 \le i \le p}} \left(\prod_{v \in V} deg_G(v) \right) \\ &= (n-2) \left(\prod_{v \in V(G)} d_G(v) \right) \left(\sum_{i=p+1}^n \frac{1}{deg_G(v_i)} \right) + (n-1) \left(\prod_{v \in V(G)} d_G(v) \right) \left(\sum_{i=1}^p \frac{1}{deg_G(v_i)} \right) \\ &= (n-2) \left(\prod_{v \in V(G)} d_G(v) \right) \left(\sum_{v \in V(G)} \frac{1}{deg_G(v)} \right) + \left(\prod_{v \in V(G)} d_G(v) \right) \left(\sum_{i=1}^p \frac{1}{deg_G(v_i)} \right) . \end{aligned}$$

The following corollary is immediate.

Corollary 2.2 Let T be a tree of order n. If v_1, v_2, \ldots, v_p are all the pendent vertices in T, then

$$\operatorname{SGut}_{n-1}(T) = (n-2)(n-p)\left(\prod_{i=1}^{p} \frac{1}{\deg_T(v_i)}\right) + (n-1)\left(\prod_{i=1}^{p} \frac{1}{\deg_T(v_i)}\right)\left(\sum_{i=1}^{p} \frac{1}{\deg_T(v_i)}\right).$$

3 Lower and upper bounds for general graphs

In this section, we give upper and lower bounds of $SGut_k(G)$.

3.1 Bounds in terms of degree

The following bounds are sharp for $SGut_k(G)$.

Theorem 3.1 Let G be a connected graph of order n. Then

$$\delta(G)^k SW_k(G) \le SGut_k(G) \le \Delta(G)^k SW_k(G),$$

with equality if and only if G is a regular graph.

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Proof. From the definition of Steiner degree distance, we have

$$\operatorname{SGut}_k(G) = \sum_{\substack{S \subseteq V(G) \\ |S|=k}} \left(\prod_{v \in S} deg_G(v) \right) d_G(S) \le \sum_{\substack{S \subseteq V(G) \\ |S|=k}} \Delta(G)^k d_G(S) = \Delta(G)^k SW_k(G)$$

and

$$\operatorname{SGut}_k(G) = \sum_{\substack{S \subseteq V(G) \\ |S|=k}} \left(\prod_{v \in S} \deg_G(v) \right) d_G(S) \ge \sum_{\substack{S \subseteq V(G) \\ |S|=k}} \delta(G)^k d_G(S) = \delta(G)^k SW_k(G) \,.$$

To show the sharpness of the upper and lower bounds, we consider a *r*-regular graph *G*. Then $\Delta(G) = \delta(G) = r$, and $\operatorname{SGut}_k(G) = r^k SW_k(G) = \Delta(G)^k SW_k(G) = \delta(G)^k SW_k(G)$.

Li et al. [19] obtained the following sharp bounds for $SW_k(G)$.

Lemma 3.1 [19] Let G be a connected graph of order n, and let k be an integer such that $2 \le k \le n$. Then

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

Moreover, the lower bound is sharp.

The following result can be easily seen.

Proposition 3.1 Let G be a connected graph of order n, and let k be an integer such that $2 \le k \le n$. Then

$$\delta(G)^k \binom{n}{k} (k-1) \le \operatorname{SGut}_k(G) \le \Delta(G)^k (k-1) \binom{n+1}{k+1}.$$

Moreover, the bounds are sharp.

Proof. From Theorem 3.1 and Lemma 3.1, we have

$$\operatorname{SGut}_k(G) \ge \delta(G)^k SW_k(G) \ge \delta(G)^k \binom{n}{k} (k-1).$$

Similarly, from Theorem 3.1 and Lemma 3.1, we have

$$\operatorname{SGut}_k(G) \le \Delta(G)^k SW_k(G) \le \Delta(G)^k (k-1) \binom{n+1}{k+1}$$

To show the sharpness of lower bound, we consider the complete graph K_n . Since $\delta(K_n) = n - 1$, it follows from Proposition 2.1 that

$$\operatorname{SGut}_k(K_n) = \binom{n}{k} (n-1)^k (k-1) = \delta(K_n)^k \binom{n}{k} (k-1).$$

To show the sharpness of upper bound, we consider the path P_2 . For k = 2, since $\Delta(P_2) = 1$, it follows from Proposition 2.2 that

$$\operatorname{SGut}_2(P_2) = 1 = \Delta(P_2)^k (k-1) \binom{n+1}{k+1}$$

3.2 Bounds in terms of order and size

For graph G having n vertices and m edges, we have the following upper and lower bounds of $SGut_k(G)$.

Theorem 3.2 Let G be a connected graph n vertices and m edges, and let k be an integer with $2 \le k \le n$. Then

$$(n-1)\left(\frac{2m}{k}\right)^k \binom{n-1}{k-1}^k \ge \operatorname{SGut}_k(G) \ge \begin{cases} 2m(k-1)\binom{n-1}{k-1} & \text{if } \delta(G) \ge 2\\ (k-1)\binom{n}{k} & \text{if } \delta(G) = 1 \end{cases}$$

Moreover, the upper and lower bounds are sharp.

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

$$(k-1)\sum_{\substack{S\subseteq V(G)\\|S|=k}} \left(\prod_{v\in S} deg_G(v)\right) \leq \mathrm{SGut}_k(G) \leq (n-1)\sum_{\substack{S\subseteq V(G)\\|S|=k}} \left(\prod_{v\in S} deg_G(v)\right)\,.$$

Let

$$M = \sum_{\substack{S \subseteq V(G) \\ |S|=k}} \left(\prod_{v \in S} deg_G(v) \right) = \sum_{\{v_1, v_2, \dots, v_k\} \subseteq V(G)} deg_G(v_1) deg_G(v_2) \dots deg_G(v_k).$$

and

$$N = \sum_{\{v_1, v_2, \dots, v_k\} \subseteq V(G)} [deg_G(v_1) + deg_G(v_2) + \dots + deg_G(v_k)]$$

Since

$$deg_G(v_1)deg_G(v_2)\dots deg_G(v_k) \le \frac{1}{k^k}[deg_G(v_1) + deg_G(v_2) + \dots + deg_G(v_k)]^k$$

it follows that

$$\begin{split} M &= \sum_{\{v_1, v_2, \dots, v_k\} \subseteq V(G)} deg_G(v_1) deg_G(v_2) \dots deg_G(v_k) \\ &\leq \frac{1}{k^k} \sum_{\{v_1, v_2, \dots, v_k\} \subseteq V(G)} [deg_G(v_1) + deg_G(v_2) + \dots + deg_G(v_k)]^k \\ &\leq \frac{1}{k^k} \left[\sum_{\{v_1, v_2, \dots, v_k\} \subseteq V(G)} (deg_G(v_1) + deg_G(v_2) + \dots + deg_G(v_k)) \right]^k \\ &\leq \frac{1}{k^k} N^k \,. \end{split}$$

For each $v \in V(G)$, there are $\binom{n-1}{k-1}$ k-subsets in G such that each of them contains v. The contribution of vertex v is exactly $\binom{n-1}{k-1} deg_G(v)$. From the arbitrariness of v, we have

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

and hence

$$\operatorname{SGut}_k(G) \le (n-1)M \le (n-1)\frac{1}{k^k}N^k \le \left(\frac{2m}{k}\right)^k \binom{n-1}{k-1}^k (n-1)^k$$

If $\delta(G) \ge 2$, then $deg_G(v_1)deg_G(v_2)\dots deg_G(v_k) \ge deg_G(v_1) + deg_G(v_2) + \dots + deg_G(v_k)$, and hence

$$\begin{aligned} \text{SGut}_k(G) &\geq (k-1) \sum_{\{v_1, v_2, \dots, v_k\} \subseteq V(G)} deg_G(v_1) deg_G(v_2) \dots deg_G(v_k) \\ &\geq (k-1) \sum_{\{v_1, v_2, \dots, v_k\} \subseteq V(G)} [deg_G(v_1) + deg_G(v_2) + \dots + deg_G(v_k)] \\ &= (k-1)N \\ &= 2m(k-1) \binom{n-1}{k-1}. \end{aligned}$$

If $\delta(G) = 1$, then

$$\operatorname{SGut}_k(G) \ge (k-1) \sum_{\{v_1, v_2, \dots, v_k\} \subseteq V(G)} \deg_G(v_1) \deg_G(v_2) \dots \deg_G(v_k) \ge (k-1) \binom{n}{k}.$$

To show the sharpness of the lower bound for $\delta = 1$ and the upper bound, we let $G = P_2$. For k = 2, we have

$$(n-1)\left(\frac{2m}{k}\right)^k \binom{n-1}{k-1}^k = 1 = \mathrm{SGut}_k(P_2) = (k-1)\binom{n}{k}.$$

To show the sharpness of the lower bound for $\delta \geq 2$, we let $G = C_3$. For k = 2, we have

$$\operatorname{SGut}_k(C_3) = 12 = 2m(k-1)\binom{n-1}{k-1}.$$

3.3 Bounds in terms of order

In this subsection we prove that the complete graph K_n gives the maximum Steiner Gutman k-index of graphs.

Theorem 3.1 Let G be a connected graph of order n. If there is a positive integer k > 0.618n, then

$$\operatorname{SGut}_k(G) \le \binom{n}{k}(n-1)^k(k-1)$$
 (1)

with equality holding if and only if $G \cong K_n$.

Proof. We have

$$k > 0.618(n-1) > \frac{\left(\sqrt{5}-1\right)(n-1)}{2} > \frac{-(n-1) + \sqrt{(n-1)^2 + 4(n^2 - 2n)}}{2}$$

that is,

$$(2k + n - 1)^{2} > (n - 1)^{2} + 4(n^{2} - 2n),$$

that is,

$$\frac{n+1}{k+1} < 1 + \frac{k}{n-2} < \left(1 + \frac{1}{n-2}\right)^k = \left(\frac{n-1}{n-2}\right)^k.$$
(2)

Again since k > 0.618(n-1), then one can easily see that

$$k(k-1) \ge n-2$$
, that is, $\left(\frac{n-1}{n-2}\right)^k > 1 + \frac{k}{n-2} \ge \frac{k}{k-1}$.

From the above, we get

$$(n-1)^{k} (k-1) > (n-2)^{k} k.$$
(3)

First we assume that $\Delta = n - 1$. If $G \cong K_n$, then by Proposition 2.1, the equality holds in (1). Otherwise, $G \ncong K_n$. For any $S \subseteq V(G)$ and |S| = k, without loss of generality, we let $S = \{u_1, u_2, \ldots, u_k\}$. Since $\Delta = n - 1$, we have two possibilities: (i) $deg_G(u_i) = n - 1$, $u_i \in S$ and (ii) $deg_G(u_i) \leq n - 2$, for any $u_i \in S$.

 $Case(i): deg_G(u_i) = n - 1, u_i \in S$. In this case the tree T induced by the edges in $\{u_i u_1, u_i u_2, \ldots, u_i u_{i-1}, u_i u_{i+1}, \ldots, u_i u_k\}$ is a Steiner tree connecting S, which implies

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 $d(S) \leq k-1$. Since |S| = k, it follows that $d_G(S) \geq k-1$. Therefore, $d_G(S) = k-1$. For each $v \in V(G)$, we have $deg_G(v) \leq n-1$. Thus we have

$$\left(\prod_{v\in S} deg_G(v)\right) d_G(S) \le (n-1)^k (k-1)$$

with equality holding if and only if $deg_G(v) = n - 1$ for any $v \in S$.

 $Case(ii): deg_G(u_i) \leq n-2$, for any $u_i \in S$. Let w be a vertex of degree n-1 as $\Delta = n-1$. In this case the tree T induced by the edges in $\{wu_1, wu_2, \ldots, wu_k\}$ is a Steiner tree connecting S. One can easily see that d(S) = k. For each $v \in S$, we have $deg_G(v) \leq n-2$. Thus we have

$$\left(\prod_{v\in S} deg_G(v)\right) d_G(S) \le (n-2)^k k$$

with equality holding if and only if $deg_G(v) = n - 2$ for any $v \in S$.

Since $G \ncong K_n$, using (3) with the above results, we get

$$\operatorname{SGut}_k(G) = \sum_{\substack{S \subseteq V(G) \\ |S|=k}} \left(\prod_{v \in S} \deg_G(v) \right) d_G(S) < \binom{n}{k} (n-1)^k (k-1) \,.$$

Next we assume that $\Delta \leq n-2$. By (2), we have

$$\frac{n+1}{k+1} < \left(\frac{n-1}{n-2}\right)^k \le \left(\frac{n-1}{\Delta}\right)^k \,.$$

From Proposition 3.1 with the above result, we have

$$\operatorname{SGut}_k(G) < \frac{k+1}{n+1} (n-1)^k (k-1) \binom{n+1}{k+1} = \binom{n}{k} (k-1) (n-1)^k.$$

4 Comparison between SDD_k and $SGut_k$ of graphs

In this section we compare between SDD_k and $SGut_k$ of graphs.

Example 1 Let S_n be the star of order $n \ (n \ge 3)$, and let k be an integer such that $2 \le k \le n$. Then

$$\operatorname{SGut}_k(S_n) = (kn - 2k + 1) \binom{n-1}{k-1}.$$

Example 2 [23] Let S_n be the star of order n. Then

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

Proposition 4.1 Let G be a connected graph of order n with minimum degree δ , and let k be an integer with $3 \le k \le n$. Let r be the number of the pendant vertices in G. (1) If $\delta(G) \ge 2$, then

$$\mathrm{SDD}_k(G) \leq \mathrm{SGut}_k(G).$$

(2) If $\delta(G) = 1$, $r + 3 \le k$ and $2^{k-r} \ge 2(k - r) + r$, then

 $\mathrm{SDD}_k(G) \leq \mathrm{SGut}_k(G).$

(3) If $\delta(G) = 1$, and r = n - 1, then

$$SDD_k(G) > SGut_k(G).$$

Proof. (1) For any $S \subseteq V(G)$ and |S| = k, we let $S = \{v_1, v_2, \ldots, v_k\}$. Let $deg_G(v_i) = x_i$ for $i \ (1 \le i \le k)$. To show $SDD_k(G) \le SGut_k(G)$, from the arbitrariness of S and the definitions, it suffices to show that $\prod_{i=1}^k x_i \ge \sum_{i=1}^k x_i$. Let $f(x_1, x_2, \ldots, x_k) = x_1 x_2 \ldots x_k - (x_1 + x_2 + \ldots + x_k)$. Since $\delta(G) \ge 2$, it follows that $x_i \ge 2$ for each $i \ (1 \le i \le k)$, and hence

$$\frac{\partial f}{\partial x_i} = x_1 x_2 \dots x_{i-1} x_{i+1} \dots x_k - 1 > 0$$

Therefore, $f(x_1, x_2, \dots, x_k)$ is a monotone increasing function. Clearly, $f(x_1, x_2, \dots, x_k) \ge f(2, 2, \dots, 2) = 2^k - 2k \ge 0$. So, we have $\text{SDD}_k(G) \le \text{SGut}_k(G)$.

(2) For any $S \subseteq V(G)$ and |S| = k, we let $S = \{v_1, v_2, \ldots, v_k\}$. Let $deg_G(v_i) = x_i$ for $i \ (1 \leq i \leq k)$. To show $SDD_k(G) \leq SGut_k(G)$, from the arbitrariness of S and the definitions, it suffices to show that $\prod_{i=1}^k x_i \geq \sum_{i=1}^k x_i$. Since there are $r \geq 1$ pendant vertices in G, we can assume that $x_1 = x_2 = \ldots = x_r = 1$. Then $x_i \geq 2$ for each $i \ (r+1 \leq i \leq k)$. Let $f(x_{r+1}, x_{r+2}, \ldots, x_k) = x_{r+1}x_{r+2} \ldots x_k - (x_{r+1} + x_{r+2} + \ldots + x_k) - r$. Then

$$\frac{\partial f}{\partial x_i} = x_{r+1}x_{r+2}\dots x_{i-1}x_{i+1}\dots x_k - 1 > 0.$$

Therefore, $f(x_{r+1}, x_{r+2}, \ldots, x_k)$ is monotone increasing. Clearly, $f(x_{r+1}, x_{r+2}, \ldots, x_k) \ge f(2, 2, \ldots, 2) = 2^{k-r} - 2(k-r) - r \ge 0$ as $2^{k-r} \ge 2(k-r) + r$. Therefore we have $\text{SDD}_k(G) \le \text{SGut}_k(G)$.

(3) If $\delta(G) = 1$ and r = n - 1, then $G = K_{1,n-1}$ is a star of order n. From Examples 1 and 2, we have $\text{SDD}_k(G) > \text{SGut}_k(G)$.

Proposition 4.2 Let G be a connected graph of order n with maximum degree Δ , and let k be an integer with $2 \le k \le n$.

(1) If $\Delta(G) \leq k-1$, then

$$\mathrm{SDD}_k(G) \leq \mathrm{SGut}_k(K_n).$$

(2) If $\Delta(G) = n - 1$, then

$$\mathrm{SDD}_k(G) \leq \mathrm{SGut}_k(K_n).$$

Proof. (1) For any $S \subseteq V(G)$ and |S| = k, since $\Delta(G) \le k - 1$, we have

$$\left[\sum_{v \in S} deg_G(v)\right] d_G(S) \le (k-1)^k d_G(S) \le (k-1)^k (n-1).$$

For this S in complete graph K_n ,

$$\left[\prod_{v\in S} deg_{K_n}(v)\right] d_{K_n}(S) = (n-1)^k (k-1).$$

Since $k \leq n$, it follows that $(k-1)^k(n-1) \leq (n-1)^k(k-1)$. From the arbitrariness of S, we have $\text{SDD}_k(G) \leq \text{SGut}_k(K_n)$.

(2) If $\Delta(G) = n - 1$, then there exists a vertex v such that $deg_G(v) = n - 1$. For any $S \subseteq V(G)$ and |S| = k, we have $v \in S$ or $v \notin S$. If $v \in S$, then $d_G(S) = k - 1$, and hence

$$\left[\sum_{v \in S} deg_G(v)\right] d_G(S) \le (n-1)^k (k-1).$$

From the arbitrariness of S, we have $\text{SDD}_k(G) \leq \text{SGut}_k(K_n)$.

If $v \notin S$, then $d_G(S) = k - 1$ or $d_G(S) = k$. If $d_G(S) = k - 1$, then it is true as the case $v \in S$. If $d_G(S) = k$, then G[S] is not connected, and there is at most one vertex of degree k - 2 in G[S]. Therefore, there are at most two vertices in S of degree less than or equal to n - 2 and all the other vertices in S are of degree at most n - 3. Then

$$\left[\sum_{v \in S} deg_G(v)\right] d_G(S) \le [(n-3)^{k-2} + 2(n-2)]k$$

It suffices to show that $[(n-3)^{k-2} + 2(n-2)]k \le (n-1)^k(k-1)$, that is,

$$\frac{k}{n-1} \left[\frac{(n-3)^{k-2}}{(n-1)^{k-1}} + \frac{2(n-2)}{(n-1)^{k-1}} \right] \le \frac{(n-3)^{k-2}}{(n-1)^{k-1}} + \frac{2(n-2)}{(n-1)^{k-1}} \le k-1.$$
(4)

One can easily see that (4) is true for $3 \le k \le n-1$. For k = n, one can easily prove that the result holds as $d_G(S) = n - 1$. For k = 2, we have

$$\left[\sum_{v \in S} deg_G(v)\right] d_G(S) \le 4(n-2) \le (n-1)^2$$

as $n \geq 3$. This completes the proof of the result.

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