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Steiner Distance in Chemical Graph Theory*

Yaping Mao[a,†], **Boris Furtula**[b,†]

[a]*School of Mathematics and Statistis, Qinghai Normal University,*
Xining, Qinghai 810008, China
`maoyaping@ymail.com`

[b]*Faculty of Science, University of Kragujevac, P. O. Box 60,*
34000 Kragujevac, Serbia
`furtula@kg.ac.rs`

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Abstract

Steiner distance $d_G(S)$ is a natural generalization of the concept of distance in a graph. For a connected graph G of order at least 2 and $S \subseteq V(G)$, $d_G(S)$ is equal to the minimum size among all connected subgraphs whose vertex sets are equal to the set S. Here, the known results on the Steiner distance parameters used in chemical graph theory such as Steiner Wiener index, Steiner degree distance, Steiner Harary index, Steiner Gutman index, Steiner hyper–Wiener index, and Steiner Hosoya polynomial are surveyed. Additionally, some conjectures and open problems are listed.

1 Introduction

All graphs in this paper are undirected, finite and simple. Definitions of graph theoretical notations and terminology, used in this survey, can be found in [7]. For a graph G, let

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†Corresponding author.

$V(G)$, $E(G)$, $e(G)$, and $\overline{G}$ denote set of vertices, set of edges, the size of G, and the complement of G, respectively. The *degree*, $deg_G(v)$, of a vertex v is equal to the number of incident edges. The *minimum degree* of G, $\delta(G)$, is the smallest degree of all vertex degrees in a graph G and the *maximum degree*, $\Delta(G)$, is the largest of all vertex degrees in G. For any subset X of $V(G)$, let $G[X]$ denote the subgraph induced by X; similarly, for any subset F of $E(G)$, let $G[F]$ denote the subgraph induced by F. We use $G \setminus X$ to denote the subgraph of G obtained by removing all the vertices of X together with the edges incident to them from G; similarly, we use $G \setminus F$ to denote the subgraph of G obtained by removing all the edges of F from G. Let K_n, P_n and C_n be the complete graph, the path, and the cycle of order n, respectively. The *connectivity*, $\kappa(G)$, of G is defined as the minimum number of vertices which deletion turns G into a disconnected or a trivial graph.

Let $f(G)$ be a graph invariant and n a positive integer, such that $n \geq 2$. The *Nordhaus–Gaddum problem* is to determine sharp bounds for $f(G)+f(\overline{G})$ and $f(G)\cdot f(\overline{G})$ for all graphs of order n, and to characterize the extremal graphs, i.e., graphs that achieve the bounds. Nordhaus–Gaddum type relations have received wide attention; see the recent survey [3] and book chapter [49].

The join, Cartesian product, lexicographic product, corona, and cluster are defined as follows.

> The *join* or *complete product* of two disjoint graphs G and H, denoted by $G \vee H$, is the graph with vertex set $V(G) \cup V(H)$ and edge set $E(G) \cup E(H) \cup \{uv \,|\, u \in V(G), v \in V(H)\}$.
>
> The *Cartesian product* of two graphs G and H, written as $G \Box H$, is the graph with vertex set $V(G) \times V(H)$, in which two vertices (u, v) and (u', v') are adjacent if and only if $u = u'$ and $(v, v') \in E(H)$, or $v = v'$ and $(u, u') \in E(G)$.
>
> The *lexicographic product* of two graphs G and H, written as $G \circ H$, is defined as follows: $V(G \circ H) = V(G) \times V(H)$, and two distinct vertices (u, v) and (u', v') of $G \circ H$ are adjacent if and only if either $(u, u') \in E(G)$ or $u = u'$ and $(v, v') \in E(H)$.
>
> The *corona* $G * H$ is obtained by taking one copy of G and $|V(G)|$ copies of H, and by joining each vertex of the i-th copy of H with the i-th vertex of G, where

$i = 1, 2, \ldots, |V(G)|$.

The *cluster* $G \odot H$ is obtained by taking one copy of G and $|V(G)|$ copies of a rooted graph H, and by identifying the root of the i-th copy of H with the i-th vertex of G, where $i = 1, 2, \ldots, |V(G)|$.

1.1 Classical distance parameters

Distance is one of the most basic concepts in the field of graph theory. If G is a connected graph and $u, v \in V(G)$, then the *distance* $d_G(u,v)$ between u and v is the length of a shortest path that connects these vertices. If v is a vertex of a connected graph G, then the *eccentricity* $e(v)$ of v is defined by $e(v) = \max\{d_G(u,v) \mid u \in V(G)\}$. Furthermore, the *radius* and *diameter* of G are defined by $\mathrm{rad}(G) = \min\{e(v) \mid v \in V(G)\}$ and $\mathrm{diam}(G) = \max\{e(v) \mid v \in V(G)\}$. These last two concepts are related by the following inequalities $\mathrm{rad}(G) \leq \mathrm{diam}(G) \leq 2\mathrm{rad}(G)$ (for more information on this topic see [27]).

1.2 Steiner distance

The distance between two vertices u and v in a connected graph G also equals the minimum size of a connected subgraph of G containing both u and v. Such a view invokes a generalization of a concept of distance. Chartrand et al. introduced such a generalization of a graph distance in 1989. They named it the *Steiner distance* of a graph [10]. 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 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* $d_G(S)$ among the vertices of S (or simply the distance of S) is the minimum size among all connected subgraphs whose vertex sets 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. Observe that $d_G(S) = \min\{e(T) \mid S \subseteq V(T)\}$, where T is subtree of G. Furthermore, if $S = \{u, v\}$, then $d_G(S) = d(u,v)$ is the classical distance between u and v. Set $d_G(S) = \infty$ when there is no S-Steiner tree in G.

Observation 1.1. *Let G be a graph of order n and k be an integer with $2 \leq k \leq n$. If $S \subseteq V(G)$ and $|S| = k$, then $d_G(S) \geq k - 1$.*

The problem of finding the Steiner distance of a set of vertices is called the *Steiner problem* and is NP-complete (see [24]). Steiner trees are well-known for their combinatorial optimization aspects and applications to network design and transportation.

1.3 Steiner eccentricity, Steiner diameter, and Steiner radius

Let n and k be two integers with the following property $2 \leq k \leq n$. The *Steiner k-eccentricity* $e_k(v)$ of a vertex v of G is defined by $e_k(v) = \max\{d(S) \mid S \subseteq V(G), |S| = k, \text{ and } v \in S\}$. The *Steiner k-radius* of G is $\mathrm{srad}_k(G) = \min\{e_k(v) \mid v \in V(G)\}$, while the *Steiner k-diameter* of G is $\mathrm{sdiam}_k(G) = \max\{e_k(v) \mid v \in V(G)\}$. Note for every connected graph G that $e_2(v) = e(v)$ for all vertices v of G and that $\mathrm{srad}_2(G) = \mathrm{rad}(G)$ and $\mathrm{sdiam}_2(G) = \mathrm{diam}(G)$.

Table 1 Classical distance parameters and Steiner distance parameters.

Distance	**Steiner distance**
$\left\{\begin{array}{l} d_G(u,v) = \min\{e(P) \mid \{u,v\} \subseteq V(P)\}, \\ \text{where } P \text{ is subpath of } G. \end{array}\right.$	$\left\{\begin{array}{l} d_G(S) = \min\{e(T) \mid S \subseteq V(T)\}, \\ \text{where } T \text{ is subtree of } G. \end{array}\right.$
Eccentricity	**Steiner k-eccentricity**
$e(v) = \max\{d_G(u,v) \mid u \in V(G)\}$	$e_k(v) = \max\{d(S) \mid S \subseteq V(G),$ $\vert S\vert = k, \text{ and } v \in S\}$
Diameter	**Steiner k-diameter**
$\mathrm{diam}(G) = \max\{e(v) \mid v \in V(G)\}$	$\mathrm{sdiam}_k(G) = \max\{e_k(v) \mid v \in V(G)\}$
Radius	**Steiner k-radius**
$\mathrm{rad}(G) = \min\{e(v) \mid v \in V(G)\}$	$\mathrm{srad}_k(G) = \min\{e_k(v) \mid v \in V(G)\}$

1.4 k-diameter

Let G be a k-connected graph, and let u, v be any pair of vertices of G. Let $P_k(u,v)$ be a family of k inner vertex-disjoint paths between u and v, i.e., $P_k(u,v) = \{P_1, P_2, \cdots, P_k\}$, where $p_1 \leq p_2 \leq \cdots \leq p_k$ and p_i denotes the number of edges of path P_i. The *k-distance* $d_k(u,v)$ between vertices u and v is the minimum p_k among all $P_k(u,v)$ and the *k-diameter* $d_k(G)$ of G is defined as the maximum k-distance $d_k(u,v)$ over all pairs u,v of vertices of G. The concept of k-diameter emerges rather naturally when one looks at the performance of routing algorithms. Its applications to network routing in distributed and parallel processing are studied and discussed by various authors including Chung [11], Hsu [36, 37], Meyer and Pradhan [61].

1.5 Three Steiner distance parameters

The *center* $C(G)$ of a connected graph G is the subgraph induced by the vertices of a graph G whose eccentricities are equal to the graph radius. The *Steiner k-center* $C_k(G)$ $(k \geq 2)$ of a connected graph G is the subgraph induced by the vertices of a graph G, each having the property that $e_k(v_i) = \mathrm{srad}_k(G)$. Hence, the Steiner 2-center of a graph is simply its center. The *Steiner k-median* of G is the subgraph of G induced by the vertices of minimum Steiner k-distance in G.

Kubicka et al. [40] defined the *Steiner interval*, $I_G(S)$ or $I(S)$, of a set S by

$$I_G(S) = \{w \in V(G) \,|\, w \text{ lies on a Steiner tree for } S \text{ in } G\}.$$

Thus if $|S| = 2$, then the Steiner interval of S is the interval between the two vertices of S.

Day et al. [17] introduced the concept of k-Steiner distance hereditary. A connected graph G is defined to be *k-Steiner distance hereditary* where $k \geq 2$, if for every connected induced subgraph H of G of order at least k and a set S of k vertices of H, $d_H(S) = d_G(S)$. Thus, the 2-Steiner distance hereditary graphs is the distance hereditary graph.

Goddard et al. [28] introduced the concept of Steiner distance stable graphs. We assume that k, ℓ, s and m are nonnegative integers such that $m \geq s \geq 2$ and $k, \ell \neq 0$. If S is a set of s vertices in a connected graph G such that $d_G(S) = m$, then S is called an *(s,m)-set*. A connected graph G is said to be *k-vertex ℓ-edge (s,m)-Steiner distance stable* if, for every (s,m)-set S of G and every set A consisting of at most k vertices of $G - S$ and at most ℓ edges of G, $d_{G-A}(S) = d_G(S)$. Thus, k-vertex ℓ-edge $(2,m)$-Steiner distance stable graphs are the $(k, \ell, \{m\})$-stable graphs.

1.6 Average Steiner distance

Let $G = (V,E)$ be a connected graph of order n. The *average distance* of G, $\mu(G)$, is defined to be the average of all distances between pairs of vertices in G, i.e.

$$\mu(G) = \binom{n}{2}^{-1} \sum_{\{u,v\} \subseteq V(G)} d_G(u,v).$$

where $d_G(u,v)$ denotes the length of a shortest u-v path in G. This parameter, introduced in architecture turned out to be a good measure for analyzing transportation networks. It indicates the average time required to transport a commodity between two destinations rather than the maximum time required, as is indicated by the diameter; see [16].

The *average Steiner distance* $\mu_k(G)$ of a graph G, introduced by Dankelmann et al. in [15], is defined as the average of the Steiner distances of all k-subsets of $V(G)$, i.e.

$$\mu_k(G) = \binom{n}{k}^{-1} \sum_{S\subseteq V(G),\ |S|=k} d_G(S).$$

If G represents a network, then the average Steiner k-distance indicates the expected number of communication links needed to connect k processors.

1.7 Steiner distance parameters in chemical graph theory

In [42], Li et al. proposed a generalization of the Wiener index using the Steiner distance. Thus, the *k-th Steiner Wiener index* $\mathrm{SW}_k(G)$ of a connected graph G is defined by

$$\mathrm{SW}_k(G) = \sum_{\substack{S\subseteq V(G)\\ |S|=k}} d_G(S)\,. \tag{1}$$

If $|V(G)| = n$, then $2 \leq k \leq n$. For $k = 2$, the Steiner Wiener index coincides with the ordinary Wiener index. It is usual to consider SW_k for $2 \leq k \leq n-1$, but the above definition implies $\mathrm{SW}_1(G) = 0$ and $\mathrm{SW}_n(G) = n-1$ for a connected graph G of order n. It should be noted that the average Steiner distance is related to the Steiner Wiener index via $\mathrm{SW}_k(G)/\binom{n}{k}$, that is,

$$\mathrm{SW}_k(G) = \sum_{S\subseteq V(G),\ |S|=k} d_G(S) = k^{-1} \sum_{v\in V(G)} d_k(v,G) = \binom{n}{k}\mu_k(G).$$

For more details on Steiner Wiener index, we refer to [31, 39, 42, 43, 57, 59, 60].

Gutman [29] devised an analogous generalization of the concept of degree distance, Eq. (2). Thus, the *k-center Steiner degree distance* $\mathrm{SDD}_k(G)$ is defined as

$$\mathrm{SDD}_k(G) = \sum_{\substack{S\subseteq V(G)\\ |S|=k}} \left[\sum_{v\in S} deg_G(v)\right] d_G(S)\ . \tag{2}$$

For more details see [29, 58].

Furtula et al. [23] introduced the Steiner Harary index. The *Steiner Harary k-index* or *k-center Steiner Harary index* $\mathrm{SH}_k(G)$ of G is defined as

$$\mathrm{SH}_k(G) = \sum_{\substack{S\subseteq V(G)\\ |S|=k}} \frac{1}{d_G(S)} \, . \tag{3}$$

More on the Steiner Harary index can be found in [23, 50].

Mao and Das [53] generalized the Gutman index. The *Steiner Gutman k-index* $\mathrm{SGut}_k(G)$ of G is defined by

$$\mathrm{SGut}_k(G) = \sum_{\substack{S\subseteq V(G)\\ |S|=k}} \left(\prod_{v\in S} deg_G(v)\right) d_G(S) \, . \tag{4}$$

Tratnik [74] generalized the hyper-Wiener index and the Hosoya polynomial. The *Steiner k-hyper-Wiener index* of G, denoted by $\mathrm{SWW}_k(G)$, is defined as

$$\mathrm{SWW}_k(G) = \frac{1}{2} \sum_{\substack{S\subseteq V(G)\\ |S|=k}} d_G(S) + \frac{1}{2} \sum_{\substack{S\subseteq V(G)\\ |S|=k}} d_G(S)^2, \tag{5}$$

and the *Steiner k-Hosoya polynomial* of G, denoted by $\mathrm{SH}_k(G,x)$ is defined as

$$\mathrm{SH}_k(G,x) = \sum_{m\geq 0} d_k(G,m)x^m,$$

where $d_k(G,m)$ denotes the number of subsets $S \subseteq V(G)$ with $|S| = k$ and $d_G(S) = m$.

The distance based topological invariants and their Steiner-distance-based generalizations are shown in the Table 2.

Table 2 Five distance parameters and their generalizations.

Wiener index	**Steiner Wiener index**
$\mathrm{W}(G) = \sum_{\{u,v\}\subseteq V(G)} d_G(u,v)$	$\mathrm{SW}_k(G) = \sum_{\substack{S\subseteq V(G)\\ \lvert S\rvert=k}} d_G(S)$
Harary index	**Steiner Harary index**
$\mathrm{H}(G) = \sum_{\{u,v\}\subseteq V(G)} \frac{1}{d_G(u,v)}$	$\mathrm{SH}_k(G) = \sum_{\substack{S\subseteq V(G)\\ \lvert S\rvert=k}} \frac{1}{d_G(S)}$
Degree distance	**Steiner degree distance**
$\mathrm{DD}(G) = \sum_{\{u,v\}\subseteq V(G)} [deg_G(u) + deg_G(v)] d_G(u,v)$	$\mathrm{SDD}_k(G) = \sum_{\substack{S\subseteq V(G)\\ \lvert S\rvert=k}} \left[\sum_{v\in S} deg_G(v)\right] d_G(S)$
Gutman index	**Steiner Gutman index**
$\mathrm{SGut}(G) = \sum_{\{u,v\}\subseteq V(G)} [deg_G(u) deg_G(v)] d_G(u,v)$	$\mathrm{SGut}_k(G) = \sum_{\substack{S\subseteq V(G)\\ \lvert S\rvert=k}} \left[\prod_{v\in S} deg_G(v)\right] d_G(S)$
Hyper-Wiener index	**Steiner hyper-Wiener index**
$\mathrm{WW}(G) = \frac{1}{2} \sum_{\{u,v\}\subseteq V(G)} [d_G(u,v) + d_G(u,v)^2]$	$\mathrm{SWW}_k(G) = \frac{1}{2} \sum_{\substack{S\subseteq V(G)\\ \lvert S\rvert=k}} [d_G(S) + d_G(S)^2]$

Let $e = uv$ be an edge of a graph G. Let $N_u(e|G)$ be the set of vertices of G which are closer to u than to v and let $N_v(e|G)$ be set of those vertices which are closer to v than to u. The set of those vertices which have equal distance from v and u is denoted by $N_0(e|G)$. More formally,

$$N_u(e|G) = \{w \in V(G) : \ d_G(w,u) < d_G(w,v)\},$$

$$N_v(e|G) = \{w \in V(G) : \ d_G(w,v) < d_G(w,u)\}$$

and

$$N_0(e|G) = \{w \in V(G) : \ d_G(w,u) = d_G(w,v)\}.$$

Let $n_u(e) = |N_u(e|G)|$, $n_v(e) = |N_v(e|G)|$ and $n_0(e) = |N_0(e|G)|$. Then the *Szeged index* of a graph G, denoted by $Sz(G)$, is defined as

$$Sz(G) = \sum_{e=uv\in E(G)} n_u(e)n_v(e),$$

and the *revised Szeged index* of a graph G, denoted by $rSz(G)$, is defined as

$$rSz(G) = \sum_{e=uv\in E(G)} (n_u(e) + n_0(e)/2)(n_v(e) + n_0(e)/2).$$

Let G be a connected graph and e an edge of G. For a positive integer k, using the concept of the Steiner distance, the following three sets of vertices of a graph G can be defined:

$$N_u(e;k) = \{S' \subseteq V(G), |S'| = k-1 \,|\, d_G(S' \cup \{u\}) < d_G(S' \cup \{v\}), \ u \notin S', \ v \notin S'\},$$

$$N_v(e;k) = \{S' \subseteq V(G), |S'| = k-1 \,|\, d_G(S' \cup \{v\}) < d_G(S' \cup \{u\}), \ v \notin S', \ u \notin S'\},$$

and

$$N_0(e;k) = \{S' \subseteq V(G), |S'| = k-1 \,|\, d_G(S' \cup \{u\}) = d_G(S' \cup \{v\}), \ u \notin S', \ v \notin S'\}.$$

Let $n_u(e;k) = |N_u(e;k)|$, $n_v(e;k) = |N_v(e;k)|$ and $n_0(e;k) = |N_0(e;k)|$. Ghorbani et al. [25] defined the *k-Steiner Szeged index* of a graph G:

$$\mathrm{Sz}_k(G) = \sum_{e=uv\in E(G)} [n_u(e;k)+1][n_v(e;k)+1].$$

Analogously, the *k-Steiner revised Szeged index* of a graph G is defined as

$$r\mathrm{Sz}_k(G) = \sum_{e=uv\in E(G)} [n_u(e;k) + n_0(e;k)/2 + 1][n_v(e;k) + n_0(e;k)/2 + 1].$$

Here, one may note that the formula of the $\mathrm{Sz}_k(G)$ does not follow the formula of the classical Szeged index. If $k = 2$, then

$$N_u(e;2) = \{w \in V(G) \,|\, d_G(u,w) < d_G(v,w),\ u \neq w, v \neq w\}.$$

It is obvious that $N_u(e;2) \neq N_u$, since $u \neq w$. By the definition of $\mathrm{Sz}_k(G)$, the classical Szeged index $Sz(G)$ can be written as

$$\mathrm{Sz}(G) = \mathrm{Sz}_2(G) = \sum_{e=uv\in E(G)} (n_u(e;2) + 1)(n_v(e;2) + 1),$$

where $N_u(e;2) = \{w \in V(G) \,|\, d_G(u,w) < d_G(v,w),\ u \neq w\}$ and $N_v(e;2) = \{w \in V(G) \,|\, d_G(v,w) < d_G(u,w),\ u \neq w\}$.

The above approach to the definition of the Szeged index reveals that the Steiner Szeged index is its natural generalization. The same also applies to the the revised Szeged index.

2 Average Steiner distance and Steiner Wiener index

It was already shown that the average Steiner distance is related to the Steiner Wiener index. The following results are proved in Dankelmann et al. [15], Li et al. [42, 43], and Li and Zhang [44].

Proposition 2.1. [15, 42, 43, 44] *Let k and n be two integers such that $2 \leq k \leq n$.*

(1) For a complete graph K_n, $\mathrm{SW}_k(K_n) = \binom{n}{k}(k-1)$.

(2) For a path P_n, $\mathrm{SW}_k(P_n) = (k-1)\binom{n+1}{k+1}$.

(3) For a star S_n, $\mathrm{SW}_k(S_n) = \binom{n-1}{k-1}(n-1)$.

(4) For a complete bipartite graph $K_{a,b}$ $(2 \leq k \leq a+b)$,

$$\mathrm{SW}_k(K_{a,b}) = \begin{cases} (k-1)\binom{a+b}{k} + \binom{a}{k} + \binom{b}{k}, & \text{if } 1 \leq k \leq a; \\ (k-1)\binom{a+b}{k} + \binom{b}{k}, & \text{if } a < k \leq b; \\ (k-1)\binom{a+b}{k}, & \text{if } b < k \leq a+b. \end{cases}$$

(5) Let T be a tree of order n, possessing p pendent vertices. Let q be the number of vertices of degree 2 in T that are adjacent to a pendent vertex. Then

$$\mathrm{SW}_{n-2}(T) = \frac{1}{2}(n^3 - 2n^2 + n - 2np + 2p - 2q).$$

(6) Let T be a graph obtained from a path P_t and a star S_{n-t+1} by identifying a pendant vertex of P_t and the center v of S_{n-t+1}, where $1 \le t \le n-1$ and $k \le n$. Then

$$\mathrm{SW}_k(T) = t\binom{n-1}{k} - \binom{t}{k+1} - \binom{n}{k+1} + \binom{n-t+1}{k+1} + (k-1)\binom{n}{k}.$$

(7) Let G be a graph obtained from a clique K_{n-r} and a star S_{r+1} by identifying a vertex of K_{n-r} and the center v of S_{r+1}. For $k \le r \le n-1-k$,

$$\mathrm{SW}_k(G) = (n-1)\binom{n-1}{k-1} - \binom{n-r-1}{k}.$$

(8) For a cycle C_n,

$$\mathrm{SW}_k(C_n) = \frac{n}{k}\sum_{x \in X_k}(n - 1 - \max\{x_0, \ldots, x_{k-1}\}).$$

(9) For a wheel W_n,

$$\mathrm{SW}_k(W_n) = \begin{cases} n-1, & \text{if } k = n; \\ n(n-2), & \text{if } k = n-1; \\ k\binom{n}{k} - n + 1 - \binom{n-1}{k-1}, & \text{if } 1 \le k \le n-2. \end{cases}$$

Dankelmann et al. [15] established a relation between $\mu_r(G)$, $\mu_{k+1-r}(G)$, and $\mu_k(G)$ for $2 \le r < k$.

Theorem 2.1. [15] *Let G be a connected weighted graph and $2 \le r \le k-1$. Then*

$$\mu_k(G) \le \mu_r(G) + \mu_{k+1-r}(G).$$

The following corollary is immediate.

Corollary 2.2. [15] *For $k \ge 3$, $\mu_k(G) \le (k-1)\mu(G)$.*

Equalities in Theorem 2.1 and Corollary 2.2 are achieved for the complete graph.

Remark 2.1. [15] *Using the same methods as those used in [35], it can be shown that for each connected graph G of order n and $3 \leq k \leq n$,*

$$\mu_k(G) \leq \frac{k+1}{k-1}\mu_{k-1}(G).$$

It remains an open problem to determine a lower bound for $\mu_k(G)$ in terms of $\mu(G)$, but it is conjectured that the smallest ratio $\mu_k(G)/\mu(G)$ taken over all connected graphs G of order n, where $n \geq k$, is attained if G is the path. More formally:

Conjecture 2.1. [15] *If G is a connected graph of order n and $3 \leq k \leq n$, then*

$$\mu_k(G) \geq 3\frac{k-1}{k+1}\mu(G).$$

In [15], Dankelmann et al. proved that the conjecture is true for $k = 3$ and $k = n$.

The following observation is immediate.

Observation 2.1. [42] *Let G be a connected graph of order n, $e \in E(G)$, and let k be an integer such that $2 \leq k \leq n$. Further, let H be a graph with vertex set $V(H) = V(G)$ and edge set $E(G) \setminus e$. Then*

$$\mathrm{SW}_k(G) \leq \mathrm{SW}_k(H).$$

This straightforwardly leads to the following result.

Proposition 2.2. [42] *Let G be a connected graph of order n, and T a spanning tree of G. Let k be an integer such that $2 \leq k \leq n$. Then*

$$\mathrm{SW}_k(G) \leq \mathrm{SW}_k(T)$$

with equality if and only if G is a tree.

2.1 Results for trees

Li et al. [42] got the formulas for Steiner Wiener index of trees when k is large.

Theorem 2.3. [42] *Let T be a tree of order n, possessing p pendent vertices. Then*

$$\mathrm{SW}_{n-1}(T) = n(n-1) - p,$$

irrespective of any other structural detail of T.

Theorem 2.4. [43] *Let T be a tree of order n, possessing p pendent vertices. Let q be the number of vertices of degree 2 in T that are adjacent to a pendent vertex. Then*

$$\mathrm{SW}_{n-2}(T) = \frac{1}{2}\big(n^3 - 2n^2 + n - 2np + 2p - 2q\big)\,.$$

Let G be any graph (not necessarily connected) with vertex set $V(G)$. Let e be an edge of G, connecting the vertices x and y. Define the sets

$$\begin{aligned} \mathcal{N}_1(e) &= \{u \,|\, u \in V(G), d(u,x) < d(u,y)\} \\ \mathcal{N}_2(e) &= \{u \,|\, u \in V(G), d(u,x) > d(u,y)\} \end{aligned}$$

and let their cardinalities be $n_1(e) = |\mathcal{N}_1(e)|$ and $n_2(e) = |\mathcal{N}_2(e)|$, respectively. In other words, $n_1(e)$ counts the vertices of G, lying closer to one end of the edge e than to its other end, and the meaning of $n_2(e)$ is analogous.

The following formula was used in the seminal paper on Wiener index [82]:

$$\mathrm{W}(T) = \sum_{e\in E(T)} n_1(e)\, n_2(e). \tag{6}$$

Li et al. [42] devised the generalization of the Eq. (6) to Steiner Wiener indices:

Theorem 2.5. [42] *Let k be an integer such that $2 \leq k \leq n$. The k-Steiner Wiener index for a tree T can be calculated using the following equation:*

$$\mathrm{SW}_k(T) = \sum_{e\in E(T)} \sum_{i=1}^{k-1} \binom{n_1(e)}{i} \binom{n_2(e)}{k-i}. \tag{7}$$

The following corollary is immediate.

Corollary 2.6. [42]

(1) Eq. 6 is obtained from Eq. (7) by setting $k = 2$.

(2) If $k = 3$, then the k-Steiner Wiener index of a tree of order n is directly related to the ordinary Wiener index:

$$\mathrm{SW}_3(T) = \frac{n-2}{2}\,\mathrm{W}(T)\ .$$

Remark 2.2. [42] *The Wiener index or the 2-Steiner Wiener index for any graph can be computed in polynomial time since one needs only to compute the distances of $\binom{n}{2}$*

pairs of vertices in a graph of order n. However, since the problem of "Steiner Tree in Graphs" is NP-complete (see [24]), it is NP-hard to compute the k-Steiner Wiener index $\mathrm{SW}_k(G)$ *for a general graph G and a general positive integer k. Recall that the problem of "Steiner Tree in Graphs" is stated as follows: For a given graph $G = (V, E)$, a weight $w(e)$ (a positive integer) for each $e \in E$, a subset $R \subseteq V$, and a positive integer B, is there a subtree of G that includes all vertices of R, such that the sum of the weights of the edges in the subtree is not greater than B? This problem remains NP-complete if all edge weights are equal.*

Vukičević and Sedlar [75] proved that the following formula for k-Steiner Wiener index of trees also holds.

Theorem 2.7. [75] *Let k be an integer such that $2 \leq k \leq n$. If T is a tree, then its k-Steiner Wiener index is equal to:*

$$\mathrm{SW}_k(T) = \sum_{e=uv \in E(T)} \left[\binom{n}{k} - \binom{n_1(e)}{k} - \binom{n_2(e)}{k} \right].$$

Dankelmann et al. [15] investigated the average k-Steiner distance of trees by establishing sharp upper and lower bounds for this parameter.

Theorem 2.8. [15] *Let T be a tree of order $n \geq k$ and $2 \leq r \leq k-1$. Then*

$$\mu_k(T) \leq \frac{n}{r} \mu_r(T).$$

Equality holds if and only if T is a star.

The following corollary is immediate Theorem 2.8.

Corollary 2.9. [15]

(1) If T is a tree of order $n \geq k$, then $\mu_k(T) \leq \frac{k}{2} \mu(T)$.

(2) If T is a tree of order $n \geq k$ and $2 \leq r \leq k-2$, then $\mu_k(T) \leq \mu_r(T) + \mu_{k-r}(T)$.

The upper and lower bounds for average Steiner distance is also obtained in the same paper [15].

Proposition 2.3. [15] *If T is a tree of order n ($2 \leq k \leq n$), then*

$$k\left(1 - \frac{1}{n}\right) \leq \mu_k(T) \leq \frac{k-1}{k+1}(n+1) .$$

Equality holds if and only if T is a star or path, respectively, or in either case if $k = n$.

Remark 2.3. [15] *For $k = 2$, Proposition 2.3 was already observed in [19] and [47].*

Theorem 2.7 implies the following lower and upper bounds for the Steiner Wiener index of a tree.

Theorem 2.10. [42] *Let T be a tree of order n, and let k be an integer such that $2 \leq k \leq n$. Then*

$$\binom{n-1}{k-1}(n-1) \leq \mathrm{SW}_k(T) \leq (k-1)\binom{n+1}{k+1}.$$

Among all trees of order n, the star S_n minimizes the k-Steiner Wiener index whereas the path P_n maximizes the k-Steiner Wiener index.

According to the classification of indices given by Vukičević and Sedlar, the k-Steiner Wiener index belongs to the Wiener-type indices [42]. More details on this classification can be found in [75].

It was shown in [79] and [90] that among trees of a given degree sequence (non-increasing sequence of vertex degrees) the following greedy tree minimizes the Wiener index.

With given vertex degrees, the greedy tree is achieved through the following "*greedy algorithm*" (here we use $deg(v)$ to denote the degree of a vertex v):

(i) Label the vertex with the largest degree as v (the root);

(ii) Label the neighbors of v as $v_1, v_2, \ldots$ assign the largest degrees available to them such that $deg(v_1) \geq deg(v_2) \geq \ldots$;

(iii) Label the neighbors of v_1 (except v) as $v_{11}, v_{12}, \ldots$ such that they take all the largest degrees available and that $deg(v_{11}) \geq deg(v_{12}) \geq \ldots$, then do the same for $v_2, v_3, \ldots$;

(iv) Repeat (iii) for all the newly labeled vertices. Always start with the neighbors of the labeled vertex with largest degree whose neighbors are not labeled yet.

For example, Figure 2.1 shows a greedy tree with degree sequence

$$(4, 4, 4, 3, 3, 3, 3, 3, 3, 3, 2, 2, 1, \ldots, 1).$$

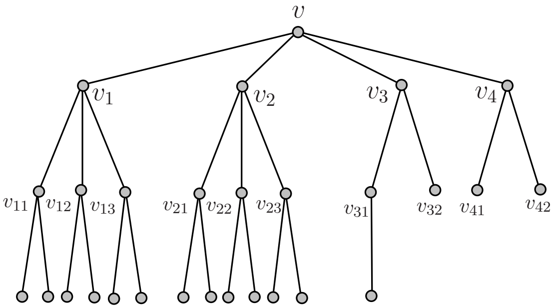

Figure 2.1 A greedy tree with degree sequence $(4,4,4,3,3,3,3,3,3,3,2,2,1,\ldots,1)$.

For convenience, let $\mathcal{T}_d$ be the set of trees with degree sequence $d = (d_1, d_2, \ldots, d_n)$. It is natural to ask the following problem:

Problem 2.1. [88] *Among trees in $\mathcal{T}_d$ for a given degree sequence d, does the greedy tree minimize the k-Steiner Wiener index for any $k \geq 2$?*

The answer to Problem 2.1 is yes for $k = 2$ as established before for the regular Wiener index. The same is true for $k = 3$ as it has been shown in Corollary 2.6 that

$$\mathrm{SW}_3(T) = \frac{n-2}{2}\,\mathrm{W}(T)\ .$$

Zhang et al. [88] stated that despite their strong belief that the greedy tree is minimizing the k-Steiner Wiener index for any k, the proof of this will not be easy to find.

A *caterpillar* is a tree whose removal of leaves result in a path, which is called the *backbone* of the caterpillar.

Theorem 2.11. [88] *If a tree T maximizes the Steiner Wiener index in $\mathcal{T}_d$, then it must be a caterpillar.*

Theorem 2.12. [88] *If a caterpillar T maximizes the Steiner Wiener index in $\mathcal{T}_d$, then the degrees of vertices on the backbone, listed from one end to the other end, form a unimodal sequence $d_1, d_2, \ldots, d_q$, i.e.,*

$$d_1 \geq d_2 \geq \cdots \geq d_j \leq \cdots \leq d_q,$$

Zhang et al. [88] conjectured that the extremal chemical trees that maximize the k-Steiner Wiener index is somewhat “balanced”.

Conjecture 2.2. [88] *Given a chemical tree with given degree sequence d as defined in [2], the k-Steiner Wiener index, for $k \geq 2$, is maximized when the chemical tree is of the structure as Figure 2.2 with*

- $x = a/2$, $y = \lfloor b/2 \rfloor$ *if a is even;*
- $x = (a-1)/2$, $y = (b+1)/2$ *if both a and b are odd;*
- $x = (a-1)/2$, $y = b/2 + 1$ *if a is odd and b is even.*

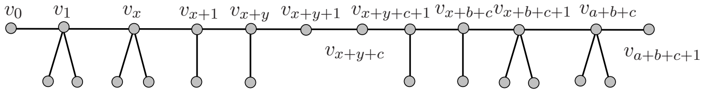

Figure 2.2 A caterpillar with maximum degree 4.

Let $\mathcal{T}_\Delta$ denote the set of trees (of order n) with given maximum degree Δ, and let $\mathcal{T}_\ell$ denote the set of trees (of order n) with ℓ leaves. An $(n-\Delta+1)$-*comet* is obtained from attaching $\Delta - 1$ pendent edges to one end of $P_{n-\Delta+1}$ (Figure 2.3 (a)).

Theorem 2.13. [88] *In $\mathcal{T}_\Delta$, the $(n-\Delta+1)$-comet maximizes the Steiner Wiener index.*

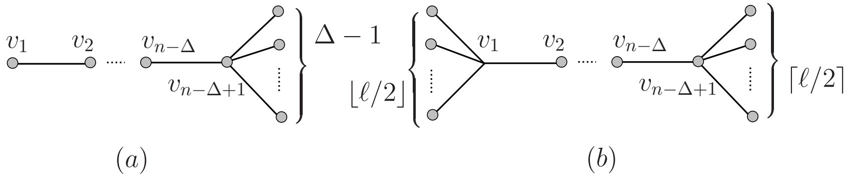

Figure 2.3 (a) $(n-\Delta+1)$-comet; (b) The dumbbell $D(n, \lfloor \ell/2 \rfloor, \lceil \ell/2 \rceil)$.

Denote $C_{n,\Delta}$ be a caterpillar of order n whose vertices are either pendent vertices or of degree Δ. Let $\mathcal{T}'_\Delta = \{T \mid T$ is a tree with n vertices, $deg(v) \in \{1, \Delta\}$, for all $x \in V(T)$, $\Delta \geq 3\}$.

Corollary 2.14. [88] *In the set $\mathcal{T}'_\Delta$, $C_{n,\Delta}$ is the extremal tree that maximizes the Steiner Wiener index.*

A *dumbbell* graph, denoted by $D(n, a, b)$, is consisting of the path P_{n-a-b} with a pendent edges attached to one end, and b pendent edges to the other.

Theorem 2.15. [88] *Let $\mathcal{T}_\ell$ be the set of trees (of order n) with ℓ leaves. The dumbbell $D(n, \lfloor \ell/2 \rfloor, \lceil \ell/2 \rceil)$ (Figure 2.3 (b)) maximizes the Steiner Wiener index in $\mathcal{T}_\ell$.*

For two integers n and d with $2 \leq d \leq n-1$, let $\mathcal{T}(n)$ be the family of trees on n vertices and $T(n,d) = \{T \in \mathcal{T}(n) : d(T) = d\}$. Clearly, $\mathcal{T}(2) = \{P_2\}$, $\mathcal{T}(3) = \{P_3\}$, $\mathcal{T}(n,2) = \{K_{1,n-1}\}$ and $\mathcal{T}(n, n-1) = \{P_n\}$. Let $T \in \mathcal{T}(n)$ and $e \in E(T)$. Denote by

$$\gamma^{(T)}(e) = \min\{n_1^{(T)}(e), n_2^{(T)}(e)\}, \quad \eta^{(T)}(e) = \max\{n_1^{(T)}(e), n_2^{(T)}(e)\}.$$

Let T and T' be two trees in $\mathcal{T}(n)$. For $\epsilon \in E(T)$ and a positive integer s, a *feasible map* from T to T' with respect to ϵ and s is a bijection $\phi : E(T) \to E(T')$ such that:

(i) $\gamma^{(T)}(\epsilon) - s = \gamma^{(T')}(\phi(\epsilon))$;

(ii) $\gamma^{(T)}(e) = \gamma^{(T')}(\phi(e))$ for $e \in E(T) \setminus \{\epsilon\}$.

Denote by $\mathcal{F}_{\epsilon,s}(T, T')$ the set of all feasible maps from T to T' with respect to ϵ and s. Lu et al. [48] gave a criterion to compare the Steiner Wiener indices of two trees.

Theorem 2.16. [48] *Let T and T' be two trees in $\mathcal{T}(n)$. If there exist $\epsilon \in E(T)$ and a positive integer s such that $\mathcal{F}_{\epsilon,s}(T, T') \neq \emptyset$, then $\mathrm{SW}_k(T) > \mathrm{SW}_k(T')$ for $2 \leq k \leq \eta^{(T)}(\epsilon) + s$ and $\mathrm{SW}_k(T) = \mathrm{SW}_k(T')$ for $\eta^{(T)}(\epsilon) + s < k \leq n-1$.*

For a tree $T \in \mathcal{T}(n)$, a vertex $u \in V(T)$ is a *star-root* if $N(u) = \{v, u_1, \ldots, u_s\}$ such that $deg(v) > 1$ and $deg(u_i) = 1$ for $1 \leq i \leq s$ and $s \geq 1$. Clearly, each tree $T \in \mathcal{T}(n)$ has at least two star-roots unless $T = K_{1,n-1}$. Let T be a tree in $\mathcal{T}(n)$ and u a star root in $V(T)$ with $N(u) = \{v, u_1, \ldots, u_s\}$ such that $deg(v) > 1$. We construct the new tree T_u from T by deleting the edges uu_i and adding the edges vu_i (see Figure 2.4). The *star-root switching* of T on u is the transformation from T to T_u, and T_u is the corresponding *star-root switching graph.* By simple observations, T_u contains one more pendent vertex than T.

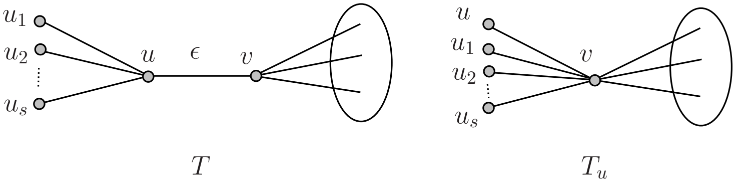

Figure 2.4 The star-root transformation of T on u.

Corollary 2.17. [48] *Let* T *be a tree in* $\mathcal{T}(n)$. *If* u *is a star-root of* T, *then* $\mathrm{SW}_k(T) > \mathrm{SW}_k(T_u)$ *for* $2 \leq k \leq n-1$.

Let $T \in \mathcal{T}(n)$ and $u \in V(T)$. Denote by $P(u) = \{v \in N(u) : deg(v) = 1\}$ and $P(u)^* = \{v \in N(u) : deg(u) > 1\}$. We say that u is a *pseudo star-root* if $|P(u)| \geq 1$ and $|P(u)^*| \geq 1$. Particularly, a star-root x is a pseudo star-root with $|P(x)^*| = 1$. Suppose that v_1 is a pseudo star-root of T. For $v_2 \in P(v_1)^*$ and $U = \{u_1, \ldots, u_s\} \subseteq P(v_1)$, we construct the new tree $T^{(U)}_{v_1 \to v_2}$ from T by deleting the edges v_1u_i and adding the edges v_2u_i for $1 \leq i \leq s$ (see Figure 2.5). The *pseudo star-root switching* of T from v_1 to v_2 with respect to U is the transformation from T to $T^{(U)}_{v_1 \to v_2}$, and $T^{(U)}_{v_1 \to v_2}$ is the corresponding *pseudo star-root switching graph.* The pseudo star-root switching is complete if $U = P(v_1)$. For convenience, denote by $T_{v_1 \to v_2} = T^{(P(v_1))}_{v_1 \to v_2}$.

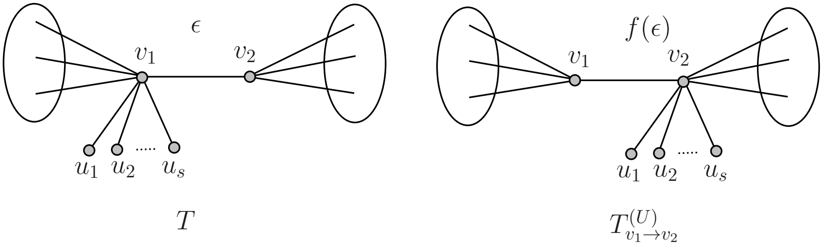

Figure 2.5 The pseudo star-root switching from v_1 to v_2 with respect to U.

Corollary 2.18. [48] *Let* T *be a tree in* $\mathcal{T}(n)$ *and* v_1 *a pseudo star-root of* T. *Let* U *be a nonempty subset of* $P(v_1)$ *and* $v_2 \in P(v_1)^*$. *If* $n_l^{(T)}(v_1v_2) \leq n_r^{(T)}(v_1v_2)$, *then*

$\mathrm{SW}_k(T) > \mathrm{SW}_k(T^{(U)}_{v_1\to v_2})$ *for* $2 \le k \le \eta^{(T)}(v_1v_2) + |U|$ *and* $\mathrm{SW}_k(T) = \mathrm{SW}_k(T^{(U)}_{v_1\to v_2})$ *for* $\eta^{(T)}(v_1v_2) + |U| < k \le n-1$.

The *caterpillar tree* with respect to $P_d = u_0u_1\ldots u_d$, denoted by $CP(s_1,\ldots,s_{d-1})$, is the tree obtained from P_d by attaching s_i new vertices to u_i for $1 \le i \le d-1$ (Figure 2.6). Especially, the path P_d itself can be regarded as the caterpillar tree $CP(\underbrace{0,0,\ldots,0}_{d-1})$ and the star $K_{1,n-1}$ can be regarded as the caterpillar tree $CP(n-3)$. Obviously, $CP(s_1,s_2,\ldots,s_{d-1}) \in \mathcal{T}(n,d)$, where $n = \sum_{i=1}^{d-1} + d + 1$. Particularly, if $s_i = 0$ for $i \ne t$ and $s_t = s \ne 0$, then such a caterpillar tree is denoted by $CP_{d,t}(s)$ (see Figure 2.6), that is,

$$CP_{d,t}(s) = CP(\underbrace{0,0,\ldots,0}_{t-1}, s, \underbrace{0,0,\ldots,0}_{d-t-1})$$

Note that $CP_{d,t}(s) \cong CP_{d,d-t}(s)$. We always assume that $t \le d/2$ in the notation $CP_{d,t}(s)$.

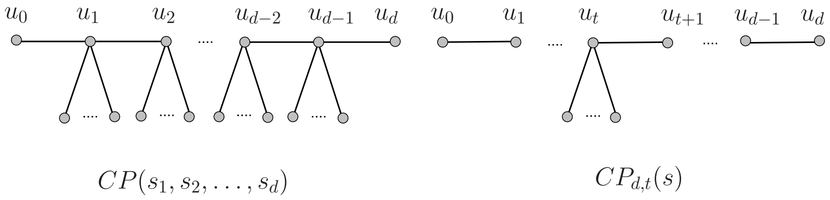

Figure 2.6 The caterpillar graphs.

Corollary 2.19. [48] *Let* $CP_{d,t}(s)$ *be a caterpillar tree with respect to* $P_d = u_0u_1\ldots u_d$ *such that* $s \ge 1$. *If* $t \le d/2 - 1$, *then*

$$\mathrm{SW}_k(CP_{d,t}(s)) > \mathrm{SW}_k(CP_{d,t+1}(s))$$

for $2 \le k \le d - t + s$ *and*

$$\mathrm{SW}_k(CP_{d,t}(s)) = \mathrm{SW}_k(CP_{d,t+1}(s))$$

for $d - t + s < k \le n - 1$.

Lu et al. [48] derived the following results.

Theorem 2.20. [48] *For* $T \in \mathcal{T}(n,d)$ *with* $3 \le d \le n-2$*, we have*

$$\mathrm{SW}_k(T) \ge \mathrm{SW}_k(CP_{d,\lfloor d/2 \rfloor}(n-d-1))$$

for $2 \le k \le n-1$*. The equality holds for all* k *if and only if* $T \cong CP_{d,\lfloor d/2 \rfloor}(n-d-1)$*.*

Theorem 2.21. [48] *For* $2 \le k \le n-d$*, the* k*-Steiner Wiener index of* $CP_{d,\lfloor d/2 \rfloor}(n-d-1)$ *is given by*

$$\mathrm{SW}_k(CP_{d,\lfloor d/2 \rfloor}(n-d-1)) = \Gamma(n,d,k),$$

where

$$\Gamma(n,d,k) = \frac{n(d+k)-k(d+1)}{n}\binom{n}{k} - 2\left[\binom{d/2+1}{k+1} + \binom{n}{k+1} - \binom{n-d/2}{k+1}\right]$$

for d *even and*

$$\begin{aligned}\Gamma(n,d,k) \;&=\; \frac{n(d+k)-k(d+1)}{n}\binom{n}{k} \\ &-\; \left[\binom{(d+3)/2}{k+1} + \binom{(d+1)/2}{k+1} + 2\binom{n}{k+1}\right. \\ &-\; \left.\binom{n-(d+1)/2}{k} - 2\binom{n-(d-1)/2}{k+1}\right]\end{aligned}$$

for d *odd.*

Corollary 2.22. [48] *For* $T \in \mathcal{T}(n,d)$ *with* $3 \le d \le n-1$*, we have*

$$\mathrm{SW}_k(T) \ge \Gamma(n,d,k)$$

for $2 \le k \le n-1$*. Furthermore, if the equality holds for all* k *then* $T \cong CP_{d,\lfloor d/2 \rfloor}(n-d-1)$*.*

2.2 Algorithmic aspect for average Steiner distance

An $O(kn^2)$ procedure is developed in [6] for calculating the k-distances of all vertices of a tree T of order n. Since the Steiner distance of any set S of k vertices contributes the same amount to the k-distance of each vertex in S, it follows that

$$\mu_k(T) = \sum_{v \in V(T)} \frac{d_k(v)}{n}\binom{n}{k}.$$

Hence, this procedure for finding $\mu_k(T)$ is much more efficient than the brute force method for calculating the Steiner distance of all $\binom{n}{k}$ sets of vertices if $n > k$.

Dankelmann et al. [15] presented an even more efficient algorithm that computes the average k-distance of a tree without first computing the k-distance of each vertex. For a graph G let $m(G)$ denote the maximum order among all components of G. This algorithm is based on the proof of Theorem 2.8, where the average k-distance of a tree is expressed implicitly in terms of the values $m(T-e)$ for $e \in E(T)$. It computes the average k-distance of a tree of order n using $O(n)$ graph operations and $O(kn)$ arithmetic operations. In [15], the *edge weight* $\omega_k(e)$ for $e \in E(T)$ is defined by

$$\omega_k(e) = \binom{n}{k} - \binom{m(T-e)}{k} - \binom{n-m(T-e)}{k}.$$

Then $\omega_k(e)$ counts the number of k-sets $S \subseteq V(T)$ that have at least one vertex in each component of $T-e$. Thus $\omega_k(e)$ equals the number of Steiner trees containing e and we have

$$\begin{aligned} \mu_k(T) &= \sum_{e\in E(T)} \omega_k(e)\binom{n}{k}^{-1} \\ &= n-1-\sum_{e\in E(T)}\left[\binom{m(T-e)}{k}+\binom{n-m(T-e)}{k}\right]\binom{n}{k}^{-1}. \end{aligned}$$

Therefore it is suffices to compute the values $m(T-e)$ for all $e \in E(T)$, which is possible in $O(n)$ time and to apply the above equlity which requires at most $O(kn)$ multiplications and divisions.

2.3 Upper and lower bounds

In [15], the range for the average k-distance of a connected graph of given order was determined by generalizing a result for $k = 2$ obtained by Entringer et al. [19], Doyle and Graver [18], and Lovász [47], independently.

Theorem 2.23. [15, 42] *Let G be a connected graph of order n and let $2 \le k \le n-1$. Then*

$$k-1 \le \mu_k(G) \le \frac{k-1}{k+1}(n+1),$$

that is,

$$\binom{n}{k}(k-1) \le \mathrm{SW}_k(G) \le (k-1)\binom{n+1}{k+1}.$$

Equality holds on the left (or right) if and only if G is $(n+1-k)$-connected (or if G is a path, respectively).

The upper bound for the average k-distance given in Theorem 2.23 can be improved for 2-connected graphs. Plesník [66] showed that the cycle of order n, C_n, is the unique 2-connected graph with given order n and maximum average distance. This result was generalized for the average k-distance in [15]. It is remarkable that Plesník's result can easily be generalized for $k = 2$ and 2ℓ-connected graphs (see [20]), which seems not to be the case for $k \geq 3$.

Theorem 2.24. [16] *Let G be a 2-connected graph of order n and let $2 \leq k \leq n$. Then*

$$\mu_k(G) \leq \mu_k(C_n).$$

Equality holds if and only if $G = C_n$, or $k \geq n - 1$.

In [66], Plesník proved that, apart from the obvious restriction $1 \leq \mu(G) \leq \mathrm{diam}(G)$, the average distance is independent of the diameter and the radius.

Theorem 2.25. [66] *Let r, d be positive integers with $d \leq 2r$ and let $t \in \Re$ such that $1 \leq t \leq d$. For every $\varepsilon > 0$ there exists a graph G with diameter d, radius r, and*

$$|\mu(G) - t| < \varepsilon.$$

An obvious question arises whether there is a similar statement for the k-diameter and the average k-distance. An answer to this question is affirmative and it is proved by Dankelmann et al. in [16].

Theorem 2.26. [16] *Let k, d he positive integers, $k \geq 2$, and let $t \in \Re$ such that $k - 1 \leq t \leq d$. For every $\varepsilon > 0$ there exists a graph G with k-diameter d and*

$$|\mu_k(G) - t| < \varepsilon.$$

Dankelmann et al. [16] pointed out that Theorem 2.26 is not a generalization of Plesník's Theorem 2.25, since it does not allow us to prescribe also the Steiner k-radius. The problem of finding such a generalization requires the determination of the possible values for the Steiner k-radius of a graph with a given Steiner k-diameter. This problem is still unsolved.

In [10] it was conjectured that the Steiner k-diameter of a graph G never exceeds $\frac{k}{k-1}\mathrm{srad}_k(G)$. This conjecture was disproved by Henning et al. [34], where the bound $\mathrm{sdiam}_k(G) \leq [2(k+1)/(2k-1)]\mathrm{srad}_k(G)$ was conjectured.

The problem of determining a sharp lower bound for the average k-distance of a connected graph with n vertices and m edges, where $k \geq 3$, is considerably more difficult than the corresponding problem for $k = 2$. The latter one was solved in [19]. The following bound shows that the complete r-partite Turán graphs are optimal in this regard. It remains an open problem to determine the graphs of given order and size that minimize the average k-distance.

Theorem 2.27. [16] *Let G be a graph of order n and size m. Then*

$$\mu_k(G) \geq k - 1 + n\binom{n - \frac{2m}{n} - 1}{k-1}\binom{n}{k}^{-1},$$

where for a real number a and a positive integer b the binomial coefficient $\binom{a}{b}$ is defined as $a(a-1)\ldots(a-b+1)/b!$.

The bound given is sharp if k is a multiple of r. It is attained by the complete r-partite Turán graph.

Tomescu and Melter [73] determined the range for the average distance of a graph of given order and chromatic number, and the corresponding extremal graphs. Dankelmann et al. in [16] showed that the same graphs are also extremal for $k \geq 3$, although there are other ones as well.

For $r < n$, let $H_{n,r}$ be the graph obtained from a complete graph K_r and a path of order $n - r$ with end vertices v_1 and v_1' by joining v_1' to one vertex of K_r. For $r = n$, let $H_{n,r}$ be the complete graph K_n and let v_1 be a vertex of K_n.

Theorem 2.28. [16] *Let G be a connected graph of order n $(2 \leq k \leq n)$ and chromatic number r and let v be a vertex of G. Then*

(1) $d_k(v, G) \leq d_k(v_1, H_{n,r})$

(2) $\mu_k(G) \leq \mu_k(H_{n,r})$,

with equality if and only if $v = v_1$ and $G = H_{n,r}$, respectively.

Dankelmann et al. in [16] remarked that Theorem 2.28 yields a sharp lower bound for the k-distance of a connected graph G of given order n and chromatic number r. From

$$e(G) \leq n^2\frac{r-1}{2r}$$

and Theorem 2.28 we have immediately

$$\mu_k(G) \geq k - 1 + n\binom{n/r-1}{k-1}\binom{n}{k}^{-1}.$$

This bound is sharp if n is a multiple of r. Examples for equality in the above equation are the r-partite Turán graph $T_{n,r}$ and, for $k > n/r$, the graph $T_{n,r} - e$.

A *segment* of a tree T is a subpath P of T such that the all internal vertices of P are of degree 2 in T and each end of P is either a leaf or a branch vertex (a vertex of degree at least 3). The *segment sequence* $(l_1, l_2, \ldots, l_m)$ of a tree is simply the sequence of the segment lengths in non-increasing order. Among various classes of trees that have been studied, the trees with a given segment sequence are of particular interest to us. Along this line, it has been shown in [45] that the *starlike tree* (obtained from identifying the ends of all segments) minimizes the Wiener index among trees of a given segment sequence. A tree whose removal of pendant segments (segments with one end being a leaf) results in a path is called a *quasi-caterpillar*. It was shown in [2] that quasi-caterpillar maximizes the Wiener index among trees of a given segment sequence. See Figure 2.7 for an illustration of these extremal structures. Zhang et al. [87] were searching for the extremal trees with respect to the Steiner Wiener index among those with a given segment sequence. They showed that the starlike and the quasi-caterpillar trees are ones with the extremal values of the Steiner Wiener index. Let $\mathcal{T}_\ell$ denote the set of trees of order n with the segment sequence $\ell = (l_1, l_2, \ldots, l_m)$.

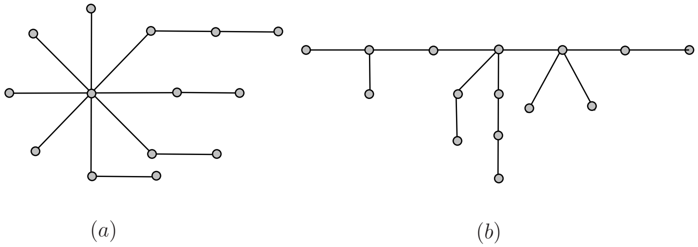

Figure 2.7 The starlike tree (top) and quasi-caterpillar (bottom) with segment sequence $(3, 2, 2, 2, 1, 1, 1, 1, 1)$.

Theorem 2.29. [87] *Among trees in $\mathcal{T}_\ell$, the starlike tree minimizes the k-Steiner Wiener* *index for any k.*

Theorem 2.30. [87] *For any k and ℓ, among trees in $\mathcal{T}_\ell$, the k-Steiner Wiener index is maximized by the quasi-caterpillar tree.*

Dankelmann [12] proved upper bounds for the Steiner Wiener index and the average Steiner distance of graphs with given order n and minimum degree δ.

Theorem 2.31. [12] *Let G be a connected graph of order n with minimum degree δ. Then G contains a spanning tree T with*

$$\mathrm{SW}_k(T) \leq \frac{3(k-1)(n+1)}{(k+1)(\delta+1)}\binom{n}{k} + \left(\frac{3\delta}{\delta+1} + 2k\right)\binom{n}{k}.$$

The following corollary is immediate.

Corollary 2.32. [12] *Let G be a connected graph of order n with minimum degree δ. Then*

$$\mathrm{SW}_k(G) \leq \frac{3(k-1)(n+1)}{(k+1)(\delta+1)}\binom{n}{k} + \left(\frac{3\delta}{\delta+1} + 2k\right)\binom{n}{k},$$

and thus

$$\mu_k(G) \leq \frac{3(k-1)(n+1)}{(k+1)(\delta+1)} + \left(\frac{3\delta}{\delta+1} + 2k\right).$$

Example 2.1. [12] *The following example is showing that the bound on the k-Steiner Wiener index in Corollary 2.32 is best possible apart from a term $O(n^k)$, and that the bound on the average k-Steiner distance is best possible apart from an additive constant. These examples are constructed for the case when $\delta+1$ is a multiple of 3, but it is not difficult to modify this construction for all values of δ. For $d \in \mathcal{N}$ define the graph $G_{d,\delta}$ by*

$$G_{d,\delta} = K_\delta + K_{(\delta+1)/3} + K_{(\delta+1)/3} + \cdots + K_{(\delta+1)/3} + K_\delta,$$

where the term $K_{(\delta+1)/3}$ appears $d-1$ times. Clearly, $|V(G_{d,\delta})| = \frac{d+5}{3}(\delta+1) - 2$, and $diam(G_{d,\delta}) = d$. Hence, for large d and constant δ we have $n = d\frac{\delta+1}{3} + O(1)$. We now bound the k-Steiner Wiener index from below.

For $i = 1, 2, \ldots, d-1$ let V_i be the set of vertices of the i-th copy of $K_{(\delta+1)/3}$, and let V_0 and V_d be subsets of cardinality $(\delta+1)/3$ of the first and last, respectively, copy of K_δ. Let $\mathcal{S}$ be the set of all k-element sets of vertices of $G_{d,\delta}$ that are contained in $\bigcup_{i=0}^{d} V_i$, and that have no two vertices in the same V_i. Let F be the path of order $d+1$ with vertices

$u_0, u_1, \ldots, u_d$. We define a mapping f that maps every set in S to a k-set of vertices of F. For $S \in \mathcal{S}$ let $f(S)$ be the subset of $V(F)$ containing those u_i for which S contains a vertex in V_i. It is clear that $d_{G_{d,\delta}}(S) = d_F(f(S))$. Since every k-set of vertices of F is the image under f of exactly $(\frac{\delta+1}{3})^k$ sets in S, we have

$$\mathrm{SW}_k(G_{d,\delta}) \geq \sum_{S\in\mathcal{S}} d_{G_{d,\delta}}(S) = \sum_{S\in\mathcal{S}} d_{P_{d+1}}(f(S)) = \sum_{\substack{S\subseteq V(G)\\|S|=k}} \left(\frac{\delta+1}{3}\right)^k d_F(S).$$

Hence, by Theorem 2.23,

$$\mathrm{SW}_k(G_{d,\delta}) \geq \left(\frac{\delta+1}{3}\right)^k \mathrm{SW}_k(F) = \left(\frac{\delta+1}{3}\right)^k \frac{(k-1)(d+2)}{k+1}\binom{d+1}{k}.$$

Now for constant k and δ and large n and d we get $n = d\frac{\delta+1}{3} + O(1)$ and thus $d = \frac{3}{\delta+1} + O(1)$. Hence $\binom{d+1}{k} = \left(\frac{3}{\delta+1}\right)^k \binom{n}{k} + O(n^{k-1})$, and so

$$\begin{aligned}\mathrm{SW}_k(G_{d,\delta}) &\geq \left(\frac{\delta+1}{3}\right)^k \frac{(k-1)(d+2)}{k+1}\left[\left(\frac{3}{\delta+1}\right)^k \binom{n}{k} + O(n^{k-1})\right]\\ &= \frac{(k-1)}{k+1}\frac{3n}{\delta+1}\binom{n}{k} + O(n^k).\end{aligned}$$

Dividing by $\binom{n}{k}$ we get

$$\mu_k(G_{d,\delta}) = \frac{(k-1)}{k+1}\frac{3n}{\delta+1} + O(1),$$

as desired.

Dankelmann [12] improved this bound for triangle-free graphs.

Theorem 2.33. [12] *Let G be a connected, triangle-free graph of order n with minimum degree δ. Then G contains a spanning tree T with*

$$\mathrm{SW}_k(T) \leq \frac{2(n+1)(k-1)}{\delta(k+1)}\binom{n}{k} + \left(\frac{4\delta-2}{\delta} + 3k + 1\right)\binom{n}{k}.$$

Corollary 2.34. [12] *Let G be a connected graph of order n with minimum degree δ. Then*

$$\mathrm{SW}_k(G) \leq \frac{2(n+1)(k-1)}{\delta(k+1)}\binom{n}{k} + \left(\frac{4\delta-2}{\delta} + 3k + 1\right)\binom{n}{k},$$

and thus

$$\mu_k(G) \leq \frac{2(n+1)(k-1)}{\delta(k+1)} + \left(\frac{4\delta-2}{\delta} + 3k + 1\right).$$

Example 2.2. [12] *The following example shows that the bound on the Steiner k-Wiener index in Corollary 2.34 is best possible apart from a term $O(n^k)$, and that the bound on the average Steiner k-distance is best possible apart from an additive constant. We only construct examples for the case that δ is even, but as in Example 2.1 it is not difficult to modify this construction for odd values of δ. For $d \in \mathcal{N}$ define the graph $H_{d,\delta}$ by*

$$H_{d,\delta} = \delta K_1 + \delta K_1 + K_{\delta/2} + K_{\delta/2} + \cdots + K_{\delta/2} + \delta K_1 + \delta K_1,$$

where the term $K_{\delta/2}$ appears $d-3$ times. Then calculations similar to those in Example 2.1 show that for constant δ and k and large n and d we have

$$\mathrm{SW}_k(H_{d,\delta}) \leq \frac{2(n+1)(k-1)}{\delta(k+1)}\binom{n}{k} + O(n^k),$$

and thus

$$\mu_k(G) \leq \frac{2n(k-1)}{\delta(k+1)} + O(1).$$

2.4 Inverse problem

The "inverse problem" in the chemical graph theory implies an answer to the following question: *Which natural numbers can be the values of an integer-valued topological index?* This problem was firstly investigated in the case of the Wiener index [21, 32, 33, 76, 78].

Li et al. [43] considered the analogous question for Steiner Wiener indices:

Problem 2.2. [43] *For a fixed k and a positive integer w, does there exist a connected graph G (or a tree T) of order $n \geq k$ such that $\mathrm{SW}_k(G) = w$ (or $\mathrm{SW}_k(T) = w$)?*

For $k = 2$, in [32, 77], it was completely solved the conjecture by Lepović and Gutman [41] for trees, where it is stated that for all but 49 positive integers w one can find a tree with Wiener index w. This is different from Problem 2.2 for trees, since Li et al. [43] considered graphs or trees with order n.

If G is a connected graph of order n, then for $k = n$, $\mathrm{SW}_k(G) = n-1$. Thus the following result is immediate.

Proposition 2.4. [43] *For a positive integer w, there exists a connected graph G of order n such that $\mathrm{SW}_n(G) = w$ if and only if $w = n-1$.*

For $k = n-1$, Li et al. [43] presented the following results.

Proposition 2.5. [43] *For a positive integer w, there exists a connected graph G of order n such that $\mathrm{SW}_{n-1}(G) = w$, if and only if $n^2 - 2n \leq w \leq n^2 - n - 2$.*

Proposition 2.6. [43] *For a positive integer w, there exists a tree T of order n such that $\mathrm{SW}_{n-1}(T) = w$ if and only if $n^2 - 2n + 1 \leq w \leq n^2 - n - 2$.*

For $k = n - 2$, Li et al. [43] derived the following result for trees.

Theorem 2.35. [43] *For a positive integer w, there exists a tree T of order n $(n \geq 5)$, possessing p pendent vertices, such that $\mathrm{SW}_{n-2}(T) = w$ if and only if $w = \frac{1}{2}\big(n^3 - 2n^2 + n - 2np + 2p - 2q\big)$, where q is the number of vertices of degree 2 in T that are adjacent to a pendent vertex, and one of the following holds:*

(1) $2 \leq q \leq \lfloor \frac{n-1}{2} \rfloor$ *and* $q \leq p \leq n - q - 1$;

(2) $q = 1$ *and* $3 \leq p \leq n - 2$;

(3) $q = 0$ *and* $4 \leq p \leq n - 1$.

Proposition 2.7. [43] *For a positive integer w, there exists a tree T of order n such that $\mathrm{SW}_k(T) = w$ if*

$$w = t\binom{n-1}{k} - \binom{t}{k+1} - \binom{n}{k+1} + \binom{n-t+1}{k+1} + (k-1)\binom{n}{k},$$

where $1 \leq t \leq n - 1$ and $k \leq n$.

Proposition 2.8. [43] *For a positive integer w, there exists a connected graph G of order n such that $\mathrm{SW}_k(G) = w$ if w satisfies one of the following conditions:*

(1) $w = t\binom{n-1}{k} - \binom{t}{k+1} - \binom{n}{k+1} + \binom{n-t+1}{k+1} + (k-1)\binom{n}{k}$, *where* $1 \leq t \leq n - 1$ *and* $k \leq n$.

(2) $w = (n-1)\binom{n-1}{k-1} - \binom{n-r-1}{k}$, *where* $k \leq r \leq n - 1 - k$ *and* $k \leq n$.

Zhang et al. [86] solved the inverse Steiner Wiener problem for $k = 3$ by proving the following.

Theorem 2.36. [86] *All but finitely many positive integers are 3-Steiner Wiener indices of graphs.*

For n large enough, every positive integer between $\mathrm{SW}_3(S_n)$ and $\mathrm{SW}_3(K_n)$ can be the 3-Steiner Wiener index of a some graph. Note that by adding edges to a star we create a graph with diameter 2. More precisely:

Theorem 2.37. [86] *For any given* $n \geq 6$ *and any* $w \in \left[2\binom{n}{3}, (n-1)\binom{n-1}{2}\right]$*, there exists a connected graph* G *with diameter* 2 *such that* $\mathrm{SW}_3(G) = w$.

Theorem 2.37 claims that the all natural numbers in the interval

$$I_n = \left[2\binom{n}{3}, (n-1)\binom{n-1}{2}\right]$$

can be values of the 3-Steiner Wiener index for $n \geq 6$. Note that

$$(n-1)\binom{n-1}{2} \geq \binom{n+1}{3}$$

when n is sufficiently large. Hence, all but finitely many positive integers are in I_n for some n. Using a computer, one can easily find the values not included in I_n and find that the following positive integers are not the 3-Steiner Wiener index of any graph:

> 1, 3, 4, 5, 6, 7, 11, 12, 13, 14, 15, 16, 17, 18, 19, 29, 31, 32, 33, 34, 35, 36, 37, 38, 39, 57, 59, 60, 63, 65, 66, 67, 68, 69.

As a consequence the stronger version of Theorem 2.31 was given.

Theorem 2.38. [86] *Except for the* 34 *numbers listed above, every positive integer is the 3-Steiner Wiener index of some simple connected graph.*

2.5 Graph products

Yeh and Gutman [85] investigated the Wiener index of graph products and obtained the following results.

Theorem 2.39. [85] *Let* G *be a connected graph with* n *vertices, and let* H *be a connected graph with* m *vertices. Then*

(1) $\mathrm{W}(G \vee H) = e(G) + e(H) + mn + 2\left[\binom{n}{2} - e(G) + \binom{m}{2} - e(H)\right]$.

(2) $\mathrm{W}(G \circ H) = m^2\left[(\mathrm{W}(G) + n) - n(e(H) + m)\right]$.

(3) $\mathrm{W}(G \square H) = m^2\,\mathrm{W}(G) + n^2\,\mathrm{W}(H)$.

(4) $\mathrm{W}(G \odot H) = m^2\, \mathrm{W}(G) + n\, \mathrm{W}(H) + m(n^2 - n)\, d(v|H)$, *where* v *is the root-vertex of* H *and*

$$d(v|H) = \sum_{u \in V(H)} d(u,v)\,.$$

(5) $\mathrm{W}(G \ominus H) = (m+1)^2\, \mathrm{W}(G) + n\big[m^2 - e(H)\big] + mn(m+1)(n-1)$.

In [57], Mao et al. studied the k-th Steiner Wiener index of the above specified graph products.

Theorem 2.40. [57] *Let* G *be a connected graph with* n *vertices, and let* H *be a connected graph with* m $(n \geq m)$ *vertices. Let* k *be an integer,* $3 \leq k \leq n+m$.

(1) *If* $k > n$, *then*

$$\mathrm{SW}_k(G \vee H) = (k-1)\binom{n+m}{k}\,.$$

(2) *If* $k \leq m$, *then*

$$\mathrm{SW}_k(G \vee H) = (k-1)\binom{n+m}{k} + \binom{n}{k} + \binom{m}{k} - x - y,$$

where x *is the number of the* k*-subsets of* $V(G)$ *such that the subgraph induced by each* k*-subset is connected, and* y *is the number of the* k*-subsets of* $V(H)$ *such that the subgraph induced by each* k*-subset is connected.*

(3) *If* $m < k \leq n$, *then*

$$\mathrm{SW}_k(G \vee H) = (k-1)\binom{n+m}{k} + \binom{n}{k} + (k-1)\binom{m}{k} - x\,.$$

Theorem 2.41. [57] *Let* G *be a connected graph with* n *vertices, and let* H *be a connected graph with* m *vertices. Let* k *be an integer,* $2 \leq k \leq nm$. *Then*

$$\begin{aligned}\mathrm{SW}_k(G \circ H) &= nk\binom{m}{k} - nx + \sum_{\ell=2}^{k}\binom{m}{r_1}\binom{m}{r_2}\cdots\binom{m}{r_\ell}\mathrm{SW}_\ell(G)\\ &\quad + \sum_{\ell=2}^{k}(k-\ell)\binom{n}{\ell}\binom{m\ell-\ell}{k-\ell}\end{aligned}$$

where $\sum_{i=1}^{\ell} r_i = k$, $r_i \geq 1$ *and* x *is the number of the* k*-subsets of* $V(H)$ *such that the subgraph induced by each* k*-subset is connected in* H.

Theorem 2.42. [57] *Let G be a connected graph with n vertices, and let H be a connected graph with m vertices. Let k be an integer with $2 \le k \le nm$. Then*

$$\sum_{x=2}^{k}\binom{m}{r_1}\binom{m}{r_2}\cdots\binom{m}{r_x}\mathrm{SW}_x(G)+\sum_{y=2}^{k}\binom{n}{s_1}\binom{n}{s_2}\cdots\binom{n}{s_y}\mathrm{SW}_y(G)\le \mathrm{SW}_k(G\Box H)$$

$$\le \frac{k}{2}\left[\sum_{x=2}^{k}\binom{m}{r_1}\binom{m}{r_2}\cdots\binom{m}{r_x}\mathrm{SW}_x(G)+\sum_{x=2}^{k}\binom{n}{s_1}\binom{n}{s_2}\cdots\binom{n}{s_y}\mathrm{SW}_y(G)\right]$$

where $\sum_{i=1}^{x} r_i = k$ and $r_i \ge 1$, and $\sum_{i=1}^{y} s_i = k$ and $s_i \ge 1$.

Remark 2.4. [57] *Suppose that $k = 2$. Then $x = y = 2$, $r_1 = r_2 = \ldots = r_x = 1$, $\sum_{i=1}^{x} r_i = 2$, $s_1 = s_2 = \ldots = s_y = 1$, $\sum_{i=1}^{y} s_i = 2$. Therefore,*

$$\mathrm{SW}_2(G\Box H) = m^2\,\mathrm{SW}_2(G) + n^2\,\mathrm{SW}_2(H)\,.$$

Thus, the upper and lower bounds in Theorem 2.42 are sharp.

Let v is the root vertex of H and

$$d(v,k|H) = \sum_{\substack{v\in V(H)\,,\,S\subseteq V(H)\\ |S|=k}} d(S)\,.$$

Theorem 2.43. [57] *Let G be a connected graph with n vertices, and let H be a connected graph with m vertices. Let k be an integer, $2 \le k \le nm$. Then*

$$\begin{aligned}\mathrm{SW}_k(G\odot H) &= n\,\mathrm{SW}_k(H)+\sum_{\ell=2}^{k}\binom{m}{r_1}\binom{m}{r_2}\cdots\binom{m}{r_\ell}\mathrm{SW}_\ell(G)\\ &+ \sum_{\ell=2}^{k}\binom{n}{\ell}\left[\sum_{j=1}^{\ell}\prod_{\substack{x=1\\x\ne j}}^{\ell}\binom{m}{r_x}d(v,k|H)\right]\end{aligned}$$

where $\sum_{x=1}^{\ell} r_x = k$, $r_x \ge 1$ and v is the root-vertex of H.

Theorem 2.44. [57] *Let G be a connected graph with n vertices, and let H be a connected graph with m vertices. Let k be an integer, $2 \le k \le nm$. Then*

$$\mathrm{SW}_k(G\ominus H)=\sum_{\ell=2}^{k}\binom{m+1}{r_1}\binom{m+1}{r_2}\cdots\binom{m+1}{r_\ell}\mathrm{SW}_\ell(G)+\binom{m}{k-1}(k-1)n$$

$$+kn\binom{m}{k}-xn+\sum_{\ell=2}^{k}\binom{n}{\ell}\left[\sum_{j=1}^{\ell}\prod_{\substack{x=1\\x\ne j}}^{\ell}\binom{m+1}{r_x}\left[\binom{m}{r_j-1}(r_j-1)+r_j\binom{m}{r_j}-x_j\right]\right]$$

where $\sum_{x=1}^{\ell} r_x = k$, $r_x \geq 1$, x *is the number of the* k*-subsets of* $V(H)$ *such that the subgraph induced by each* k*-subset is connected in* H, *and* x_j *is the number of the* r_j*-subsets of* $V(H)$ *such that the subgraph induced by each* r_j*-subset is connected in* H.

Remark 2.5. *One can see that Theorems Theorem 2.40, 2.41, 2.42, 2.43, and 2.44 are extensions* $(1), (2), (3), (4), (5)$ *of Theorem 2.39, respectively. In all considered cases, for* $k = 2$, *the new results can be reduced to already known ones.*

2.6 Nordhaus–Gaddum-type results

In [89], Zhang and Wu studied the Nordhaus–Gaddum problem for the Wiener index and proved that for $G \in \mathcal{G}(n)$,

$$3\binom{n}{2} \leq \mathrm{W}(G) + \mathrm{W}(\overline{G}) \leq \frac{1}{6}(n^3 + 3n^2 + 2n - 6)\,.$$

Mao et al. [59] investigated the analogous problem for the Steiner Wiener index.

Theorem 2.45. [59] *Let* $G \in \mathcal{G}(n)$ *be a connected graph with a connected complement* $\overline{G}$. *Let* k *be an integer such that* $3 \leq k \leq n$. *Then:*

(1)

$$\binom{n}{k}(2k - 1 - x) \leq \mathrm{SW}_k(G) + \mathrm{SW}_k(\overline{G}) \leq \max\{n + k - 1, 4k - 2\}\binom{n}{k}$$

where if $n \geq 2k - 2$, *then* $x = 0$; $x = 1$ *for positive integer,*

(2)

$$(k-1)^2\binom{n}{k}^2 \leq \mathrm{SW}_k(G) \cdot \mathrm{SW}_k(\overline{G}) \leq \max\{k(n-1), (2k-1)^2\}\binom{n}{k}^2$$

Moreover, the lower bounds are sharp.

For $k = n$, the following result is immediate.

Observation 2.2. [59] *Let* $G \in \mathcal{G}(n)$ *be a connected graph with a connected complement* $\overline{G}$. *Then*

(1)

$$\mathrm{SW}_n(G) + \mathrm{SW}_n(\overline{G}) = 2n - 2\,;$$

(2)

$$\mathrm{SW}_n(G) \cdot \mathrm{SW}_n(\overline{G}) = (n-1)^2\,.$$

For $k = n-1$, they derived [59] the following result.

Proposition 2.9. [59] *Let $G \in \mathcal{G}(n)$ $(n \geq 5)$ be a connected graph with a connected complement $\overline{G}$.*

(1) *If G and $\overline{G}$ are both 2-connected, then $\mathrm{SW}_{n-1}(G) + \mathrm{SW}_{n-1}(\overline{G}) = 2n(n-2)$ and $\mathrm{SW}_{n-1}(G) \cdot \mathrm{SW}_{n-1}(\overline{G}) = n^2\,(n-2)^2$.*

(2) *If $\kappa(G) = 1$ and $\overline{G}$ is 2-connected, then $\mathrm{SW}_{n-1}(G) + \mathrm{SW}_{n-1}(\overline{G}) = 2n(n-2) + p$ and $\mathrm{SW}_{n-1}(G) \cdot \mathrm{SW}_{n-1}(\overline{G}) = n(n-2)(n^2-2n+p)$, where p is the number of cut vertices in G.*

(3) *If $\kappa(G) = \kappa(\overline{G}) = 1$, $\Delta(G) \leq n-3$, and G has a cut vertex v with pendent edge uv such that $G-u$ contains a spanning complete bipartite subgraph, and $\Delta(\overline{G}) \leq n-3$ and $\overline{G}$ has a cut vertex q with pendent edge pq such that $G-p$ contains a spanning complete bipartite subgraph, then $\mathrm{SW}_{n-1}(G) + \mathrm{SW}_{n-1}(\overline{G}) = 2(n-1)^2$ and $\mathrm{SW}_{n-1}(G) \cdot \mathrm{SW}_{n-1}(\overline{G}) = (n-1)^4$.*

(4) *If $\kappa(G) = \kappa(\overline{G}) = 1$, $\Delta(\overline{G}) = n-2$, $\Delta(G) \leq n-3$ and G has a cut vertex v with pendent edge uv such that $G-u$ contains a spanning complete bipartite subgraph, then*

$$\mathrm{SW}_{n-1}(G) + \mathrm{SW}_{n-1}(\overline{G}) = 2(n-1)^2 \quad \textit{or} \quad \mathrm{SW}_{n-1}(G) + \mathrm{SW}_{n-1}(\overline{G}) = 2(n-1)^2 + 1$$

and

$$\mathrm{SW}_{n-1}(G) \cdot \mathrm{SW}_{n-1}(\overline{G}) = (n-1)^4 \quad \textit{or} \quad \mathrm{SW}_{n-1}(G) \cdot \mathrm{SW}_{n-1}(\overline{G}) = (n-1)^2\,(n^2-2n+2)\,.$$

(5) *If $\kappa(G) = \kappa(\overline{G}) = 1$, $\Delta(G) = \Delta(\overline{G}) = n-2$, then*

$$2(n-1)^2 \leq \mathrm{SW}_{n-1}(G) + \mathrm{SW}_{n-1}(\overline{G}) \leq 2(n-1)^2 + 2$$

and

$$(n-1)^4 \leq \mathrm{SW}_{n-1}(G) \cdot \mathrm{SW}_{n-1}(\overline{G}) \leq (n^2-2n+2)^2\,.$$

For $k = 3$ and $n \geq 10$, from Theorem 2.45, one can see that

$$5\binom{n}{3} \leq \mathrm{SW}_3(G) + \mathrm{SW}_3(\overline{G}) \leq (n+2)\binom{n}{3} \quad \text{and}$$

$$4\binom{n}{3}^2 \leq \mathrm{SW}_3(G) \cdot \mathrm{SW}_3(\overline{G}) \leq 3(n-1)\binom{n}{3}^2\,.$$

Mao et al. [59] improved these bounds and proved the following result.

Theorem 2.46. [59] *Let* $G \in \mathcal{G}(n)$ $(n \geq 4)$ *be a connected graph with a connected complement* $\overline{G}$. *Then*

(1)

$$5\binom{n}{3} \leq \mathrm{SW}_3(G) + \mathrm{SW}_3(\overline{G})$$

$$\leq \begin{cases} 7\binom{n}{3} - 3n + 8, & \text{if } n = 6,7, \text{ and } sdiam_3(G) = 5, \\ & \text{or } n = 6,7, \text{ and } sdiam_3(\overline{G}) = 5; \\ 2\binom{n+1}{4} + 2\binom{n-3}{3} + \frac{1}{2}(7n^2 - 35n + 48), & \text{otherwise.} \end{cases}$$

(2)

$$6\binom{n}{3}^2 + (n-2)\binom{n}{3} - (n-2)^2$$

$$\leq \mathrm{SW}_3(G) \cdot \mathrm{SW}_3(\overline{G})$$

$$\leq \begin{cases} \frac{1}{4}\left[7\binom{n}{3} - 3n + 8\right]^2, & \text{if } n = 6,7, \text{ and } sdiam_3(G) = 5; \\ & \text{or } n = 6,7, \text{ and } sdiam_3(\overline{G}) = 5; \\ \left[\binom{n+1}{4} + \binom{n-3}{3} + \frac{1}{4}(7n^2 - 35n + 48)\right]^2, & \text{otherwise.} \end{cases}$$

Moreover, the bounds are sharp.

2.7 Steiner Wiener index and Steiner betweenness centrality

The *betweenness centrality* $B(v)$ of a vertex $v \in V(G)$ is defined as the sum of the fraction of all pairs of shortest paths that pass through v across all pairs of vertices in a graph:

$$B(v) = \sum_{x,y \in V(G)-v,\ x \neq y} \frac{\sigma_{x,y}(v)}{\sigma_{x,y}},$$

where $\sigma_{x,y}$ denotes the number of all shortest paths between vertices x and y in a graph G and $\sigma_{x,y}(v)$ denotes the number of all shortest paths between vertices x and y in graph G passing through the vertex v.

In a case when a graph models a social or communication network, as the name suggests, it measures the centrality of a vertex in a graph, by the influence of a vertex in the dissemination of information over a network. It has been independently introduced by Anthonisse [1] and by Freeman [22], and, among other applications, has been applied to detect communities in networks [26, 63].

For a graph G, let $n(G)$ denote the number of its vertices. For a forest (acyclic graph) F with $p > 1$ connected components $T_1, T_2, \ldots, T_p$, denote by $N_k(F)$ the sum over all partitions of k into at least two nonzero parts of products of combinations distributed among the p components of F:

$$N_k(F) = \sum_{\ell_1+\ell_2+\ldots+\ell_p=k,\ 0\le\ell_1,\ell_2,\ldots,\ell_p<k} \binom{n(T_1)}{\ell_1}\binom{n(T_2)}{\ell_2}\cdots\binom{n(T_p)}{\ell_p}.$$

For a tree T, we define $N_k(T) = 0$. Note that by the definition $\binom{n}{0} = 1$ and $\binom{n}{k} = 0$ whenever $n < k$.

Kovše [39] derived the following result for Steiner Wiener index.

Theorem 2.47. [39] (1) *Let T be a tree on n vertices. Then*

$$\mathrm{SW}_k(T) = \sum_{e\in E(T)} N_k(T-e).$$

(2) *Let T be a tree on n vertices. Then*

$$\mathrm{SW}_k(T) = \sum_{v\in V(T)} N_k(T-v) + (k-1)\binom{n}{k}.$$

The *Steiner k-betweenness centrality* $B_k(v)$ of a vertex $v \in V(G)$ is defined as the sum of the fraction of all k-Steiner trees that include v as its non-terminal vertex across all combinations of k vertices of G:

$$B_k(v) = \sum_{S\in V(G)\setminus\{v\},\ |S|=k} \frac{\sigma_S(v)}{\sigma_S},$$

where σ_S denotes the number of all Steiner trees between vertices of S in a graph G and $\sigma_S(v)$ denotes the number of all Steiner trees between vertices of S in a graph G that include also the vertex v as a non-terminal vertex.

Theorem 2.48. [39] (1) *Let G be a connected graph on n vertices. Then*

$$\mathrm{SW}_k(G) = \sum_{v\in V(G)} B_k(v) + (k-1)\binom{n}{k}.$$

For a graph G on n vertices the *average k-Steiner betweenness* $\overline{B_k}(G)$ is defined as

$$\overline{B_k}(G) = \frac{1}{n}\sum_{v\in V(G)} B_k(v).$$

Corollary 2.49. [39] *Let G be a connected graph on n vertices. Then*

$$\overline{B_k}(G) = \frac{1}{n}\binom{n}{k}(\mu_k(G) - k + 1).$$

2.8 Chemical applications of Steiner Wiener index

The Wiener index was originally devised as a tool for predicting the boiling points of alkanes at standard pressure [82]. Eventually, the quality of topological indices was tested by correlating them with boiling points of alkanes [62, 68, 71, 72]. In view of this, the Steiner Wiener indices were also subjected to the same test. The following results are published in [31].

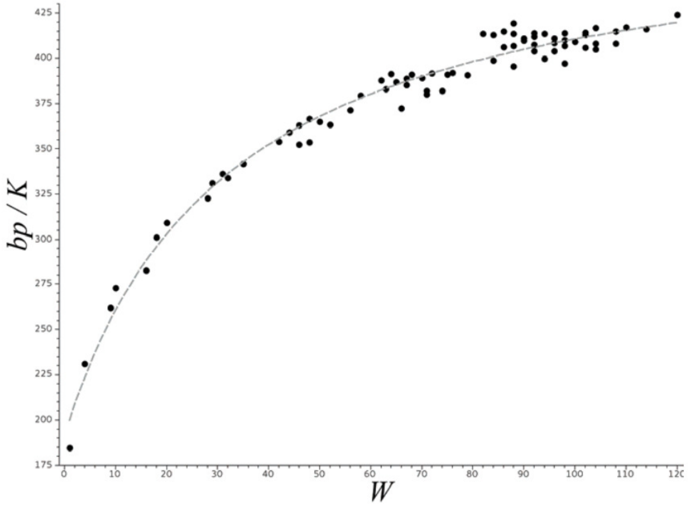

Figure 2.8 Correlation between normal boiling points (bp/K) and Wiener index (W) for the set of all isomeric alkanes with 2 to 9 carbon atoms. The curve passing through the data-points is specified by Eq. (8). Statistical data pertaining to this correlation are found in Tables I and II, for $k = 2$.

Figure 2.8 is reproducing the well known [62] plot of the normal boiling points vs. the Wiener index. The curve passing through the data-points is of the form

$$bp \approx bp_{calc}(W^*) = \frac{a + bW^*}{1 + cW^*}\,, \tag{8}$$

where $W^* = W$ and where a, b, c are fitting parameters. The correlation between the experimental and calculated boiling points (i.e., between bp and bp_{calc}, cf. Eq. (8)), is shown in Figure 2.9.

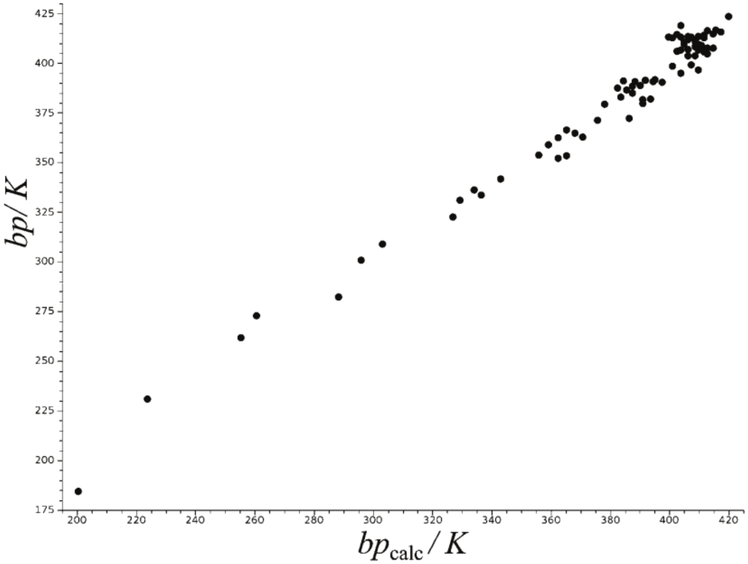

Figure 2.9 Correlation between the calculated boiling points (bp_{calc}, according to Eq. (8), $W^* = W$) and the experimental boiling points (bp) for the same compounds as in Figure 2.8. Statistical data pertaining to this correlation are found in Tables 3 and 4, for $k = 2$.

Table 3 Fitting parameters in formulas (8) and (9), for $k = 2, 3, \ldots, 9$. The (a, b, c)-values were obtained by means of the scaled Levenberg-Marquardt algorithm; see [64]. The λ-values are those for which the respective correlation coefficients are maximal, cf. Figure 2.9. The parameters of the best approximation are bolded.

k	a	b	c	λ
2	191.328	15.104	0.031	–
3	192.480	14.547	0.031	0.023
4	193.704	14.820	0.032	0.044
5	191.287	16.476	0.037	0.063
6	186.764	18.773	0.043	0.127
7	**181.255**	**21.421**	**0.049**	**0.392**
8	180.547	20.834	0.047	0.802
9	187.788	16.790	0.036	1.400

Table 4 Statistical data for the correlations between boiling points and the topological indices, $k = 2, 3, \ldots, 9$; R =correlation coefficient, ARE =average relative error (in %), MRE = maximal observed relative error (in %). By boldface are indicated the data for the best approximation. For details, see Eqs. (8) and (9) and the text .

k	R	ARE	MRE
2	0.98954	1.45	8.42
3	0.98957	1.45	8.83
4	0.99018	1.41	9.46
5	0.99135	1.33	8.58
6	0.99256	1.23	6.80
7	**0.99323**	**1.18**	**4.63**
8	0.99273	1.23	4.19
9	0.99149	1.33	6.98

The replacement of W^* by SW_k in the Eq. (8) did not show any improvement. Then, the following modification of the Wiener index was used:

$$W^* = \mathrm{W} + \lambda \mathrm{SW}_k, \tag{9}$$

and use the variable W^* in combination with Eq. (8). For each fixed choice of k, $k = 3, 4, \ldots, 8$, the parameter λ was varied, and its value determined to maximize the correlation coefficient for the linear correlation between bp and $bp_{calc}(W^*)$. In all studied cases, an optimal value for λ exists at which the correlation coefficients attain a maximum; a characteristic example is shown in Figure 2.10.

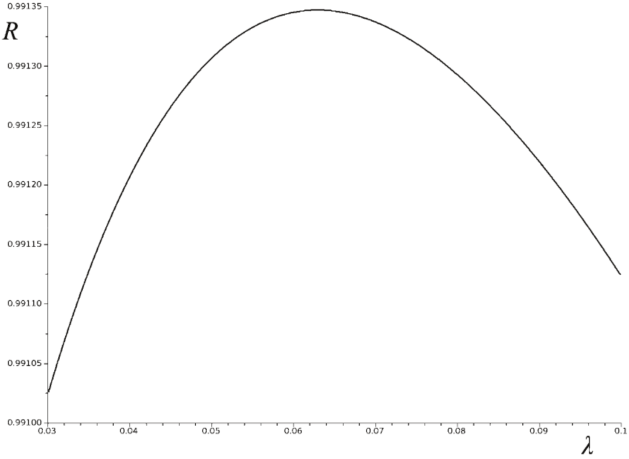

Figure 2.10 The λ-dependence of the correlation coefficient R for the correlation between bp and bp_{calc} for the case $k = 5$. The maximum is attained at $\lambda = 0.063$, cf. Table 3.

The results thus obtained are presented in Tables 3 and 4, and in Figures. 2.11 and 2.12.

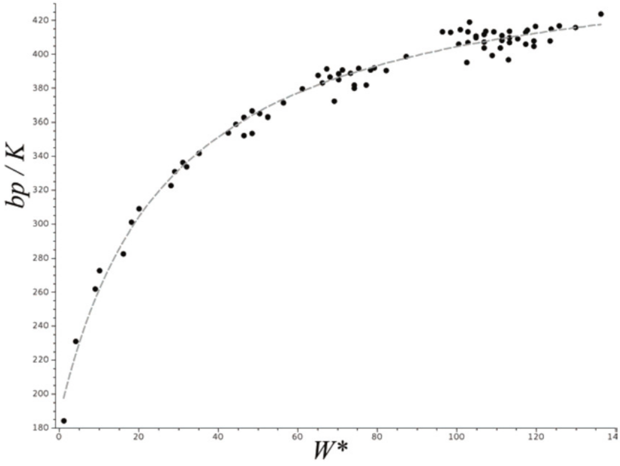

Figure 2.11 Normal boiling points (bp/K) vs. $W + \lambda SW_7$ for the same alkanes as in Figure 2.8. As the data in Tables 3 and 4 show, the choice $k = 7$ provides the best agreement between bp and bp_{calc}, cf. Eqs. (8) and (9).

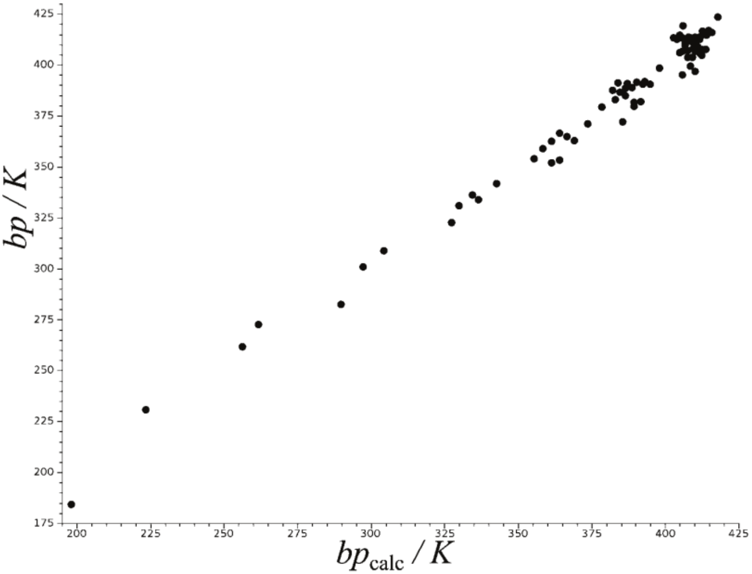

Figure 2.12 The best correlation between bp and bp_{calc}, was obtained by Eqs. (8) and (9) for $k = 7$. Statistical data pertaining to this correlation are to be found in Tables 3 and 4.

Although Figures 2.11 and 2.12 look a lot alike the Figures 2.9 and 2.10, the average and maximal relative errors of predictions are 20% and 50% smaller, respectively. Therefore, it may be claimed that the multicenter-distance-contributions improve the model of predicting physico–chemical properties (shown in Figure 2.9), but only to a limited extent.

3 Steiner degree distance

The degree distance (DD) is a recently adopted name for the part of the MTI index (also known as the Schultz index), which carries information rather different from already known topological molecular descriptors. Since DD is an index based on the topological distance, besides the vertex degree, its definition can be generalized by using the Steiner distance instead. The Steiner degree distance was elaborated in a couple of recent papers, and the main results are summarized in the next few subsections.

3.1 Results for special graphs

It is needless to say that all formulas presented in this subsection are also valid for the ordinary degree distance, a.k.a. when $k=2$.

Theorem 3.1. [58] *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 $2 \leq k \leq n-2$ or $2 \leq k \leq a+b-2$,*

$$\begin{aligned}
\mathrm{SDD}_k(S_n) &= (2kn-n-3k+2)\binom{n-1}{k-1} \\
\mathrm{SDD}_k(P_n) &= \frac{2(k-1)(kn-1)}{k+1}\binom{n}{k} \\
\mathrm{SDD}_k(K_n) &= n(n-1)^2\binom{n-2}{k-2}
\end{aligned}$$

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

Gutman [29] derived the following results for trees.

Theorem 3.2. [29] *Let T be a tree of order n with edge set $E(T)$. Then for $2 \leq k \leq n$, the k-center Steiner degree distance of T obeys the identity*

$$\mathrm{SDD}_k(T) = \sum_{e \in E(T)} \sum_{i=1}^{k-1} \left[\binom{n_1(e)-1}{i-1}(2n_1(e)-1)\binom{n_2(e)}{k-i} + \binom{n_2(e)-1}{k-i-1}(2n_2(e)-1)\binom{n_1(e)}{i} \right]. \tag{10}$$

For $k=3$, using Theorem 3.2, Gutman [29] obtained the following result.

Theorem 3.3. [29] *Let T be a tree of order n. Then*

$$\mathrm{SDD}_3(T) = (3n-7)\mathrm{W}(T) - \frac{1}{2}n(n-1)(n-3).$$

Redžepović, Mao, Wang and Furtula [67] derived the following results.

Theorem 3.4. [67] *Let* G *be a graph of order* n *and size* m *. Then*

$$\mathrm{SDD}_3(G) \geq \frac{n-3}{2}\,\mathrm{SDD}_2(G) + m \cdot \mathrm{W}(G) \tag{11}$$

with equality attained in the case of trees.

Theorem 3.5. [67] *Let* T *be a tree of order* n *. Then,*

$$\mathrm{SDD}_4(T) \approx \frac{14n^2 - 77n + 105}{12}\,\mathrm{W}(T) - \frac{(n-1)(n-3)}{12}\left(\frac{3}{4}n^2 - 4n - 2\right) \tag{12}$$

The quality of approximation, shown in the Eq. (12), was tested with the help of a computer, and obtained results are given in Table 5.

Table 5 Coefficients of correlations (R) and average relative error (ARE) of the approximation given in Eq. (12).

n	# of trees	R	ARE
8	23	0.9990	1.50%
9	47	0.9989	1.48%
10	106	0.9989	1.52%
11	235	0.9989	1.61%
12	551	0.9989	1.74%
13	1301	0.9989	1.88%
14	3159	0.9989	2.02%
15	7741	0.9989	2.15%

Using the data from Table 5, Redžepović et al. [67] corroborate their claim that the almost all variations noticed in the values of $\mathrm{SDD}_4(T)$ could be explained by the model based on the Wiener index.

3.2 Formulas for large k

The following observation is immediate.

Observation 3.1. [58] *Let* G *be the connected graph of order* n *and size* m*. Then directly from the definition of* $\mathrm{SDD}_n(G)$*, Eq. (2), it follows*

$$\mathrm{SDD}_n(G) = 2m(n-1).$$

In [51], Mao obtained the following result.

Lemma 3.1. [51] *Let G be a connected graph of order n. Then* $\mathrm{sdiam}_{n-1}(G) = n-2$ *if and only if G is 2-connected.*

Mao, Wang, Gutman, and Klobučar [58] showed how to compute $\mathrm{SDD}_{n-1}(G)$.

Theorem 3.6. [58] *Let G be a connected graph of order n , size m , and vertex-connectivity $\kappa(G)$.*

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

$$\mathrm{SDD}_{n-1}(G) = 2m(n-2)(n-1)\,. \tag{13}$$

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

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

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

In [58], Mao et al. presented the following expression of $\mathrm{SDD}_{n-1}(T)$.

Theorem 3.7. [58] *Let T be a tree of order n, possessing p pendent vertices. Then*

$$\mathrm{SDD}_{n-1}(T) = 2(n-1)^3 - p(2n-3) \tag{15}$$

irrespective of any other structural detail of T.

3.3 Lower and upper bounds for general graphs

The bounds stated as Proposition 3.1, follow immediately from the the definitions of the Steiner Wiener index, Eq. (1), and Steiner degree distance, Eq. (2).

Proposition 3.1. [58] *Let G be a connected graph of order n. Then*

$$k\delta(G)\mathrm{SW}_k(G) \leq \mathrm{SDD}_k(G) \leq k\Delta(G)\mathrm{SW}_k(G)$$

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

Mao et al. [58] derived the following bounds for $\mathrm{SDD}_k(G)$.

Theorem 3.8. [58] *Let G be a connected graph of order n and size m. Then*

$$2m\binom{n-1}{k-1}(k-1) \leq \mathrm{SDD}_k(G) \leq 2m\binom{n-1}{k-1}(n-1) \tag{16}$$

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

Proposition 3.2. [58] *Let G be a connected graph of order n. Then*

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

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

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 Proposition 3.2 and Theorem 3.1 that

$$\mathrm{SDD}_k(K_n) = n(n-1)^2\binom{n-2}{k-2} = \binom{n}{k}k(n-1)(k-1) = k\delta(K_n)\,\mathrm{SW}_k(K_n).$$

To show the sharpness of the upper bound, we consider the path P_2. Since $\delta(P_2) = 1$, it follows from Proposition 3.2 and Theorem 3.1 that

$$\mathrm{SDD}_2(P_n) = \mathrm{DD}(P_n) = 2 = 2\Delta(P_2)\,\mathrm{SW}_2(P_2)\,.$$

Redžepović et al. [67] derived the following upper and lower bounds for Steiner distance.

Theorem 3.9. [67] *Let G be a connected graph, and $S = \{v_1, v_2, \ldots, v_k\} \subseteq V(G)$. Then*

$$\frac{\sum\limits_{i=1}^{k} d_G(S-v_i)+2}{k} \le d_G(S) \le \frac{\sum\limits_{i=1}^{k} d_G(S-v_i)}{k} + \mathrm{diam}(G).$$

The lower and upper bounds are attained for the P_n and the K_n, respectively.

Additionally, in [67] the following result is presented.

Theorem 3.10. [67] *Let G be a connected graph of order n, size m. Denote by δ minimum degree and by Δ maximum degree in a set of connected graphs. Then*

$$\begin{aligned}
&\frac{n-k+1}{k}[\mathrm{SDD}_{k-1}(G)+\delta\,\mathrm{SW}_{k-1}(G)] + \frac{4m}{k}\binom{n-1}{k-1}\\
\le\ & \mathrm{SDD}_k(G)\\
\le\ & \frac{n-k+1}{k}[\mathrm{SDD}_{k-1}(G)+\Delta\,\mathrm{SW}_{k-1}(G)] + 2m\binom{n-1}{k-1}\mathrm{diam}(G).
\end{aligned}$$

For K_n the upper bound is attained.

As we have seen, we can not show the sharpness of lower bound in Theorem 3.10, but for dense graphs, we can improve the above lower bound and show the sharpness of new bound.

Theorem 3.11. [67] *Let G be a connected graph of order n and size m. If $\kappa(G) \geq n-k+1$, then*

$$\begin{aligned}
& \frac{n-k+1}{k}[\mathrm{SDD}_{k-1}(G)+\delta\,\mathrm{SW}_{k-1}(G)]+2m\binom{n-1}{k-1} \\
\leq\ & \mathrm{SDD}_k(G) \\
\leq\ & \frac{n-k+1}{k}[\mathrm{SDD}_{k-1}(G)+\Delta\,\mathrm{SW}_{k-1}(G)]+2m\binom{n-1}{k-1}\mathrm{diam}(G).
\end{aligned}$$

The upper bound is attained for K_n.

3.4 Results for graph products

Mao et al. [54] derived the exact expression of $\mathrm{SDD}_k(G \vee H)$.

Theorem 3.12. [54] *Let G, H be two connected graphs of order a, b $(a \leq b)$, respectively. Let k be an integer with $3 \leq k \leq a+b$.*

(1) *If $1 \leq k \leq a$, then*

$$\begin{aligned}
\mathrm{SDD}_k(G \vee H) &= k\binom{a}{k} - x - 2e(G)\binom{a-1}{k-1} - \sum_{i=1}^{x}\left(\sum_{v \in S_i} deg_G(v)\right) + k\binom{b}{k} - y \\
&- 2e(H)\binom{b-1}{k-1} - \sum_{i=1}^{y}\left(\sum_{v \in S_i'} deg_H(v)\right) \\
&+ 2(k-1)[e(G)+e(H)+ab]\binom{a+b-1}{k-1} \\
&- (k-1)ab\binom{a-1}{k-1} - (k-1)ab\binom{b-1}{k-1},
\end{aligned}$$

where $S_1, S_2, \ldots, S_x$ are all the k-subsets of $V(G)$ such that $G[S_i]$ $(1 \leq i \leq x)$ is connected, and $S_1', S_2', \ldots, S_y'$ are all the k-subsets of $V(H)$ such that $H[S_i']$ $(1 \leq i \leq y)$ is connected.

(2) *If $a < k \leq b$, then*

$$\begin{aligned}
\mathrm{SDD}_k(G \vee H) &= ak^2\binom{b}{k} - akx + 2e(H)\binom{b-1}{k-1} - \sum_{i=1}^{x}\left(\sum_{v \in S_i} deg_H(v)\right) \\
&+2(k-1)[e(G)+e(H)+ab]\binom{a+b-1}{k-1} - (k-1)ab\binom{a-1}{k-1} \\
&-(k-1)ab\binom{b-1}{k-1} - (k-1)\cdot 2e(G)\binom{a-1}{k-1},
\end{aligned}$$

where $S_1, S_2, \ldots, S_x$ *are all the* k*-subsets of* $V(H)$ *such that* $H[S_i]$ $(1 \leq i \leq x)$ *is connected.*

(3) *If* $b < k \leq a+b$*, then*

$$\begin{aligned}\mathrm{SDD}_k(G \vee H) &= 2(k-1)e(G)\left[\binom{a+b-1}{k-1} - \binom{a-1}{k-1}\right] - (k-1)ab\left[\binom{a-1}{k-1}\right.\\ &\left.+\binom{b-1}{k-1}\right] + 2(k-1)e(H)\left[\binom{a+b-1}{k-1} - \binom{b-1}{k-1}\right].\end{aligned}$$

The upper and lower bounds of $\mathrm{SDD}_k(G \square H)$ are also given in [54].

Theorem 3.13. [54] *Let* G, H *be two connected graphs of order* a, b $(a \leq b)$*, respectively. Let* k *be an integer with* $3 \leq k \leq a+b$*. Then*

$$X \leq \mathrm{SDD}_k(G \square H) \leq \left\lceil \frac{k-1}{2} \right\rceil X,$$

where

$$\begin{aligned}X &= \sum_{i=1}^{k} b\binom{b-1}{r_1-1}\binom{b}{r_2}\cdots\binom{b}{r_i}\mathrm{SDD}_i(G) + \sum_{j=1}^{k} a\binom{a-1}{s_1-1}\binom{a}{s_2}\cdots\binom{a}{s_j}\mathrm{SDD}_j(H)\\ &+2e(H)\sum_{i=1}^{k} b\binom{b-1}{r_1-1}\binom{b}{r_2}\cdots\binom{b}{r_i} i\mathrm{SW}_i(G)\\ &+2e(G)\sum_{j=1}^{k} a\binom{a-1}{s_1-1}\binom{a}{s_2}\cdots\binom{a}{s_j} j\mathrm{SW}_j(H), \text{ and}\end{aligned}$$

$\sum_{p=1}^{i} r_p = k$, $\sum_{q=1}^{j} s_q = k$, $r_p \geq 1$ $(1 \leq p \leq i)$, $s_q \geq 1$ $(1 \leq q \leq j)$.

3.5 Prediction potential of Steiner degree distance indices

Since the beginning of the application of topological indices in chemistry, they have been using primarily for modeling the physico–chemical properties of molecules. The first topological index ever introduced (Wiener index) demonstrated its prediction power on the boiling points of a set of alkanes [82]. This is probably one of the main reasons why the newly introduced topological indices are subjected to testing their predictive ability on the sets of boiling points of alkanes.

It was noticed that in the case of a set of alkane isomers, the correlation between the Wiener index and boiling points is of unacceptably low quality. Since there exists the linear relation between the Wiener and the degree distance indices for isomeric alkanes [30], the same low quality correlation of the boiling points and $\mathrm{DD}(G)$ is being exposed.

Hoping that the Steiner degree distance indices would show better prediction power than the “ordinary” degree distance, and bearing in mind the above mentioned facts, the examination of correlations with the boiling points of isomeric alkanes was conducted in [67]. In particular, the boiling points of octanes were modeled with the $\mathrm{SDD}_k(G)$ indices for $k = 2, 3, \ldots, 7$, using the linear equation described in the caption of Table 6. The coefficient of determination was used as a measure of the explanation of the variance in data. Results are given in Table 6.

Table 6 The determination coefficients of modeling the boiling points of octanes by the linear model $\alpha \cdot \mathrm{SDD}_x + \beta \cdot \mathrm{SDD}_y + \varepsilon$, where $x, y \in \{2, 3, \ldots, 7\}$.

		R^2					
		SDD_2	SDD_3	SDD_4	SDD_5	SDD_6	SDD_7
R^2	SDD_2	29.15%	29.15%	65.78%	65.78%	65.61%	64.81%
	SDD_3		29.15%	65.78%	65.78%	65.61%	64.81%
	SDD_4			33.13%	65.78%	65.58%	64.68%
	SDD_5				40.20%	65.41%	64.26%
	SDD_6					47.63%	63.22%
	SDD_7						53.66%

Data from Table 6 are telling us that the linear model with $\mathrm{SDD}_k(G)$ as a sole parameter cannot be used for describing the variance in the boiling points of alkanes. The best such model with $\mathrm{SDD}_7(G)$ explains only 50% of boiling points’ variance. The same coefficients of determination, obtained for $\mathrm{SDD}_2(G)$ and $\mathrm{SDD}_3(G)$, are expected because of the existence of the linear relationship between these two indices. An explanation of variance in the set of boiling points of octanes is increasing among one-parameter linear models with an increase of k. This was explained in [67] that the Steiner degree distance with larger k are more sensitive on the branching in the alkanes. The two-parameter linear models that exhibit the highest value of the R^2 are observed for $\mathrm{SDD}_2(G)$ (or $\mathrm{SDD}_3(G)$) and $\mathrm{SDD}_4(G)$ (or $\mathrm{SDD}_5(G)$). These models, in comparison with one-parameter models, improve the explanation of variance in the set of boiling points by more than twice.

4 Steiner Gutman index

Inspired by the already introduced invariants based on the Steiner distance, Mao and Das introduced the $\mathrm{SGut}_k(G)$ in 2018 [53]. The following result was presented in the very first paper on the Steiner Gutman index.

Proposition 4.1. [53] *Let K_n be the complete graph of order n, and let k be an integer such that $2 \leq k \leq n$. Then*

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

By the similar method, authors in [58] derived the result for complete bipartite graphs.

Theorem 4.1. [53] *Let $K_{a,b}$ be the complete bipartite graph of order $a+b$ $(1 \leq a \leq b)$, and let k be an integer such that $2 \leq k \leq a+b$. Then*

$$\mathrm{SGut}_k(K_{a,b}) = \begin{cases} ka^k\binom{b}{k} + kb^k\binom{a}{k} + (k-1)\sum\limits_{x=1}^{k-1}\binom{a}{x}\binom{b}{k-x}b^x a^{k-x} & \text{if } 1 \leq k \leq a \\ ka^k\binom{b}{k} + (k-1)\sum\limits_{x=1}^{a}\binom{a}{x}\binom{b}{k-x}b^x a^{k-x} & \text{if } a < k \leq b \\ (k-1)\sum\limits_{x=1}^{a}\binom{a}{x}\binom{b}{k-x}b^x a^{k-x} & \text{if } b < k \leq a+b. \end{cases}$$

From the Theorem 4.1 the following corollary can be deduced.

Corollary 4.2. [53] *Let S_n be the star of order n $(n \geq 3)$, and let k be an integer such that $2 \leq k \leq n$. Then*

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

Mao and Das derived the equality, shown in Proposition 4.2, for the calculation of the Steiner Gutman index of paths of order n.

Proposition 4.2. [53] *Let P_n be the path of order n, and let k be an integer such that $2 \leq k \leq n-2$. Then*

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

For $k = n$, the following result is immediate.

Observation 4.1. [53] *Let G be the connected graph of order n. Then*

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

In [51], Mao obtained the following result.

Lemma 4.1. [51] *Let G be a graph. Then* $\mathrm{sdiam}_{n-1}(G) = n-2$ *if and only if G is 2-connected.*

Mao and Das [53] gave the expression of $\mathrm{SGut}_{n-1}(G)$ for a graph G.

Proposition 4.3. [53] *Let G be a connected graph of order n.*

(1) *If G is 2-connected, then*

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

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

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

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

The following corollary is immediate.

Corollary 4.3. [53] *Let T be a tree of order n. If $v_1, v_2, \ldots, v_p$ are all the pendent vertices in T, then*

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

4.1 Lower and upper bounds for general graphs

The following bounds are sharp for $\mathrm{SGut}_k(G)$.

Theorem 4.4. [53] *Let G be a connected graph of order n, and let k be an integer with $2 \le k \le n$. Then*

$$\delta(G)^k \mathrm{SW}_k(G) \le \mathrm{SGut}_k(G) \le \Delta(G)^k \mathrm{SW}_k(G),$$

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

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

The following result can be easily seen.

Proposition 4.4. [53] *Let G be a connected graph of order n, and let k be an integer such that $2 \leq k \leq n$. Then*

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

Moreover, the bounds are sharp.

To show the sharpness of the lower bound, we consider the complete graph K_n. Since $\delta(K_n) = n-1$, it follows from Proposition 4.1 that

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

To show the sharpness of the upper bound, we consider the path P_2. For $k = 2$, since $\Delta(P_2) = 1$, it follows from Proposition 4.2 that

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

For graph G having n vertices and m edges, they derived the following upper and lower bounds of $\mathrm{SGut}_k(G)$.

Theorem 4.5. [53] *Let G be a connected graph n vertices and m edges, and let k be an integer with $2 \leq k \leq n$. Then*

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

Moreover, the upper and lower bounds are sharp.

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

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

Wang et al. [81] derived lower and upper bounds on $\mathrm{SGut}_k(G)$ in terms of n, m, maximum degree Δ and minimum degree δ:

Proposition 4.5. [81] *Let G be a connected graph of order $n \geq 3$ with m edges and maximum degree Δ, minimum degree δ. Also let k be an integer with $2 \leq k \leq n$. Then*

$$2m(n-1)\binom{n-1}{k-1}\frac{\Delta^{k-1}}{k} \geq \mathrm{SGut}_k(G) \geq \begin{cases} 2m(k-1)\binom{n-1}{k-1}\frac{\delta^{k-1}}{k} & \text{if } \delta \geq 2 \\ k\binom{p}{k} + 2^q(k-1)\left[\binom{n}{k} - \binom{p}{k}\right] & \text{if } \delta = 1, \end{cases}$$

where p is the number of pendent vertices in G, and $q = \max\{k-p, 1\}$. The equality of upper bound holds if and only if G is a regular graph with $k = n$. The equality of lower bound holds if and only if G is a regular $(n-k+1)$-connected graph of order n $(\delta \geq 2)$ or G is a path of order n and $k = n$ $(\delta = 1)$ or G is a path of order 3 and $k = 2$ when $(\delta = 1)$.

Mao and Das [53] proved that the complete graph K_n gives the maximum k-Steiner Gutman index of graphs.

Theorem 4.6. [53] *Let G be a connected graph of order n. If there is a positive integer $k > 0.618n$, then*

$$\mathrm{SGut}_k(G) \leq \binom{n}{k}(n-1)^k(k-1) \tag{17}$$

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

4.2 Comparison between $\mathbf{SDD}_k$ and $\mathbf{SGut}_k$ of graphs

The comparison between SDD_k and SGut_k of graphs was examined in [53].

Example 4.1. [53] *Let S_n be the star of order n $(n \geq 3)$, and let k be an integer such that $2 \leq k \leq n$. Then*

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

By Theorem 3.1 and Example 4.1, they derived the following proposition.

Proposition 4.6. [53] *Let G be a connected graph of order n with minimum degree δ, and let k be an integer with $3 \leq k \leq n$. Let p be the number of the pendent vertices in G.*

(1) *If $\delta(G) \geq 2$, then*

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

(2) *If $\delta(G) = 1$, $p \leq k$ and $2^{k-p} \geq 2(k-p) + p$, then*

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

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

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

Proposition 4.7. [53] *Let* G *be a connected graph of order* n *with minimum degree* δ, *and let* k *be an integer with* $3\leq k\leq n$.

(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*

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

4.3 Nordhaus–Gaddum-type results

Wang et al. [81] derived the Nordhaus–Gaddum-type results on $\mathrm{SGut}_k(G)$.

Theorem 4.7. [81] *Let* G *be a connected graph of order* n *with* m *edges, maximum degree* Δ, *minimum degree* δ *and a connected* $\overline{G}$. *Also let* k *be an integer with* $2\leq k\leq n$. *Then*

(1)

$$\mathrm{SGut}_k(G)+\mathrm{SGut}_k(\overline{G})\leq (n-1)^2\binom{n}{k}s_1^{k-1}$$

and

$$\mathrm{SGut}_k(G)\cdot \mathrm{SGut}_k(\overline{G})\leq 2m(n^2-n-2m)(n-1)^2\binom{n-1}{k-1}^2\frac{\Delta^{k-1}\,(n-\delta-1)^{k-1}}{k^2},$$

where $s_1=\max\{\Delta,\, n-\delta-1\}$. *Moreover, the upper bounds are sharp.*

(2)

$$\mathrm{SGut}_k(G)+\mathrm{SGut}_k(\overline{G})$$
$$\geq \begin{cases} (n-1)(k-1)\binom{n}{k}\,t_1^{k-1} & \text{if } \delta\geq 2,\ \Delta\leq n-3\\ 2m(k-1)\binom{n-1}{k-1}\frac{\delta^{k-1}}{k}+k\binom{n}{k} & \text{if } \delta\geq 2,\ \Delta=n-2\\ k\binom{n}{k}+[n(n-1)-2m](k-1)\binom{n-1}{k-1}\frac{(n-\Delta-1)^{k-1}}{k} & \text{if } \delta=1,\ \Delta\leq n-3\\ 2k\binom{n}{k} & \text{if } \delta=1,\ \Delta=n-2, \end{cases}$$

where $t_1=\min\{\delta,\, n-\Delta-1\}$.

(3)

$$\mathrm{SGut}_k(G)\cdot\mathrm{SGut}_k(\overline{G})$$

$$\geq \begin{cases} 2m(n^2-n-2m)(k-1)^2\binom{n-1}{k-1}^2\frac{\delta^{k-1}\,(n-\Delta-1)^{k-1}}{k^2} & \text{if } \delta\geq 2,\ \Delta\leq n-3\\ 2m(k-1)\binom{n}{k}\binom{n-1}{k-1}\delta^{k-1} & \text{if } \delta\geq 2,\ \Delta=n-2\\ [n(n-1)-2m](k-1)\binom{n}{k}\binom{n-1}{k-1}(n-\Delta-1)^{k-1} & \text{if } \delta=1,\ \Delta\leq n-3\\ k^2\binom{n}{k}^2 & \text{if } \delta=1,\ \Delta=n-2. \end{cases}$$

To show the sharpness of the upper bound and the lower bound, we consider the following example.

Example 4.2. [81] *For* $\delta(G)\geq 2$, $\Delta\leq n-3$, *we let* G *and* $\overline{G}$ *be two* $\frac{n-1}{2}$*-regular graphs of order* n, *where* n *is odd. If* $k=n$, *then* $\mathrm{SGut}_k(G)=(n-1)(\frac{n-1}{2})^n$, $\mathrm{SGut}_k(\overline{G})=(n-1)(\frac{n-1}{2})^n$, $s_1=\max\{\Delta,\,n-\delta-1\}=\frac{n-1}{2}$, $\Delta\,(n-\delta-1)=(\frac{n-1}{2})^2$, $t_1=\min\{\delta,\,n-\Delta-1\}=\frac{n-1}{2}$, *and* $\delta\,(n-\Delta-1)=(\frac{n-1}{2})^2$. *Furthermore, we have* $\mathrm{SGut}_k(G)+\mathrm{SGut}_k(\overline{G})=2(n-1)(\frac{n-1}{2})^n=(n-1)^2\binom{n}{k}s_1^{k-1}$, $\mathrm{SGut}_k(G)\cdot\mathrm{SGut}_k(\overline{G})=(n-1)^2(\frac{n-1}{2})^{2n}=2m(n^2-n-2m)(n-1)^2\binom{n-1}{k-1}^2\frac{\Delta^{k-1}\,(n-\delta-1)^{k-1}}{k^2}$, $\mathrm{SGut}_k(G)+\mathrm{SGut}_k(\overline{G})=2(n-1)(\frac{n-1}{2})^n=(n-1)(k-1)\binom{n}{k}t_1^{k-1}$ *and* $\mathrm{SGut}_k(G)\cdot\mathrm{SGut}_k(\overline{G})=(n-1)^2(\frac{n-1}{2})^{2n}=2m(n^2-n-2m)(k-1)^2\binom{n-1}{k-1}^2\frac{\delta^{k-1}\,(n-\Delta-1)^{k-1}}{k^2}$.

The following corollary is immediate from above theorem.

Corollary 4.8. [81] *Let* G *be a connected graph of order* $n\geq 4$ *with maximum degree* Δ *and minimum degree* δ. *Then*

(1)

$$(n-1)^2\binom{n}{k}s_1^{k-1}\geq \mathrm{SGut}_k(G)+\mathrm{SGut}_k(\overline{G})$$

$$\geq \begin{cases} (n-1)(k-1)\binom{n}{k}\,t_1^{k-1} & \text{if } \delta\geq 2,\ \Delta\leq n-3\\ n(k-1)\binom{n-1}{k-1}\frac{\delta^k}{k}+k\binom{n}{k} & \text{if } \delta\geq 2,\ \Delta=n-2\\ k\binom{n}{k}+n(k-1)\binom{n-1}{k-1}\frac{(n-\Delta-1)^k}{k} & \text{if } \delta=1,\ \Delta\leq n-3\\ 2k\binom{n}{k} & \text{if } \delta=1,\ \Delta=n-2, \end{cases}$$

where $s_1=\min\{\Delta,\,n-\delta-1\}, t_1=\min\{\delta,\,n-\Delta-1\}$;

(2)

$$n^2\binom{n-1}{k-1}^2\frac{\Delta^{k-1}\,(n-\delta-1)^{k-1}\,(n-1)^4}{4k^2}\geq \mathrm{SGut}_k(G)\cdot \mathrm{SGut}_k(\overline{G})$$

$$\geq\begin{cases} n^2(k-1)^2\binom{n-1}{k-1}^2\frac{\delta^k\,(n-\Delta-1)^k}{k^2} & \text{if } \delta\geq 2,\ \Delta\leq n-3\\ n(k-1)\binom{n}{k}\binom{n-1}{k-1}\delta^k & \text{if } \delta\geq 2,\ \Delta=n-2\\ n(k-1)\binom{n}{k}\binom{n-1}{k-1}\,(n-\Delta-1)^k & \text{if } \delta=1,\ \Delta\leq n-3\\ k^2\binom{n}{k}^2 & \text{if } \delta=1,\ \Delta=n-2.\end{cases}$$

Using the famous inequality given in [65], the following lower and upper bounds on $\mathrm{SGut}_k(G)\cdot\mathrm{SGut}_k(\overline{G})$ in terms of n, Δ and δ can be obtained.

Theorem 4.9. [81] *Let G be a connected graph of order n with maximum degree Δ, minimum degree δ and a connected $\overline{G}$. Also let k be an integer with $2\leq k\leq n$. Then*

$$\mathrm{SGut}_k(G)\cdot\mathrm{SGut}_k(\overline{G})\geq\begin{cases}(k-1)^2\,\delta^k\,(n-\delta-1)^k\,\binom{n}{k}^2 & \text{if } \Delta+\delta\leq n-1,\\ (k-1)^2\,\Delta^k\,(n-\Delta-1)^k\,\binom{n}{k}^2 & \text{if } \Delta+\delta\geq n-1\end{cases}$$

with equality holding if and only if G is a regular graph with $d_G(S)=d_{\overline{G}}(S)=k-1$ for any $S\subseteq V(G)$, $|S|=k$, and

$$\mathrm{SGut}_k(G)\cdot\mathrm{SGut}_k(\overline{G})\leq\frac{(n-1)^{2k+2}}{2^{2k+2}}\binom{n}{k}^2\left[\left(\frac{\Delta\,(n-\delta-1)}{\delta\,(n-\Delta-1)}\right)^k+\left(\frac{\delta\,(n-\Delta-1)}{\Delta\,(n-\delta-1)}\right)^k+2\right],$$

The equality holds if and only if G is a $\left(\frac{n-1}{2}\right)$-regular graph with $k=n$, n is odd.

Lower and upper bounds for $\mathrm{SGut}_k(G)+\mathrm{SGut}_k(\overline{G})$ in terms of n, Δ and δ (shown in the Theorem 4.10) are firstly published in [81].

Theorem 4.10. [81] *Let G be a connected graph of order n with maximum degree Δ, minimum degree δ and a connected $\overline{G}$. Also let k be an integer with $2\leq k\leq n$. Then*

$$\mathrm{SGut}_k(G)+\mathrm{SGut}_k(\overline{G})\geq\begin{cases}2\,(k-1)\,\delta^{k/2}\,(n-\delta-1)^{k/2}\,\binom{n}{k} & \text{if } \Delta+\delta\leq n-1,\\ 2\,(k-1)\,\Delta^{k/2}\,(n-\Delta-1)^{k/2}\,\binom{n}{k} & \text{if } \Delta+\delta\geq n-1\end{cases}$$

with equality holding if and only if G is a regular graph with $d_G(S)=d_{\overline{G}}(S)=k-1$ for any $S\subseteq V(G)$, $|S|=k$, and

$$\mathrm{SGut}_k(G)+\mathrm{SGut}_k(\overline{G})\leq(n-1)\left[\Delta^k+(n-\delta-1)^k\right]\binom{n}{k}$$

with equality holding if and only if G is a regular graph with $k=n$.

5 Steiner Harary Index

The Harary index was introduced at the beginning of the nineties of the last century. It is emphasizing the stronger influence of atoms that are close to each other. Recall that the Harary index is defined as

$$\mathrm{H}(G)=\sum_{i<j}\frac{1}{d_G(v_i,v_j)}, \tag{18}$$

and the Steiner Harary 3-index is defined as

$$\mathrm{SH}_3(G)=\sum_{i<j<k}\frac{1}{d_G(v_i,v_j,v_k)}. \tag{19}$$

In the same way, the k^{th} Steiner Harary index gives priority to k atoms that are close to each other. In the next few subsections, results on the Steiner Harary index will be outlined.

5.1 Results for some special graphs

Mao [50] derived the following results on the Steiner Harary index.

Proposition 5.1. [50] *Let K_n be the complete graph of order n, and let k be an integer such that $2\le k\le n$. Then $\mathrm{SH}_k(K_n)=\frac{1}{k-1}\binom{n}{k}$.*

Proposition 5.2. [50] *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*

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

From the above proposition, Mao [50] derived the following corollary.

Corollary 5.1. [50] *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*

$$\mathrm{SH}_k(S_n)=\frac{kn-n+k}{k^2(k-1)}\binom{n-1}{k-1}.$$

Proposition 5.3. [50] *Let P_n be the path of order n $(n\ge 3)$, and let k be an integer such that $2\le k\le n$. Then*

$$\mathrm{SH}_k(P_n)=n\sum_{k-1\le t\le n-1}\frac{1}{t}\binom{t-1}{k-2}-\binom{n-1}{k-1}.$$

5.2 Lower and upper bounds for general graphs

The following proposition is immediate.

Proposition 5.4. [50] *Let* G *be a connected graph of order* n*,* $e \in E(G)$*, and let* k *be an integer such that* $2 \leq k \leq n$*. Furthermore, let* F *be the graph with vertex set* $V(F) = V(G)$ *and edge set* $E(G) \setminus e$*. Then*

$$\mathrm{SH}_k(F) \leq \mathrm{SH}_k(G).$$

This straightforwardly leads to the following theorem:

Proposition 5.5. [50] *Let* G *be a connected graph of order* n*, and* T *a spanning tree of* G*. Let* k *be an integer such that* $2 \leq k \leq n$*. Then*

$$\mathrm{SH}_k(T) \leq \mathrm{SH}_k(G)$$

with equality if and only if G *is a tree.*

Lower and upper bounds for the Steiner Harary index of trees are presented in the next theorem.

Theorem 5.2. [50] *Let* T *be a tree of order* n*, and let* k *be an integer such that* $2 \leq k \leq n$*. Then*

$$n \sum_{k-1 \leq t \leq n-1} \frac{1}{t}\binom{t-1}{k-2} - \binom{n-1}{k-1} \leq \mathrm{SH}_k(T) \leq \frac{kn-n+k}{k^2(k-1)}\binom{n-1}{k-1}.$$

Among all trees of order n*, the star* S_n *maximizes the* k*-Steiner Harary index whereas the path* P_n *minimizes the* k*-Steiner Harary index.*

Theorem 5.3. [50] *Let* G *be a connected graph of order* n*, and let* k *be an integer such that* $2 \leq k \leq n$*. Then*

$$n \sum_{k-1 \leq t \leq n-1} \frac{1}{t}\binom{t-1}{k-2} - \binom{n-1}{k-1} \leq \mathrm{SH}_k(G) \leq \frac{1}{k-1}\binom{n}{k}.$$

5.3 On Steiner Harary indices of trees

For $k = n-1$ and $k = n-2$, Mao [50] proved the following results.

Theorem 5.4. [50] *Let T be a tree of order n, possessing p pendent vertices. Then*

$$\mathrm{SH}_{n-1}(T) = \frac{n^2-2n-p}{(n-1)(n-2)}, \tag{20}$$

irrespective of any other structural detail of T.

Theorem 5.5. [50] *Let T be a tree of order n, possessing p pendent vertices. Let q be the number of vertices of degree 2 in T such that each of them is adjacent to a pendent vertex. Then*

$$\mathrm{SH}_{n-2}(T) = \left[\binom{p}{2}+q\right]\frac{1}{n-3} + \binom{n-p}{2}\frac{1}{n-1} + \frac{pn-p^2-q}{n-2}\,. \tag{21}$$

5.4 Nordhaus–Gaddum-type results

Wang et al. [80] obtained the following result for general k.

Theorem 5.6. [80] *Let $G \in \mathcal{G}(n)$ and let k be an integer such that $3 \le k \le n$. Then:*

(1) $\binom{n}{k}\frac{2k-2}{\max\{k(n-1),(2k-1)^2\}} \le \mathrm{SH}_k(G) + \mathrm{SH}_k(\overline{G}) \le \frac{(n+k-2)\binom{n}{k}}{(k-1)^2}$.

(2) $\frac{1}{\max\{k(n-1),(2k-1)^2\}}\binom{n}{k}^2 \le \mathrm{SH}_k(G)\cdot\mathrm{SH}_k(\overline{G}) \le \frac{1}{(k-1)^2}\binom{n}{k}^2$. *The lower bounds are sharp.*

For $k = n$, the following result is immediate.

Observation 5.1. [80] *Let $G \in \mathcal{G}(n)$. Then*

$$\mathrm{SH}_n(G) + \mathrm{SH}_n(\overline{G}) = \frac{2}{n-1} \quad \mathrm{SH}_n(G)\cdot\mathrm{SH}_n(\overline{G}) = \frac{1}{(n-1)^2}.$$

For $k = n-1$, they [80] obtained the following result.

Proposition 5.6. [80] *Let G be a graph of order n ($n \ge 5$).*

(1) *If G and $\overline{G}$ are both 2-connected, then*

$$\mathrm{SH}_{n-1}(G) + \mathrm{SH}_{n-1}(\overline{G}) = \frac{2n}{n-2} \quad \textit{and} \quad \mathrm{SH}_{n-1}(G)\cdot\mathrm{SH}_{n-1}(\overline{G}) = \frac{n^2}{(n-2)^2}.$$

(2) *If $\kappa(G) = 1$ and $\overline{G}$ is 2-connected, then*

$$\mathrm{SH}_{n-1}(G) + \mathrm{SH}_{n-1}(\overline{G}) = \frac{p}{n-1} + \frac{2n-p}{n-2}$$

and

$$\mathrm{SH}_{n-1}(G)\cdot\mathrm{SH}_{n-1}(\overline{G}) = \frac{pn}{(n-1)(n-2)} + \frac{n(n-p)}{(n-2)^2},$$

where p is the number of cut vertices in G.

(3) *If $\kappa(G) = \kappa(\overline{G}) = 1$, $\Delta(G) \leq n-3$, and G has a cut vertex v with pendent edge uv such that $G-u$ contains a spanning complete bipartite subgraph, and $\Delta(\overline{G}) \leq n-3$ and $\overline{G}$ has a cut vertex q with pendent edge pq such that $G-p$ contains a spanning complete bipartite subgraph, then*

$$\mathrm{SH}_{n-1}(G) + \mathrm{SH}_{n-1}(\overline{G}) = \frac{2n^2-2n-2}{(n-1)(n-2)} \text{ and } \mathrm{SH}_{n-1}(G) \cdot \mathrm{SH}_{n-1}(\overline{G}) = \frac{(n^2-n-1)^2}{(n-1)^2(n-2)^2}.$$

(4) *If $\kappa(G) = \kappa(\overline{G}) = 1$, $\Delta(\overline{G}) = n-2$, $\Delta(G) \leq n-3$ and G has a cut vertex v with pendent edge uv such that $G-u$ contains a spanning complete bipartite subgraph, then*

$$\mathrm{SH}_{n-1}(G) + \mathrm{SH}_{n-1}(\overline{G}) = \frac{2n^2-2n-2}{(n-1)(n-2)} \quad or \quad \mathrm{SH}_{n-1}(G) + \mathrm{SH}_{n-1}(\overline{G}) = \frac{2n^2-2n-3}{(n-1)(n-2)}$$

and

$$\mathrm{SH}_{n-1}(G) \cdot \mathrm{SH}_{n-1}(\overline{G}) = \frac{(n^2-n-1)^2}{(n-1)^2(n-2)^2} \quad or \quad \mathrm{SH}_{n-1}(G) \cdot \mathrm{SH}_{n-1}(\overline{G}) = \frac{(n^2-n-1)(n+1)}{(n-1)^2(n-2)}.$$

(5) *If $\kappa(G) = \kappa(\overline{G}) = 1$, $\Delta(G) = \Delta(\overline{G}) = n-2$, then*

$$\frac{2(n+1)}{n-1} \leq \mathrm{SH}_{n-1}(G) + \mathrm{SH}_{n-1}(\overline{G}) \leq \frac{2n^2-2n-2}{(n-1)(n-2)}$$

and

$$\frac{(n+1)^2}{(n-1)^2} \leq \mathrm{SH}_{n-1}(G) \cdot \mathrm{SH}_{n-1}(\overline{G}) \leq \frac{(n^2-n-1)^2}{(n-1)^2(n-2)^2}.$$

In [80], they improved the bounds of Theorem 5.6 for $k = 3$ and proved the following result.

Theorem 5.7. [80] *Let $G \in \mathcal{G}(n)$ with $n \geq 4$. Then*

(1)

$$\begin{aligned} \frac{5}{6}\binom{n}{3} &\geq \mathrm{SH}_3(G) + \mathrm{SH}_3(\overline{G}) \\ &\geq \begin{cases} \frac{7}{10}\binom{n}{3} + \frac{11}{60}n - \frac{1}{2} & \text{if } n = 6,7, \text{ and } sdiam_3(G) = 5 \\ & \text{or } n = 6,7, \text{ and } sdiam_3(\overline{G}) = 5 \\ \frac{1}{2}\binom{n-3}{3} - \sum_{i=2}^{n-1} \frac{n}{i} + \frac{7n^2-23n+20}{6} & \text{otherwise.} \end{cases} \end{aligned}$$

(2)

$$\begin{aligned} \frac{25}{144}\left[\binom{n}{3}^2\right] &\geq \mathrm{SH}_3(G) \cdot \mathrm{SH}_3(\overline{G}) \\ &\geq \left[\frac{1}{n-1}\binom{n}{3} + \frac{(n-3)(n-2)}{2(n-1)}\right]\left[\frac{1}{2}\binom{n}{3} - \frac{(n-3)(n-2)}{2(n-1)}\right] \end{aligned}$$

Bounds are sharp.

5.5 Chemical applications of Steiner Harary index

Furtula et al. [23] presented two discouraging results. In Figure 5.1 is shown the correlation between the Harary and three–center Harary indices in the case of octanes. Figure 5.2a shows the correlation between the Harary index and standard enthalpy of formation (ΔH_f°) of the same set of molecules, while the Figure 5.2b is displaying the analogous plot for the three–center Harary index. Good linear correlation between H and H_3 (cf. Figure 5.1) indicates that there is no statistical difference between the two correlations shown in Figure 5.2.

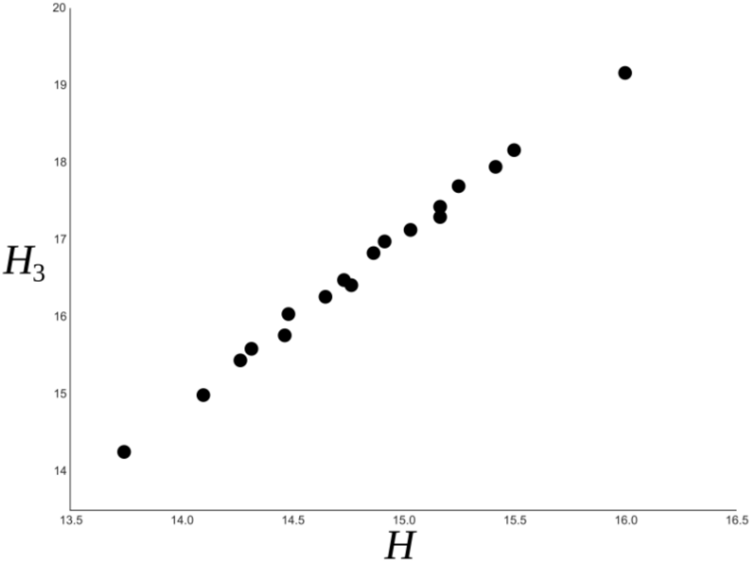

Figure 5.1 Correlation between the three-center Harary index H_3, Eq. (19), and the ordinary Harary index H, Eq. (18) for the set of isomeric octanes (18 data points); the correlation coefficient is $R = 0.9980$.

A remarkable improvement in modeling the enthalpy of formation of octanes is obtained by using the linear combination of these two Harary indices, namely $\mathrm{H} + \lambda \mathrm{H}_3$. Figure 5.3 is showing this correlation, where the optimized value λ is equal to = -0.443.

Analogous improvements have been found also in the case of a number of other physico-chemical properties of octanes. The respective statistical data are collected in Table 7.

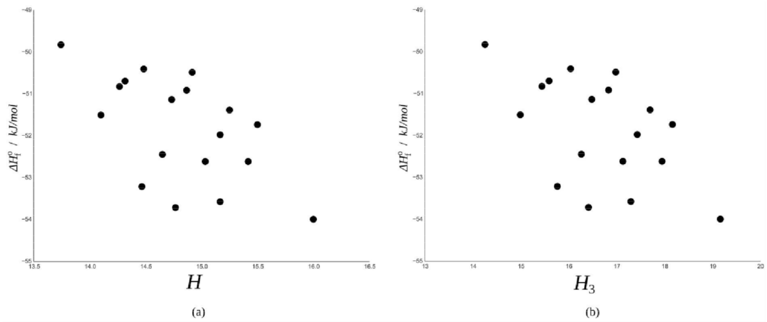

Figure 5.2 (*a*) Correlation between the standard enthalpy of formation (ΔH_f°) of isomeric octanes [38] and the ordinary Harary index H; $R = 0.576$. (*b*) Analogous correlation with the three-center Harary index H$_3$; $R = -0.528$.

Table 7 Correlation coefficients for the correlation between physico-chemical properties of octane isomes [38] and Harary index (R(H)), three-center Harary index ($R(\mathrm{SH}_3)$), and the linear combination thereof ($R(\mathrm{H} + \lambda \mathrm{SH}_3)$); ($\Delta H_f^o$) =standard enthalpy of formation, S^o =standard entropy, ΔH_{ev} =enthalpy of evaporation, BP =boiling point at atmospheric pressure, CT =critical temperature, CP =critical pressure, $\log P$ =logarithm of octanol/water partition coefficient; in the last column is the optimized value of the parameter λ for which $R(\mathrm{H} + \lambda \mathrm{SH}_3)$ is maximal..

Property	R(H)	$R(\mathrm{SH}_3)$	$R(\mathrm{H} + \lambda \mathrm{SH}_3)$	λ
ΔH_f^o	-0.576	-0.542	0.928	-0.433
S^o	-0.929	-0.914	0.954	-0.356
ΔH_{ev}	-0.779	-0.745	0.928	-0.414
BP	-0.573	-0.533	0.831	-0.429
CT	-0.111	-0.063	0.756	-0.451
CP	0.505	0.540	0.754	-0.483
$\log P$	-0.184	-0.192	0.223	-0.503

If the topological indices H and SH$_3$ were exactly linearly correlated, then their linear combination would not result in any improvement. From the data shown in Table 7 we see that in some cases significant improvements are obtained, which may be viewed as a kind of (convenient) surprise. This especially is the case for formation enthalpy, critical temperature, and critical pressure. Remarkably, whereas the indices H and SH$_3$ are completely uncorrelated with critical temperature, i.e., $R(\mathrm{H}) \approx R(\mathrm{SH}_3) \approx 0$, their linear combination results in a moderately good correlation, $R(\mathrm{H} + \lambda \mathrm{SH}_3) > 0.75$.

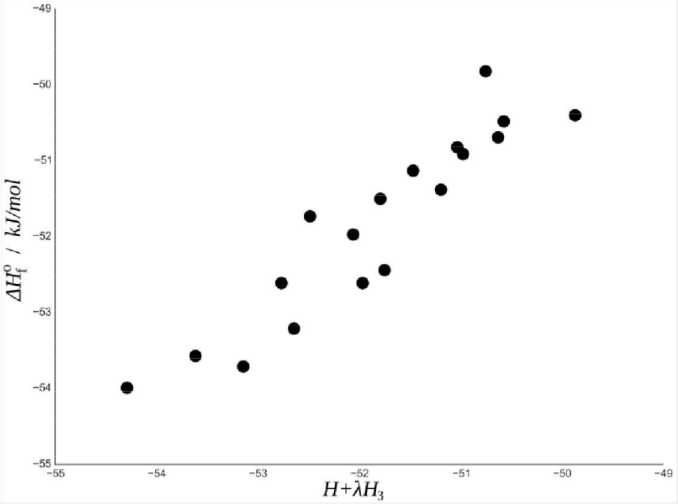

Figure 5.3 Correlation between the standard enthalpy of formation (ΔH_f°) of octanes [38] and the linear combination H + λH$_3$. The best results are obtained for $\lambda = -0.433$ in which case the correlation coefficient increases to $R = 0.928$.

In all cases, the linear combination of H and H$_3$ improves the quality of the correlations. However, in some cases, the gain is minor and insignificant. This (necessarily) happens for properties that are well correlated with H and H$_3$ (e.g., entropy), but also when the initial correlations are weak (e.g. partition coefficient).

A noteworthy fact is that the optimized value of the parameter λ is nearly equal for all physico-chemical properties examined, and is always negative-valued.

6 Steiner (revised) Szeged index

The Steiner (revised) Szeged index was recently proposed as an generalizations of already existing Szeged and revised Szeged indices. In the following pages, the results derived for these indices will be shown.

Li and Zhang [44] derived the Steiner Szeged index of cycles and wheels.

Theorem 6.1. [44] (1) *For a cycle C_n,*

$$\mathrm{Sz}_k(C_n) = n\left(1 + \sum_{j=1}^{n-k} \sum_{\substack{r+sj=n-k-j+1\\(r,s)\in\mathbb{N}^2}} (-1)^s \left[\binom{k+r-2}{r}\binom{k-1}{s} - \binom{k+r-3}{r}\binom{k-2}{s}\right]\right)^2$$

where $2 \leq k \leq n-1$ *and* $k \in \mathbb{N}$.

(2) *For a wheel* W_n,

$$\mathrm{Sz}_k(W_n) = \begin{cases} 2n-2 & \text{if } n-2 \leq k \leq n-1, \\ (n-1)\left[\binom{n-2}{k-1} + 5 - k\right] & \text{if } 2 \leq k \leq n-3. \end{cases}$$

6.1 Results for trees

Ghorbani et al., in the seminal paper [25], investigated the behavior of these indices in the case of trees. The following result is easy to obtain.

Theorem 6.2. [25] *For a tree* T,

$$\mathrm{Sz}_k(T) = \sum_{e=uv\in E(T)} \left[\binom{n_u(e)-1}{k-1} + 1\right]\left[\binom{n_v(e)-1}{k-1} + 1\right],$$

where $2 \leq k \leq |V(T)| - 1$.

Note that for $k = 2$, $\mathrm{Sz}_2(T) = \sum_{e=uv\in E(T)} n_u(e)n_v(e) = \mathrm{Sz}(T)$, which is exactly the classical Szeged index.

Some examples are given as follows.

Example 6.1. [25] *Let* $P_n = u_1u_2\cdots u_iu_{i+1}\cdots u_n$ *be a path with* n *vertices, and let* $e = u_iu_{i+1}$ *be an edge of this path. Then* $P_n - e$ *has two subpaths* P_i *and* P_{n-i}. *So we have* $n_{u_i}(e) = i$ *and* $n_{u_{i+1}}(e) = n - i$. *Thence,*

$$\mathrm{Sz}_k(P_n) = \sum_{i=1}^{n-1} \left[\binom{i-1}{k-1} + 1\right]\left[\binom{n-i-1}{k-1} + 1\right].$$

Since any $(k-1)$*-subset* S *of* $V(T) \setminus \{u, v\}$ *satisfies* $d_T(S \cup \{u\}) = d_T(S \cup \{v\})$ *if and only if both* $S \cap T_u \neq \emptyset$ *and* $S \cap T_v \neq \emptyset$, *then we can deduce that*

$$n_0(e;k) = \sum_{j=1}^{k-2} \binom{i-1}{j}\binom{n-i-1}{k-j-1}.$$

From this one can give an explicit formula for the $r\mathrm{Sz}_k(P_n)$.

Example 6.2. [25] *For the star* S_{n+1} *on* $n+1$ *vertices with a central vertex* u *and the other pendent vertices* $u_1, u_2, \cdots, u_n$, *take an edge* $e = uu_i$. *Then* $S_{n+1} \setminus e$ *has two subgraphs* $T_{u_i} = P_1$ *and* $T_u = S_n$. *So we have* $n_{u_i}(e) = 1$ *and* $n_u(e) = n$. *Therefore,*

$$\mathrm{Sz}_k(S_{n+1}) = \sum_{i=1}^{n} \left[\binom{n-1}{k-1} + 1\right] = n\binom{n-1}{k-1} + n.$$

Since any $(k-1)$-subset S of $V(S_{n+1}) - \{u, u_i\}$ satisfies $d_T(S \cup u) = d_T(S \cup u_i)$ if and only if both $S \cap T_u \neq \emptyset$ and $S \cap T_{u_i} \neq \emptyset$, then we have $n_0(e;k) = 0$ for any $e = uu_i$ because $T_{u_i} - u_i = \emptyset$, and hence there is no such S. Therefore, we have

$$r\mathrm{Sz}_k(S_{n+1}) = \mathrm{Sz}_k(S_{n+1}) = n\binom{n-1}{k-1} + n.$$

Above equation will be also derived in the next section using symmetry of graphs.

Remark 6.1. [25] *For $k = 2$, the Steiner Szeged index Sz_2 of a tree is equal to the Szeged index Sz, and the Steiner Wiener index SW_2 is equal to the Wiener index W, and hence the Steiner Szeged index Sz_2 of a tree is equal to the Steiner Wiener index SW_2 of a tree since $\mathrm{Sz} = \mathrm{W}$ for a tree. However, for $k \geq 3$, one can see from Examples 6.1 and 6.2 that the Steiner Szeged index Sz_k of a tree is not equal to the Steiner Wiener index SW_k of a tree.*

Conjecture 6.1. [25] *For any two trees T and T', $\mathrm{Sz}_k(T) \leq \mathrm{Sz}_k(T')$ if and only if $\mathrm{Sz}(T) \leq \mathrm{Sz}(T')$?*

Li and Zhang [44] proved that this conjecture is not true. To disprove it, they first calculated $\mathrm{Sz}(P_n)$, $\mathrm{Sz}(S_n)$, $\mathrm{Sz}_{n-1}(P_n)$ and $\mathrm{Sz}_{n-1}(S_n)$; see the following:

$$\mathrm{Sz}(P_n) = \frac{n^3 - n}{6}, \quad \mathrm{Sz}(S_n) = (n-1)^2, \quad \mathrm{Sz}_{n-1}(P_n) = n + 1, \quad \mathrm{Sz}_{n-1}(S_n) = 2n - 2.$$

When n is relatively large, $\mathrm{Sz}(P_n) > \mathrm{Sz}(S_n)$ if and only if $\mathrm{Sz}_{n-1}(P_n) < \mathrm{Sz}_{n-1}(S_n)$. When n is large enough and k approaches to n (assume $k = n - t$), $\mathrm{Sz}_k(P_n) = \Omega(n^{t-1})$ and $\mathrm{Sz}_k(S_n) = \Omega(n^t)$, and hence $\mathrm{Sz}_k(P_n) < \mathrm{Sz}_k(S_n)$ in many cases.

Liu and Das [46] derived the following results for trees.

Theorem 6.3. [46] *Let T be a tree of order n. Then*

$$r\mathrm{Sz}_k(T) = \frac{n-1}{4}\left[\binom{n-2}{k-1} + 2\right]^2 - \frac{1}{4}\sum_{e=uv \in E(T)} \left[\binom{n_u(e)-1}{k-1} - \binom{n_v(e)-1}{k-1}\right]^2.$$

A *double star* $DS(p,q)$ is a tree obtained from two disjoint stars S_{p+1} and S_{q+1} by joining their center with an edge. If n is the number of vertices of $DS(p,q)$, then $n = p + q + 2$.

Corollary 6.4. [46] *Let $DS(p,q)$ be a double star. Then*

$$r\mathrm{Sz}_k(DS(p,q)) = (p+q+1)\left[\binom{p+q}{k-1} + 1\right] + \frac{1}{4}\binom{p+q}{k-1}^2 - \frac{1}{4}\left[\binom{p}{k-1} - \binom{q}{k-1}\right]^2.$$

In [46], they also gave a lower bound on $\mathrm{Sz}_3(T)$ in terms of n when $n \geq 9$.

Theorem 6.5. [46] *Let T be a tree of order $n \geq 9$. Then*

$$\mathrm{Sz}_k(T) \geq \left\lceil \frac{n-1}{2} \right\rceil \left[\binom{n-2}{2} + 1 \right] + \left\lfloor \frac{n-1}{2} \right\rfloor \left[\binom{n-3}{2} + 1 \right]$$

with equality holding if and only if $T \cong S'_n$, where S'_n is a tree of order n with center vertex v such that $T \setminus \{v\} = \lfloor n/2 \rfloor K_2$ (when n is odd) or $T \setminus \{v\} = \lfloor (n-1)/2 \rfloor K_2 \cup K_1$ (when n is even).

By $S(n_1, n_2, \ldots, n_q)$ we denote the *starlike tree* that has a vertex v_1 of degree $q \geq 3$ and the following property

$$S(n_1, n_2, \ldots, n_q) - v_1 = P_{n_1} \cup P_{n_2} \cup \ldots \cup P_{n_q}.$$

This tree has $n_1 + n_2 + \cdots + n_q + 1 = n$ vertices. Clearly, the parameters $n_1, n_2, \ldots, n_q$ determine the starlike tree up to isomorphism. In what follows, it will be assumed that $n_1 \geq n_2 \geq \cdots \geq n_q \geq 1$.

Theorem 6.6. [46] *Let $S(n_1, n_2, \ldots, n_q)$ be a starlike tree of order $n \geq 10$. Then*

$$\mathrm{Sz}_3(S(n_1, n_2, \ldots, n_q)) \leq \sum_{i=1}^{n-1} \left[\binom{i-1}{2} + 1 \right] \left[\binom{n-i-1}{2} + 1 \right]$$

with equality holding if and only if $S(n_1, n_2, \ldots, n_q) \cong P_n$.

Liu and Das [46] stated that the following conjecture.

Conjecture 6.2. [46] *Let G be a connected graph of order n. Then G is a star graph if and only if $n_0(e;k) = n_u(e;k) = 0$, $n_v(e;k) = \binom{n-2}{k-1}$ or $n_0(e;k) = n_v(e;k) = 0$, $n_u(e;k) = \binom{n-2}{k-1}$ for any edge $e = uv \in E(G)$.*

Problem 6.1. [46] *Which graph gives the maximum value of $\mathrm{Sz}_3(T)$ among the trees T of order n.*

6.2 Results for graphs with symmetry

Let G be a group and Ω be a non-empty set. An action of G on Ω, denoted by $(G|\Omega)$, induces a group homomorphism φ from G into the symmetric group S_Ω on Ω, where

$\varphi(g)^\alpha = g^\alpha$, $(\alpha \in \Omega)$. The *orbit* of an element $\alpha \in \Omega$ is denoted by α^G and it is defined as the set of all $\alpha^g, g \in G$.

A bijection σ on the vertex set of a graph Γ is named an *graph automorphism* if it preserves the edge set of Γ. In other words, σ is a graph automorphism of Γ if for an edge $e = uv$ of Γ, also the $\sigma(e) = \sigma(u)\sigma(v)$ is an edge of Γ. Let $Aut(\Gamma)$ be the set of all graph automorphisms of Γ. Then $Aut(\Gamma)$ under the composition of mappings forms a group. A graph Γ is called *vertex-transitive* if $Aut(\Gamma)$ acting on $V(G)$ has one orbit. The edge-transitive graph can be similarly defined by considering $Aut(\Gamma)$ acting on $E(G)$.

Theorem 6.7. [25] *Let $E_1, E_2, \ldots, E_r$ be the orbits of a graph Γ under the action of $Aut(\Gamma)$ on the edge set $E(\Gamma)$ of Γ. Suppose $e = uv$ and $f = xy$ are two arbitrary edges of E_i $(1 \le i \le r)$. Then*

$$\{n_u(e;k), n_v(e;k)\} = \{n_x(f;k), n_y(f;k)\}.$$

The following corollary is immediate.

Corollary 6.8. [25] *Let $E_1, E_2, \ldots, E_r$ be the orbits of a graph Γ under the action of $Aut(\Gamma)$ on the edge set $E(\Gamma)$ of Γ and $u_iv_i = e_i \in E_i$. Then*

$$\mathrm{Sz}_k(\Gamma) = \sum_{i=1}^{r} |E_i|(n_{u_i}(e_i;k) + 1)(n_{v_i}(e_i;k) + 1),$$

and

$$r\mathrm{Sz}_k(\Gamma) = \sum_{i=1}^{r} |E_i|(n_{u_i}(e_i;k) + n_0(e_i;k)/2 + 1)(n_{v_i}(e_i;k) + n_0(e_i;k)/2 + 1).$$

Example 6.3. [25] *Suppose K_n is the complete graph on n vertices. It is not difficult to see that for any $uv = e \in E(K_n)$, we have $n_u(e;k) = n_v(e;k) = 0$ and $n_0(e;k) = \binom{n-2}{k-1}$. Then*

$$\mathrm{Sz}_k(K_n) = \sum_{e=uv \in E(K_n)} (n_u(e;k) + 1)(n_v(e:k) + 1) = |E(K_n)| = n(n-1)/2,$$

and

$$\begin{aligned} r\mathrm{Sz}_k(K_n) &= \sum_{e=uv \in E(K_n)} (n_u(e;k) + n_0(e;k)/2 + 1)(n_v(e;k) + n_0(e;k)/2 + 1) \\ &= |E(K_n)|\binom{n-2}{k-1}^2. \end{aligned}$$

Example 6.4. [25] *Suppose* $K_{1,n}$ *is the star graph on* $n+1$ *vertices. Let* $V(K_{1,n}) = \{u, u_1, \ldots, u_n\}$ *and* $E(K_{1,n}) = \{\{u,u_1\}, \ldots, \{u,u_n\}\}$. *Again* $K_{1,n}$ *is edge-transitive and for any edge* $uu_i = e_i \in E(K_{1,n})$, *we have* $n_u(e;k) = \binom{n-1}{k-1}$, $n_{u_i}(e;k) = 0$ *and* $n_0(e;k) = 0$. *Then*

$$r\mathrm{Sz}_k(K_{1,n}) = \mathrm{Sz}_k(K_{1,n}) = \sum_{e\in E(K_n)} \left[\binom{n-1}{k-1} + 1\right] = n\binom{n-1}{k-1} + n.$$

For complete multipartite graphs, we can get the exact value for the kth Steiner Szeged index.

Theorem 6.9. [25] *Let* $\Gamma = K_{a_1,a_2,\ldots,a_m}$ *be a complete multipartite graph and let* k *be an integer such that* $k \le a_i$ $(1 \le i \le m)$. *Then*

$$\mathrm{Sz}_k(\Gamma) = \sum_{i=1}^{m-1}\sum_{j=i+1}^{m} a_i a_j \left[\binom{a_i-1}{k-1} + 1\right]\left[\binom{a_j-1}{k-1} + 1\right],$$

and

$$r\mathrm{Sz}_k(\Gamma) = \sum_{i=1}^{m-1}\sum_{j=i+1}^{m} a_i a_j \left[\binom{a_i-1}{k-1} + n_0(e;k)/2 + 1\right]\left[\binom{a_j-1}{k-1} + n_0(e;k)/2 + 1\right],$$

where $B = V(\Gamma) - (A_i \cup A_j)$ *and*

$$n_0(e;k) = \binom{|B|}{k-1} + \sum_{p=1}^{a_i-2}\sum_{q=1}^{k-1-p}\binom{a_i-2}{p}\binom{a_j-1}{q}\binom{|B|}{k-1-(p+q)}.$$

6.3 Formulas for large k

For trees, we have the following formula for $k = n-1$.

Theorem 6.10. [25] *Let* T *be a tree of order* n *with* p *pendent edges. Then*

$$\mathrm{Sz}_{n-1}(T) = n + p - 1 \quad \textit{and} \quad r\mathrm{Sz}_{n-1}(T) = 2p + \frac{9}{4}(n-p-1).$$

Remark 6.2. [25] *Notice that the derivative function* $(r\mathrm{Sz}_{n-1})'(T)$ *is less than zero, and thus, the function* $r\mathrm{Sz}_{n-1}(T) = 2p + \frac{9}{4}(n-p-1)$ *is strictly increasing. Let* $\mathcal{T}_n$ *be all of trees with* n *vertices. Among all elements of* $\mathcal{T}_n$, *the star graph* S_n *and the path graph* P_n *has the minimum and the maximum value of* $r\mathrm{Sz}_{n-1}$, *respectively.*

Theorem 6.11 is a generalization of Theorem 6.10.

Theorem 6.11. [25] *Let* G *be a connected graph of order* n *and size* m *with* p *pendent edges. Then*

$$\mathrm{Sz}_{n-1}(G) = p + m \quad \textit{and} \quad r\mathrm{Sz}_{n-1}(G) = 2p + \frac{9}{4}(m-p).$$

6.4 Upper and lower bounds

In [25] the following upper and lower bounds are derived for general graphs.

Theorem 6.12. [25] *Let n, k be two integers with $2 \leq k \leq n-1$, and let G be a graph of order n and size m.*

(1) *If G is $(n-k)$-connected, then* $\mathrm{Sz}_k(G) = m$.

(2) *If G is not $(n-k)$-connected, then*

$$m \leq \mathrm{Sz}_k(G) \leq m\left(\left\lceil \frac{1}{2}\binom{n-2}{k-1} \right\rceil + 1\right)\left(\left\lfloor \frac{1}{2}\binom{n-2}{k-1} \right\rfloor + 1\right).$$

Let $e = uv$ be an edge of G, we define

$$D(u|e) = \sum_{\substack{S \subseteq V(G),\ |S|=k-1 \\ u,v \notin S}} d_G(S \cup \{u\}).$$

Theorem 6.13. [46] *Let G be a connected graph of order n and size m. Then*

$$r\mathrm{Sz}_k(G) \leq \frac{m}{4}\left[\binom{n-2}{k-1} + 2\right]^2$$

Equality holds if and only if $D(u|e) = D(v|e)$ for every edge $e = uv$ in G.

The following two corollaries are immediate.

Corollary 6.14. [46] *If G is $(n-k)$-connected graph of order n and size m, then*

$$r\mathrm{Sz}_k(G) \leq \frac{m}{4}\left[\binom{n-2}{k-1} + 2\right]^2.$$

Corollary 6.15. [46] *Let G be a connected graph of order n and size m. Then*

$$r\mathrm{Sz}_k(G) \leq \frac{m}{4}\left[\binom{n-2}{k-1} + 2\right]^2$$

Equality holds if and only if $D(u|e) = D(v|e)$ and $n_0(e;k) = 0$ for every edge $e = uv$ in G.

Liu and Das [46] gave a lower bound on $r\mathrm{Sz}_k(G)$ and $\mathrm{Sz}_k(G)$ of graph G.

Theorem 6.16. [46] *Let G be a connected graph of order n and size m. Then*

$$r\mathrm{Sz}_k(G) \geq m\left[\binom{n-2}{k-1} + 1\right]$$

Equality holds if and only if $n_0(e;k) = n_u(e;k) = 0$, $n_v(e;k) = \binom{n-2}{k-1}$ or $n_0(e;k) = n_v(e;k) = 0$, $n_u(e;k) = \binom{n-2}{k-1}$ for every edge $e = uv$ in G.

The following corollary is immediate.

Corollary 6.17. [46] *Let G be a connected graph of order n. Then*

$$r\mathrm{Sz}_k(G) \geq (n-1)\left[\binom{n-2}{k-1}+1\right],$$

with equality if and only if $G \cong S_n$.

Theorem 6.18. [46] *Let G be a connected graph of order n with m edges and p pendent vertices. Then*

$$\mathrm{Sz}_k(G) \geq m + p\binom{n-2}{k-1}.$$

In [46], they considered the difference between $r\mathrm{Sz}_k(G)$ and $\mathrm{Sz}_k(G)$.

Theorem 6.19. [46] *Let G be a connected graph of order n and size m. Then*

$$r\mathrm{Sz}_k(G) - \mathrm{Sz}_k(G) \leq \frac{m}{4}\left[\binom{n-2}{k-1}+4\right]\binom{n-2}{k-1}$$

6.5 Nordhaus–Gaddum-type results

Liu and Das [46] gave Nordhaus–Gaddum-type results on the kth Steiner Szeged index $\mathrm{Sz}_k(G)$ and the kth Steiner revised Szeged index $r\mathrm{Sz}_k(G)$ of graph G.

Theorem 6.20. [46] *Let G be a connected graph of order n with connected complement $\overline{G}$. Then*

(1)

$$\frac{n(n-1)}{2}\left[\binom{n-2}{k-1}+1\right] \leq r\mathrm{Sz}_k(G) + r\mathrm{Sz}_k(\overline{G}) \leq \frac{n(n-1)}{8}\left[\binom{n-2}{k-1}+2\right]^2,$$

(2)

$$\frac{(n-2)(n-1)^2}{2}\left[\binom{n-2}{k-1}+1\right]^2 < r\mathrm{Sz}_k(G)\cdot r\mathrm{Sz}_k(\overline{G}) \leq \frac{n^2(n-1)^2}{256}\left[\binom{n-2}{k-1}+2\right]^4.$$

One can easily see that the left equality holds in Theorem 6.20 if and only if $G \cong S_n$ or $\overline{G} \cong S_n$. Since both G and $\overline{G}$ are connected, the left inequality in Theorem 6.20 is strict.

Theorem 6.21. [46] *Let G be a connected graph of order n with p pendent vertices. Then*

$$\frac{n(n-1)}{2} + p\binom{n-2}{k-1} \leq \mathrm{Sz}_k(G) + \mathrm{Sz}_k(\overline{G}) \leq \frac{n(n-1)}{8}\left[\binom{n-2}{k-1}+2\right]^2.$$

Corollary 6.22. [46] *Let G be a connected graph of order n. Then*

$$\mathrm{Sz}_k(G) + \mathrm{Sz}_k(\overline{G}) \geq \frac{n(n-1)}{2}.$$

7 Steiner hyper–Wiener index and Steiner Hosoya polynomial

In 2002, Cash showed the relation between the Hosoya polynomial and the hyper–Wiener index, see [9]. Tratnik [74] generalized this result and showed that it holds also for the k-Steiner hyper-Wiener index and the k-Steiner Hosoya polynomial where k is a positive integer such that $k \leq |V(G)|$.

Tratnik [74] noticed the obvious connection between the k-Steiner Wiener index and the k-Steiner Hosoya polynomial.

Theorem 7.1. [74] *Let G be a connected graph and k a positive integer such that $k \leq |V(G)|$. Then*

$$\mathrm{SW}_k(G) = \mathrm{SHP}'_k(G,1).$$

In [74], Tratnik derived the following results.

Theorem 7.2. [74] *Let G be a connected graph and k a positive integer such that $k \leq |V(G)|$. Then*

$$\mathrm{SWW}_k(G) = \mathrm{SHP}'_k(G,1) + \frac{1}{2}\mathrm{SHP}''_k(G,1).$$

Theorem 7.3. [74] (1) *For complete graphs K_n,*

$$\mathrm{SHP}_k(K_n,x) = \binom{n}{k} x^{k-1}, \quad \mathrm{SWW}_k(K_n) = \binom{k}{2}\binom{n}{k}.$$

(2) *For paths P_n,*

$$\mathrm{SHP}_k(P_n,x) = \sum_{j=k-1}^{n-1} (n-j)\binom{j-1}{k-2} x^j, \quad \mathrm{SWW}_k(P_n) = \binom{k}{2}\binom{n+2}{k+2}.$$

Two edges $e_1 = u_1v_1$ and $e_2 = u_2v_2$ of a connected graph G are in relation Θ, $e_1 \Theta e_2$, if

$$d_G(u_1,u_2) + d_G(v_1,v_2) \neq d_G(u_1,v_2) + d_G(u_1,v_2).$$

This relation is known as Djoković–Winkler relation. The relation Θ is reflexive and symmetric, but not necessarily transitive. We denote its transitive closure (i.e. the smallest transitive relation containing Θ) by Θ^*.

The *hypercube* Q_n of dimension n is defined in the following way: all vertices of Q_n are presented as n-tuples $(x_1, x_2, \ldots, x_n)$ where $x_i \in \{0,1\}$ for each i, $1 \leq i \leq n$, and two vertices of Q_n are adjacent if the corresponding n-tuples differ in precisely one position.

A subgraph H of a graph G is called an *isometric subgraph* if for each $u, v \in V(H)$ it holds $d_H(u,v) = d_G(u,v)$. Any isometric subgraph of a hypercube is called a *partial cube.*

If G is a partial cube with Θ-classes $E_1, E_2, \ldots, E_d$, denote by U_i and U_i' the connected components of the graph $G - E_i$, where $i \in \{1, \ldots, d\}$. For any $i, j \in \{1, \ldots, d\}$, $i \neq j$, set

$$N_{ij}^{00} = V(U_i) \cap V(U_j), \; N_{ij}^{01} = V(U_i) \cap V(U_j'),$$
$$N_{ij}^{10} = V(U_i') \cap V(U_j), \; N_{ij}^{11} = V(U_i') \cap V(U_j').$$

Cardinalities of such defined sets are denoted as $n_{ij}^{kl} = |N_{ij}^{kl}|$, where $i, j \in \{1, \ldots, d\}$, $i \neq j$, and $k, l \in \{0, 1\}$. Let also be $n_i^0 = |V(U_i)|$, $n_i^1 = |V(U_i')|$ for $i \in \{1, \ldots, d\}$.

For a connected graph G, the $\overline{\mathrm{WW}}(G)$ is equal to the sum of squares of distances between all the pairs of vertices, i.e.

$$\overline{\mathrm{WW}}(G) = \sum_{\{u,v\} \subseteq V(G)} d_G(u,v)^2.$$

For a graph G, $O_2(G) = \{(u,v) \in V(G)^2 \mid u \neq v\}$, and $O_3(G) = \{(u,v,w) \in V(G)^3 \mid u \neq v, \; u \neq w, \; v \neq w\}$. For a connected graph G with at least three vertices,

$$\widehat{\mathrm{WW}}(G) = \sum_{(u,v,w) \in O_3(G)} d_G(u,v) d_G(u,w).$$

Tratnik [74] proved how the 3-Steiner hyper-Wiener index of a modular graph G can be obtained from $\mathrm{W}(G)$, $\overline{\mathrm{WW}}(G)$, and $\widehat{\mathrm{WW}}(G)$.

Theorem 7.4. [74] *Let G be a modular graph with at least three vertices. Then*

$$\mathrm{SWW}_3(G) = \frac{|V(G)| - 2}{4} \mathrm{W}(G) + \frac{|V(G)| - 2}{8} \mathrm{WW}(G) + \frac{1}{8} \widehat{\mathrm{WW}}(G).$$

Theorem 7.5. [74] *Let G be a modular graph and a partial cube with at least three vertices and let d be the number of Θ-classes of G. Then*

$$
\begin{aligned}
\mathrm{SWW}_3(G) &= \frac{3|V(G)|-6}{8}\sum_{i=1}^{d} n_i^0 n_i^1 + \frac{|V(G)|-2}{4}\sum_{i=1}^{d}\sum_{j=i+1}^{d}(n_{ij}^{11}n_{ij}^{00}+n_{ij}^{01}n_{ij}^{10}) \\
&\quad + \frac{1}{8}\sum_{i=1}^{d}[n_i^0 n_i^1(n_i^1-1)+n_i^1 n_i^0(n_i^0-1)] \\
&\quad + \frac{1}{4}\sum_{i=i}^{d-1}\sum_{j+1}^{d}[3n_{ij}^{00}n_{ij}^{01}n_{ij}^{10}+3n_{ij}^{00}n_{ij}^{01}n_{ij}^{11}+3n_{ij}^{00}n_{ij}^{10}n_{ij}^{11}+3n_{ij}^{01}n_{ij}^{10}n_{ij}^{11} \\
&\quad + n_{ij}^{00}n_{ij}^{11}(n_{ij}^{11}-1)+n_{ij}^{01}n_{ij}^{10}(n_{ij}^{10}-1)+n_{ij}^{10}n_{ij}^{01}(n_{ij}^{01}-1)+n_{ij}^{11}n_{ij}^{00}(n_{ij}^{00}-1)]
\end{aligned}
$$

The *grid graph* $G_{m,n}$ is defined as the Cartesian product of two paths P_m and P_n, i.e. $G_{m,n} = P_m \Box P_n$.

Proposition 7.1. [74] *Let $G_{m,n}$ be a grid graph such that m and n are integers greater or equal to 2. Then*

$$\mathrm{SWW}_3(G_{m,n}) = \frac{1}{12}(m^4n^3 + m^3n^4 - 3m^3n^2 - 3m^2n^3 + 2m^2n + 2mn^2).$$

Theorem 7.6. [74] *Let $G_{m,n}$ be a grid graph such that m and n are integers greater or equal to 3. Then*

$$
\begin{aligned}
\mathrm{SWW}_3(G_{m,n}) &= \frac{1}{360}(9m^5n^3 + 15m^4n^4 + 9m^3n^5 + 15m^4n^3 + 15m^3n^4 - 30m^4n^2 \\
&- 50m^3n^3 - 30m^2n^4 + 26m^3n - 45m^3n^2 - 45m^2n^3 + 45m^2n^2 \\
&+ 26mn^3 + 30m^2n + 30mn^2 - 20mn).
\end{aligned}
$$

For any $n \geq 3$ it holds

$$\mathrm{SWW}_3(G_{2,n}) = \frac{1}{15}(3n^5 + 10n^4 - 25n^2 + 12n).$$

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