Cut Method: Update on Recent Developments and Equivalence of Independent Approaches

Sandi Klavžar\textsuperscript{1,2,3} \hspace{1cm} M. J. Nadjafi-Arani\textsuperscript{4}

October 18, 2014

\textsuperscript{1} Faculty of Mathematics and Physics, University of Ljubljana, Slovenia
\textsuperscript{2} Faculty of Natural Sciences and Mathematics, University of Maribor, Slovenia
\textsuperscript{3} Institute of Mathematics, Physics and Mechanics, Ljubljana, Slovenia
sandi.klavzar@fmf.uni-lj.si
\textsuperscript{4} Faculty of Mathematical Science, University of Kashan, Kashan, I. R. Iran
mjnajafiarani@gmail.com

Abstract

The cut method is a powerful tool for the investigation of distance-based (and some other) molecular structure-descriptors. In this paper a survey on the recent developments of the method is given. The instances of the standard cut method for the Wiener index, the Szeged index, the PI index, the generalized terminal Wiener index, the Gutman index, the edge-Wiener index, and the edge-Szeged index are described, where a standard cut method is a method that applies to partial cubes. It is pointed out that the standard cut method was recently independently discovered a couple of times. Numerous proper extensions of the standard cut method are presented. The method extends to $\ell_1$-graphs, graphs with a non-trivial canonical metric representation, graphs with transitive relation $\Theta$, and partial Hamming graphs. The instances of these extended cut methods include the Wiener index, the degree distance, distance moments, and the colored Wiener index.

Keywords: Cut method, topological index, QSPR/QSAR, partial cube, Wiener index, Szeged index, PI index, terminal Wiener index, isometric embedding, distance moment, colored Wiener index.

1 INTRODUCTION

The cut method turned out to be very useful in the investigation of molecular structure-descriptors, called topological indices. These indices are used in theoretical chemistry for the design of quantitative structure-property relations (QSPR) and
quantitative structure-activity relations (QSAR), see the books [1, 2, 3], the recent book chapter [4], and articles [5, 6, 7]. For the role of distance-sum-based molecular descriptors in a drug discovery process we refer to [8]. Moreover, very recently Putz et al. [9] used colored representations of some central distance-based topological indices (which are also the most important indices of this article) to provide novel topo-reactive or structure-reactivity indices with applications to polycyclic aromatic hydrocarbons. For another related and relevant applications of molecular distances (via the so called Wiener topological potential) see [10].

The cut method in a general form reads as follows [11]. If \( G \) is a (molecular) graph, then

1. partition the edge set of \( G \) into classes \( F_1, \ldots, F_k \), called cuts, such that each of the graphs \( G - F_i \), \( 1 \leq i \leq k \), consists of at least two connected components; and then

2. use properties of the components of the graphs \( G - F_i \) to derive a required property of \( G \).

The cut method demonstrated its usefulness especially for those topological indices that are based on the distances in the molecular graphs, the common name for such indices is distance-based topological indices. Their history goes back to 1947, when Harold Wiener [12] used the distances in the molecular graphs of alkanes to calculate their boiling points. This pioneering research led to the topological index named Wiener index that became one of the most popular molecular structure-descriptors. It found numerous applications for QSPR and was applied elsewhere, say in crystallography, communication theory, facility location, etc., cf. [13]. Other important distance-based topological indices introduced later include the hyper-Wiener index [14, 15], the Szeged index [16, 17], the edge-Szeged index [18], Wiener-type indices [19], the PI index [20], to name just some of the central ones. For the state of the art on the distance in molecular graphs see the recent books [21, 22].

The power of the cut method stems from the fact that in a way it enables to obtain distance-based topological indices of families of chemical graphs without actually calculating the distances between pairs of vertices. Based on the class of molecular graphs to which a cut method applies, we will distinguish two kinds of the method. We will say that a cut method is standard if it applies to the molecular graphs that allow isometric embeddings into hypercubes; these graphs are known as partial cubes. Cut methods that apply to classes larger than partial cubes will be called extended cut methods.

Several researchers share an opinion that a mathematical method should be considered as important only if it has been independently discovered/applied at least a couple of times. When it comes to independent discoveries, they are often due to the fact that in different fields of science, as well as sometimes within the same field, researchers speak different scientific language, in particular use different
notions for the same objects. Anyhow, if a certain method was applied several times and/or being independently introduced by different groups, it is clear that the method is useful and applicable.

The above “multiple-discovery” phenomena is certainly true for the cut method. The first goal of this survey article is to overview the developments after 2008 as in that year the first survey [11] on the cut method was published. Unfortunately it did not reach all that came across the method later on. Accordingly, our second goal is to point out that several seemingly different approaches are equivalent in the sense that they apply to the same class of (molecular) graphs.

The paper is organized as follows. At the end of this section we recall some definitions from graph theory. In the next section partial cubes and the standard cut method are presented. The instances of the standard cut method for the Wiener index, the Szeged index, the PI index, and the generalized terminal Wiener index, are explicitly given and some specific applications listed. In Section 3 we follow with instances of the cut method for the Gutman index, the edge-Wiener index, and the edge-Szeged index. These methods were recently developed for a certain class of graphs that turned out to be precisely the class of partial cubes. In other words, these cut methods are instances of the standard cut method. In addition, we present yet another independent approach for the Wiener index, Szeged index, and PI index, that also turned out to be equivalent to the standard cut method. In the final, longest section of the paper, proper extensions of the standard cut method are presented. The classes of graphs that appear there larger than partial cubes are $\ell_1$-graphs, graphs with a non-trivial canonical metric representation, graphs with transitive relation $\Theta$, and partial Hamming graphs, while the topological indices for which extended cut methods are developed are the Wiener index, the degree distance, distance moments, and the colored Wiener index.

Let $G = (V(G), E(G))$ be a connected graph. Then the distance $d_G(u, v)$ between vertices $u, v \in V(G)$ is the number of edges on a shortest $u, v$-path. A subgraph $H$ of a graph $G$ is convex if for any vertices $u, v$ of $H$, any shortest path in $G$ between $u$ and $v$ lies completely in $H$. Similarly, $H$ is an isometric subgraph of $G$ if $d_H(u, v) = d_G(u, v)$ holds for any vertices $u, v$ of $H$. Clearly, a convex subgraph is isometric but not the other way around. A graph $G = (V(G), E(G))$ is bipartite if $V(G)$ can be partitioned into subsets $X$ and $Y$ such that each edge of $G$ has one end-vertex in $X$ and the other end-vertex in $Y$. The $n$-cube $Q_n$, $n \geq 1$, is the graph whose vertex set consists of all binary strings of length $n$, two strings being adjacent if they differ in precisely one position. Finally, the degree of a vertex $u \in V(G)$ will be denoted by $\deg(u)$.
2 STANDARD CUT METHOD

In this section we present the standard cut method and its instances for the Wiener index, the Szeged index, the PI index, and the generalized terminal Wiener index. Some applications are also listed.

For the standard cut method we need to introduce partial cubes and the Djoković-Winkler relation $\Theta$, the two key notions of the method. Let $G$ be a connected graph, then $G$ is called a \textit{partial cube} if its vertices $u$ can be labeled with binary strings $\ell(u)$ of a fixed length, such that

$$d_G(u, v) = H(\ell(u), \ell(v))$$

holds for any vertices $u$ and $v$ of $G$, where $H(\ell(u), \ell(v))$ is the Hamming distance between the binary strings $\ell(u)$ and $\ell(v)$, that is, the number of positions in which $\ell(u)$ and $\ell(v)$ differ. One can easily see that partial cubes are bipartite graphs.

The edges $e = xy$ and $f = uv$ are in the Djoković-Winkler relation $\Theta$ [23, 24] if

$$d_G(x, u) + d_G(y, v) \neq d_G(x, v) + d_G(y, u).$$

The relation $\Theta$ is reflexive and symmetric, but not transitive in general. For example, $\Theta$ is not transitive on the complete bipartite graph $K_{2,3}$. On the other hand, the relation $\Theta$ is transitive when $G$ is partial cube. The transitive closure of $\Theta$ is denoted by $\Theta^*$. It is not difficult to see that an edge $e$ of an isometric cycle $C$ of $G$ is in relation $\Theta$ with its antipodal edge(s) on $C$ and all the edges of an odd cycle will be in the same $\Theta^*$-class. The following result of Winkler is the theoretical base for the cut method, cf. the book [25] and references therein.

\textbf{Theorem 2.1} [24] \textit{Let $G$ be a partial cube. Then relation $\Theta$ partitions the edge set $E(G)$ into $\Theta$-classes $F_1, \ldots, F_k$, where edges $e$ and $f$ lie in a common class $F_i$ if and only if $e \Theta f$. Moreover, for any index $i$, the graph $G - F_i$ consists of precisely two connected components.}

The oldest and one of the most thoroughly studied distance-based molecular structure-descriptors is the Wiener index [12]. Hosoya [26] extended the original definition from trees to all connected graphs $G$ as follows:

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

This topological index has also been extensively studied in the mathematical literature in terms of the average distance $\mu(G) = \frac{2}{n(n-1)}W(G)$, cf. [27]. For more information on the Wiener index see the reviews [28, 29].

Using the partition from Theorem 2.1, the first instance of the cut method is the following theorem.
Theorem 2.2 [30] Let $G$ be a partial cube and let $F_1, \ldots, F_k$ be its $\Theta$-classes. Let $n_1(F_i)$ and $n_2(F_i)$ be the number of vertices in the two connected components of $G - F_i$. Then

$$W(G) = \sum_{i=1}^{k} n_1(F_i) \cdot n_2(F_i).$$

Theorem 2.2 was applied in several papers to obtain closed expressions for the Wiener index of families of benzenoid and other chemical graphs, cf. [31, 32], as well as for other purposes, cf. [33]. Khalifeh, Yousefi-Azari, and Ashrafi [34] made a step forward in the way how Theorem 2.2 can be applied. Their application was done on certain carbon nanocones, but can in principle be applied to other molecular graphs that admit “enough” symmetry and a “nice” decomposition into isometric subgraphs.

Carbon nanocones were discovered by Ge and Sattler [35] in 1994. These are constructed from a graphene sheet by removing a 60 wedge and joining the edges a cone with a single pentagonal defect at the apex. Removing additional wedges introduces more such defects and reduces the opening angle. A cone with six pentagons has an opening angle of zero and is just a nanotube with one open end. Let $G[n] = \text{CNC}_5[n]$, $n \geq 0$, be the one-pentagonal carbon nanocone, that is, a nanocone that consists of a central pentagon and $n$ rings of concentric hexagons around the pentagon. In particular, $G[0]$ is the 5-cycle. In Fig. 1 one-pentagonal carbon nanocone $G[1]$ is shown, together with the half-edges that indicate how $G[1]$ grows into $G[2]$ by adding a ring of 10 additional hexagons to it.

Figure 1: One-pentagonal carbon nanocone $G[1]$ together with half-edges that grow towards $G[2]$

Clearly, $G[n]$ is not bipartite and hence not a partial cube. Consequently, at the first sight, Theorem 2.2 is not applicable. However, $G[n]$ can be partitioned into natural isometric subgraphs that are partial cubes. Then using the theorem on these
subgraphs and appropriately combining the results, it was deduced in [34] that

$$W(G[n]) = \frac{62}{3} n^5 + \frac{310}{3} n^4 + \frac{1205}{6} n^3 + \frac{1135}{6} n^2 + 86n + 15. \quad (1)$$

To present additional instances of the standard cut method we first need some definitions. Let $e = uv$ be an edge of a (connected) graph $G$, and define the sets $N_u(e)$ and $N_v(e)$ as follows:

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

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

The number of elements of $N_u(e)$ and $N_v(e)$ are denoted by $n_u(e)$ and $n_v(e)$, respectively. Thus, $n_u(e)$ counts the vertices of $G$ lying closer to the vertex $u$ than to $v$. The meaning of $n_v(e)$ is analogous. In addition to the sets $N_u(e)$ and $N_v(e)$, let $N_0(e)$ be the set of vertices equidistant from both ends of the edge $uv$. Set $n_0(e) = |N_0(e)|$. Note that for any edge $e$ of $G$, $n_u(e) \geq 1$ and $n_v(e) \geq 1$ because $u \in N_u(e)$ and $v \in N_v(e)$. The following property of the Wiener index of a tree $W(T)$ goes back to [12] and also follows immediately from Theorem 2.1. Motivated by this property, Gutman [16] introduced the Szeged index of a graph $G$ as

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

Evidently, $Sz(T) = W(T)$ holds for any tree $T$.

Now, let $F$ be a $\Theta$-class of a partial cube $G$ and let $uv \in F$. It is easily seen that the connected components of $G - F$ are precisely the subgraphs of $G$ induced by the sets $N_u(e)$ and $N_v(e)$. Hence applying Theorem 2.1 we get:

**Theorem 2.3** [11, 36] Let $G$ be a partial cube and let $F_1, \ldots, F_k$ be its $\Theta$-classes. Let $n_1(F_i)$ and $n_2(F_i)$ be the number of vertices in the two connected components of $G - F_i$. Then

$$Sz(G) = \sum_{i=1}^{k} |F_i| \cdot n_1(F_i) \cdot n_2(F_i).$$

For a recent application of Theorem 2.3 (as well as of Theorem 2.2) on certain polyomino chains, triangular benzenoids, and nanostar dendrimers, see [37].

The PI index of a (molecular) graph $G$ was introduced in [20] as

$$PI(G) = \sum_{e=uv \in E(G)} m_u(e) + m_v(e),$$
where $m_u(e)$ denotes the number of edges of $G$ whose distance to $u$ is smaller than the distance to $v$. The standard cut method for the PI index was first proved by John, Khadikar, and Singh:

**Theorem 2.4** [38] Let $G$ be a partial cube and let $F_1, \ldots, F_k$ be its $\Theta$-classes. Then

$$\text{PI}(G) = |E(G)|^2 - \sum_{i=1}^{k} |F_i|^2 .$$

Actually, Theorem 2.4 was stated in [38] only for the standard chemical prototype of partial cubes, the benzenoid hydrocarbons, however, knowing the essence of the cut method it easily extends to all partial cubes.

We now present a wide generalization of Theorem 2.4. By abuse of language, for the edge $e = uv$ we identify $N_u(e)$ with the subgraph of $G$ induced by the vertices from $N_u(e)$. A partition $T_1, \ldots, T_k$ of $E(G)$ is called a PI-partition of $E(G)$ [39] if for any $1 \leq i \leq k$ and for any edges $e = xy$ and $f = uv$ that belong to $T_i$ we have $N_u(e) = N_x(f)$ and $N_v(e) = N_y(f)$. For $X \subseteq V(G)$, let $\partial X$ denote the set of edges of $G$ with one end vertex in $X$ and the other not in $X$. Then we have:

**Theorem 2.5** [39] Let $T_1, \ldots, T_k$ be a PI-partition of $E(G)$ and let $e_i = uv \in T_i$, $1 \leq i \leq k$, be representatives of $T_i$. Then

$$\text{PI}(G) = |E(G)|^2 - \sum_{i=1}^{k} |T_i| \cdot (|T_i| + |E(N_0(e_i))| + |\partial(N_0(e_i))|) .$$

Moreover, if $G$ is bipartite, then

$$\text{PI}(G) = |E(G)|^2 - \sum_{i=1}^{k} |T_i|^2 .$$

The bipartite case of Theorem 2.5 was deduced also in [40] and applied in [41] to determine extremal catacondensed hexagonal systems with respect to the PI index.

In 2009, the concept of the terminal Wiener index was introduced by Gutman, Furtula, and Petrović [42]. Independently (a couple of years later) Székely, Wang, and Wu [43] came with the same idea. If $P \subseteq V(G)$ is the set of pendant vertices (alias leaves) of a (connected) graph $G$, then the terminal Wiener index of $G$ is defined with:

$$TW(G) = \sum_{\{u,v\} \subseteq P} d_G(u,v) .$$

In words, the terminal Wiener index is the sum of the distances between all pairs of pendant vertices of $G$. If $G$ has at most one pendant vertex, then $TW(G) = 0$. Clearly, the applicability of this molecular structure-descriptor is restricted to graphs
with many pendant vertices such as trees [44]. For more information on the terminal Wiener index see the survey [45], as well as the very recent survey on the graphs extremal with respect to distance-based topological indices [46].

In 2013, Ilić and Ilić [47] generalized the terminal Wiener index by setting, for any $r \geq 1$,

$$TW_r(G) = \sum_{\{u,v\} \in V(G), \deg(u) = \deg(v) = r} d_G(u,v).$$

Clearly, $TW_1(G) = TW(G)$. The standard cut method for the generalized terminal Wiener index reads as follows:

**Theorem 2.6** [47, Theorem 5.1] Let $G$ be a partial cube and let $F_1, \ldots, F_k$ be its $\Theta$-classes. Let $r \geq 1$ and let $n_1^{(r)}(F_i)$ and $n_2^{(r)}(F_i)$ be the number of vertices of degree $r$ in the two connected components of $G - F_i$. Then

$$TW_r(G) = \sum_{i=1}^{k} n_1^{(r)}(F_i) \cdot n_2^{(r)}(F_i).$$

As a sample chemical application we state a closed expression for $TW_3$ of the coronene/circumcoronene homologous series $H_k$, $k \geq 1$. This series is a particular, but important class of chemical graphs that is often used as a test for the efficiency of a proposed method. The first terms of this series are $H_1 = \text{benzene}$, $H_2 = \text{coronene}$, $H_3 = \text{circumcoronene}$, and $H_4 = \text{circumcircumcoronene}$. The first graph of this sequence is thus the 6-cycle, while for $H_k$, $k \geq 2$, is obtained from $H_{k-1}$ by attaching an outer ring of hexagons to it. In Fig. 2 the first three graphs from this series are depicted.

![Figure 2: Coronene/circumcoronene graphs $H_1$, $H_2$, and $H_3$: benzene, coronene, and circumcoronene](image)

Now we have:
Corollary 2.7 [47] $TW_3(H_k) = \frac{1}{5}(k-1)k(2k-1)(82k^2 - 82k - 19)$.

3 EQUIVALENT FORMS OF THE STANDARD CUT METHOD

In this section we present the cut methods developed for the Gutman index, the edge-Wiener index, and the edge-Szeged index. When being introduced, they were aimed to apply to a certain new class of graphs, but as we will see, it is just the class of partial cubes. At the end of the section yet another independent approach that also leads to partial cubes will be presented.

The Gutman index [48] (see also [49, 50] and references therein) of a connected graph $G$ is defined as

$$\text{Gut}(G) = \sum_{\{u,v\} \subseteq V(G)} \text{deg}(u) \cdot \text{deg}(v) \cdot d_G(u,v).$$

Let $D_G(e, f)$ denote the distance between edges $e$ and $f$, that is, the distance between the vertices $e$ and $f$ in the line graph $L(G)$ [51]. Recall that for an edge $e = uv$ the quantity $m_u(e)$ denotes the number of edges of $G$ whose distance to $u$ is smaller than the distance to $v$. Then the edge-Wiener index [51, 52, 53] and the edge-Szeged index [18] of $G$ are defined as follows:

$$W_e(G) = \sum_{\{e,f\} \subseteq E(G)} D_G(e, f),$$

$$Sz_e(G) = \sum_{e = uv \in E(G)} m_u(e) \cdot m_v(e).$$

Khalifeh, Yousefi-Azari and Ashrafi in [34] developed the cut method for the degree-distance index (see Section 4.3) and the Gutman index, while in the subsequent paper [40] they followed with the cut method for the edge-Wiener index and the edge-Szeged index. Their approach involves a class of graphs that was proved in [54] to be the class of partial cubes. To describe their approach we first need to introduce the notion of a convex cut.

Recall that a subgraph $H$ of a graph $G$ is convex if for any vertices $u, v$ of $H$, any shortest path $P$ in $G$ between $u$ and $v$ lies completely in $H$. Suppose now that $C$ is a cut of $G$ such that $G - C$ consists of two components. Then we say that $C$ is a convex cut if both components of $G - C$ are convex subgraphs of $G$.

The cut method from [34, 40] was developed for graphs that admit a partition $\{F_i\}$ of the edge set such that $G \setminus F_i$ is a two component graph with convex components; in other words, for graphs that admit a partition of the edge set into convex cuts. These graphs can be characterized as partial cubes:
Proposition 3.1 [54, Proposition 2.1] Let $G$ be a connected graph. Then $G$ admits a partition of $E(G)$ into convex cuts if and only if $G$ is a partial cube.

Therefore, the cut methods from [34, 40] are standard cut methods. The corresponding results read as follows.

Theorem 3.2 Let $G$ be a partial cube and let $F_1, \ldots, F_k$ be its $\Theta$-classes. Let $m_1(F_i)$ and $m_2(F_i)$ be the number of edges in the two connected components of $G - F_i$. Then

(i) [34] $\text{Gut}(G) = 2|E(G)|^2 + \sum_{i=1}^{k} (4 \cdot m_1(F_i) \cdot m_2(F_i) - |F_i|^2)$.

(ii) [40] $W_e(G) = \sum_{i=1}^{k} m_1(F_i) \cdot m_2(F_i)$.

(iii) [40] $Sz_e(G) = \sum_{i=1}^{k} |F_i| \cdot m_1(F_i) \cdot m_2(F_i)$.

Note that Theorem 3.2(ii) and Theorem 3.2(iii) are completely parallel to Theorems 2.2 and 2.3, respectively.

Several applications of the standard cut method appeared recently, apparently being unaware of Proposition 3.1. For instance, in [55] Theorems 2.2, 2.3, and 2.4 were applied to obtain the corresponding topological indices of phenylazomethine dendrimers $S_n$, $n \geq 0$. The seminal paper for these dendrimers with a tetraphenylmethane core is [56], their structure should be clear from Fig. 3. It shows $S_1$ together with the half-edges towards $S_2$. Note that in $S_2$ there are 16 additional hexagons. The phenylazomethine dendrimer $S_0$ consists of the inner four hexagons.

![Figure 3: The phenylazomethine dendrimer $S_1$](image)
The obtained results are:
\[ W(S_n) = 13520n \cdot 4^n - 1820n \cdot 2^n - 14040 \cdot 4^n + 181616 \cdot 2^n - 3328, \]
\[ Sz(S_n) = 15548n \cdot 4^n - 2093n \cdot 2^n - 16146 \cdot 4^n + 2143 \cdot 2^n - 3838, \]
\[ PI(S_n) = 3600 \cdot 4^n - 3948 \cdot 2^n + 1080. \]

For yet additional application of Theorem 3.2 (again without mentioning the original source(s) of the theorem) see [57].

Very recently, Manuel et al. [58] introduced the so-called I-partition of a graph \( G \) as a partition \( \{S_1, \ldots, S_k\} \) of the edge set of \( G \) such that each \( S_i \) is an edge cut of \( G \) and the removal of edges of \( S_i \) leaves \( G \) into two components \( G_i \) and \( G_i' \) and the following holds:

(i) For any two vertices \( u, v \in G_i \), a shortest path between \( u \) and \( v \) has no edges in \( S_i \).

(ii) For any two vertices \( u, v \in G_i' \), a shortest path between \( u \) and \( v \) has no edges in \( S_i \).

(iii) For any two vertices \( u \in G_i \) and \( v \in G_i' \), a shortest path between \( u \) and \( v \) has exactly one edge in \( S_i \).

The conditions (i) and (ii) can be clearly reformulated by saying that \( G_i \) and \( G_i' \) are convex subgraphs. Moreover, it is not difficult to see that, as proved by Ilić in [59], the condition (iii) is redundant, that is, it follows from the first two conditions. It follows that the main theorem of [58] is an independent discovery of Theorem 2.2. Moreover, Al-Fozan et al. [60, 61] also independently rediscovered the standard cut method for the PI index and the Szeged index.

4 EXTENDED CUT METHODS

In this section we review different extensions of the standard cut method. The extensions generalize the standard cut method for a given topological index to a larger class of (molecular) graphs. The extensions are presented in the chronological order of their discoveries.

4.1 WIENER INDEX OF \( \ell_1 \)-GRAPHS

The first extension of the standard cut method beyond partial cubes is due to Chepoi, Deza, and Grishukhin [62]. They have generalized Theorem 2.2 to the so-called \( \ell_1 \)-graphs (to be defined below). In the bipartite case, \( \ell_1 \)-graphs coincide with partial cubes, hence their generalization is important in the non-bipartite case which indeed contains many chemical graphs.
By definition, $\ell_1$-graphs are graphs whose shortest-path metric can be isometrically embedded into an $\ell_1$-space. In order to have a graph-theoretical description of these graphs, we need the following definition. Let $\lambda \in \mathbb{N}$ and let $G$ and $H$ be two graphs. Then $H$ is scale $\lambda$-embeddable into $G$ if there exists a mapping $\alpha : V(H) \to V(G)$ such that for all vertices $u, v \in V(H)$,

$$d_G(\alpha(u), \alpha(v)) = \lambda \cdot d_H(u, v).$$

Assouad and Deza [63] proved the key characterization of $\ell_1$-graphs:

- A graph $G$ is an $\ell_1$-graph if and only if $G$ is scale $\lambda$-embeddable into a hypercube for some $\lambda \geq 1$.

Furthermore, Deza and Tuma [64] proved that the $\ell_1$-graphs can also be characterized as follows.

- A graph $G$ is an $\ell_1$-graph if and only if $G$ admits a collection $\mathcal{C}(G)$ of (not necessarily different) convex cuts of $G$ such that every edge of $G$ is cut by precisely $\lambda$ cuts from $\mathcal{C}(G)$.

The announced generalization of Theorem 2.2 now reads as follows:

**Theorem 4.1** [62, Proposition 5] Let $G$ be a scale $\lambda$-embeddable into a hypercube and let $\mathcal{C}(G)$ be the collection of convex cuts defining this embedding. Then

$$W(G) = \frac{1}{\lambda} \sum_{F \in \mathcal{C}(G)} n_1(F) \cdot n_2(F).$$

In order to determine the Wiener index of irregular convex triangular hexagons, Shiu, Lam, and Poon [65] extended the standard cut method to homogeneous $n$-gonal nets and in this way independently discovered the extended cut method of Theorem 4.1 (for $\lambda = 2$). Another application of Theorem 4.1 was given in [66] (called $k$-division method) to reprove the above-mentioned result from [65]. Moreover, the Szeged index and the vertex PI index were also determined.

Theorem 4.1 is quite powerful, so it is unfortunate that until now it was applied very rarely. A reason for this fact could be that $\ell_1$-graphs might appear “unfriendly” to the chemical community. To overcome this difficulty let us apply the theorem to the chemical graph from [67] shown in Fig. 4, let us denote it with $L$.

We can construct a collection of 12 convex cuts of $L$ such that every edge of $L$ will be cut by precisely two cuts from the collection as follows. In Fig. 4, five convex cuts of this collection are shown; these are the convex cuts that cut the edges of the lower pentagon, each the edges of it precisely twice. Five more cuts that cut the edges of the upper pentagon are constructed in an analogous way. Finally, to this collection of 10 cuts, we twice add the cut consisting of the three middle vertical...
edges. (Recall that some cuts in a collection of convex cuts are allowed to repeat, actually this is the reason why we are speaking about a “collection of convex cuts” and not about a “set of convex cuts”.) This collection of convex cuts prove that $L$ is an $\ell_1$-graph and we can thus apply Theorem 4.1 for which we must, for each convex cut, multiply the numbers of vertices in the connected components after the cut is removed, and add up the contributions of all cuts (and divide by 2 because each edge lies in two cuts). Hence,

$$W(L) = \frac{1}{2} \left( 2 \cdot (4 \cdot 10 + 4 \cdot 10 + 2 \cdot 12 + 5 \cdot 9 + 5 \cdot 9) + 2 \cdot (7 \cdot 7) \right) = 243.$$ 

A very rich source of chemical $\ell_1$-graphs is the book [68] which could hence be used as a source for possible further applications of Theorem 4.1.

### 4.2 Wiener Index via Canonical Metric Representation

In this subsection we first present the main result from [69] (Theorem 4.2) which widely generalizes Theorem 2.2. It applies to any graph that admits a non-trivial $\Theta^*$-partition (for an explanation of this statement see below). After presenting the result some applications will be given. Afterwards a two-fold generalization of Theorem 4.2, put forward very recently in [54], will be stated (Theorem 4.3).

To understand the results of this subsection, some preparation is needed. First recall from Section 2 the definition of the relation $\Theta$, the fact (Theorem 2.1) that $\Theta$ is an equivalence relation on partial cube, that for general graphs this need not be the case, and that the transitive closure $\Theta^*$ of $\Theta$ is an equivalence relation. Therefore $\Theta^*$ partitions the edge set of a given graph into equivalence classes, call this partition the $\Theta^*$-partition. This partition can be trivial meaning that $\Theta^*$ consists of a single equivalence class. For instance, $\Theta^*$ is trivial on all complete graphs and all complete bipartite graphs $K_{n,m}$, $n$, $m \geq 2$, as soon as at least one of $n$ and $m$ is bigger than 2.

Let $G$ be a graph and let $\{F_1, \ldots, F_k\}$ be the $\Theta^*$-partition of $G$. For any $j$, $1 \leq j \leq k$, let $G/F_j$ be the quotient graph defined as follows [70]. The vertex set of
$G/F_j$ consists of the connected components of the graph $G - F_j$ (that is, the graph obtained by removing $F_j$ from $G$), two components $C$ and $C'$ being adjacent if there exists an edge $uv \in F_j$ such that $u \in C$ and $v \in C'$. In addition, let $(G/F_j, w_j)$ be a vertex weighted graph, where $w_j : V(G/F_j) \to \mathbb{N}$ is the function that assigns to a vertex (= connected component) $C$ of $G/F_j$ the number of vertices in $C$. The last concept we need is the Wiener index $W(G, w)$ of a vertex weighted graph $(G, w)$ which is defined as [71]:

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

Clearly, if all the weights are 1, then $W(G, w) = W(G)$. Now we are ready to state:

**Theorem 4.2** [69] *For any connected graph $G$,*

$$W(G) = \sum_{j=1}^{k} W(G/F_j, w_j).$$

Let $G$ be a partial cube. Then by Theorem 2.1, the $\Theta^*$-partition coincides with the $\Theta$-partition and, moreover, each quotient graph $G/F_j$ is isomorphic to the complete graph on two vertices. But then, denoting the connected components of $G - F_j$ with $C$ and $C'$, the summation in (2) has only one term:

$$W(G/F_j, w_j) = \left|C\right| \cdot \left|C'\right| \cdot 1.$$

It follows that in the case when $G$ is a partial cube, Theorem 4.2 reduces to Theorem 2.2.

Let us list some applications of Theorem 4.2. Recall from Section 2 that in [34] the Wiener index of one-pentagonal carbon nanocones $G[n]$ was computed by means of partitioning $G[n]$ into appropriate isometric subgraphs and then applying Theorem 2.2. This result was confirmed in [72] by an application of Theorem 4.2. In this way the result was obtained in a more routine way. Similarly, a one-heptagonal nanocone $L[n]$ is the nanocone $L[n] = \text{CNC}_7[n]$ that consists of a central heptagon and $n$ rings of concentric hexagons around the heptagon. It can be easily visualized with the help of Fig. 1, where the inner pentagon is replaced with a hexagon. Of course, in the $L[n]$, the first layer of hexagons contains seven copies of it, the second layer contains 14 hexagons, ... In [73] Theorem 4.2 was applied to obtain the following closed expression for the Wiener index of the one-heptagonal nanocones:

$$W(L[n]) = \frac{238}{5} n^5 + \frac{2821}{6} n^4 + \frac{917}{2} n^3 + \frac{3311}{15} n + 42.$$

As another example, Yarahmadi and Fath-Tabar [74] used Theorem 4.2 to calculate the Wiener index of $N$-branched phenylacetylenes dendrimers.
We conclude this subsection with yet further generalization of Theorem 4.2. The generalization is two-fold. First, we may start with an arbitrary vertex weighted graph. And second, we can consider any coarser partition of the $\Theta^*$-partition $F$, where we say that a partition $E = \{E_1, \ldots, E_r\}$ of $E(G)$ is coarser than $F$ if each set $E_j$ is the union of one or more $\Theta^*$-classes of $G$. Then we have:

**Theorem 4.3** [54] Let $(G, w)$ be a connected, vertex weighted graph, and let $E = \{E_1, \ldots, E_r\}$ be a partition of $E(G)$ coarser than $F$. Then

$$W(G, w) = \sum_{j=1}^{r} W(G/E_j, w_j),$$

where $w_j : V(G/E_j) \to \mathbb{R}^+$ is defined by $w_j(C) = \sum_{x \in C} w(x)$, for all connected components $C$ of $G \setminus E_j$.

### 4.3 Degree Distance of Partial Hamming Graphs

Let $G$ be a (connected, molecular) graph. Then the degree distance [48, 75] of $G$ is defined as

$$DD(G) = \sum_{\{u,v\} \subseteq V(G)} (\deg(u) + \deg(v)) d_G(u, v).$$

The degree distance may be considered as a weighted version of the Wiener index similar (but not equal!) to (2). For recent developments on the degree distance we refer to [76, 77, 78] and references therein.

We now present a cut method result from [79] that is important from two reasons. The first is that the cut method was used for a topological index that involves the degrees of vertices, thus extending the cut method beyond the distance-based topological indices. The second reason is that the cut method is applied to a new class of graph, partial Hamming graphs, to be defined next.

The Cartesian product $G_1 \Box \cdots \Box G_k$ of graphs $G_1, \ldots, G_k$ has the vertex set $V(G_1) \times \cdots \times V(G_k)$, vertices $(g_1, \ldots, g_k)$ and $(g'_1, \ldots, g'_k)$ being adjacent if they differ in exactly one position, say in $i$th, and $g_i g'_i$ is an edge of $G_i$. See [25] for more information on the Cartesian (and other) product(s) of graphs. Recall that a subgraph $H$ of a graph $G$ is isometric if $d_H(u, v) = d_G(u, v)$ holds for any vertices $u, v$ of $H$. Now, a partial Hamming graph is a graph that is an isometric subgraph of some Cartesian product of complete graphs.

Before stating the main result of [79], let’s put the partial Hamming graphs into the previous framework. The simplest Cartesian product of $k$ complete graphs is $K_2 \Box \cdots \Box K_2$ and it is not difficult to see that it is isomorphic to the $k$-dimensional hypercube $Q_k$. Since the isometric subgraphs of hypercubes are partial cubes, partial Hamming graphs extend the class of partial cubes.
Let now $G$ be a partial Hamming graph, let $\{F_1 \ldots, F_k\}$ be the $\Theta^*$-partition of $G$, and let $G/F_i$, $1 \leq i \leq k$, be the corresponding quotient graphs (see Section 4.2).

For $i = 1, \ldots, k$ set in addition $V(G/F_i) = \{C^{(i)}_1, \ldots, C^{(i)}_{r_i}\}$, that is, $C^{(i)}_1, \ldots, C^{(i)}_{r_i}$ are the connected components of the graph $G - F_i$. For $i = 1, \ldots, k$ and $j = 1, \ldots, r_i$, set finally $\deg(C^{(i)}_j)$ to be the sum of degrees in $G$ of the vertices from $C^{(i)}_j$. Using these notations we can state:

**Theorem 4.4** [79] *If $G$ is a partial Hamming graph, then*

$$DD(G) = \sum_{i=1}^{k} \sum_{j=1}^{r_i} \deg(C^{(i)}_j) (|V(G)| - |C^{(i)}_j|).$$

Independently and at the same time Khalifeh, Yousefi-Azari, and Ashrafi [34, Theorem 5, first statement] obtained Theorem 4.4 in the bipartite case, that is, for partial cubes. In other words, they have developed the standard cut method for the degree distance index.

### 4.4 Distance Moments

In 1997, Gutman [19] generalized the Wiener index by setting

$$W_\lambda(G) = \sum_{\{u,v\} \subseteq V(G)} d_G(u,v)^\lambda,$$

where $\lambda$ is some real number, cf. [80]. When $\lambda$ is a positive integer, $W_\lambda(G)$ is called the $\lambda$-th distance moment of $G$ [81]. The distance moment is clearly a fundamental metric graph concept. Observe first that $W_1(G) = W(G)$. Also, the special cases $W_{-2}$, $W_{-1}$, $\frac{1}{2} W_2 + \frac{1}{2} W_1$, and $\frac{1}{6} W_3 + \frac{1}{2} W_2 + \frac{1}{3} W_1$ are known in the literature as the Harary index [82], the reciprocal Wiener index [83], the hyper-Wiener index [14, 15], and the Tratch-Stankevich-Zefirov index [81, 84], respectively. Moreover, it was demonstrated in [85] that the $n$th order Wiener index $W^{(n)}$ [87] can be expressed using distance moments and Stirling numbers. See also [88] for a related concept of walk numbers.

Hence, to compute the above mentioned topological indices of chemical graphs it suffices to compute the corresponding distance moments. We will now show how this task can be performed on graphs with transitive relation $\Theta$. This class is another proper superclass of partial cubes.

Let $G$ be a graph with transitive $\Theta$ and let $F_1, \ldots, F_k$ be the $\Theta$-classes of $G$. Then for any $1 \leq i \leq k$, the graph $G - F_i$ consists of two or three connected components denoted $C^{(i)}_1$, $C^{(i)}_2$, and $C^{(i)}_3$. If there are only two such components we assume that $C^{(i)}_3$ is the empty graph. For any $p \geq 1$, for any pairwise different $i_1, i_2, \ldots, i_p \in \{1, \ldots, k\}$ and for any $j_1, j_2, \ldots, j_p \in \{1, 2, 3\}$ let

$$n_{i_1,i_2,\ldots,i_p}^{j_1,j_2,\ldots,j_p} = \left| V\left(C^{(i_1)}_{j_1}\right) \cap V\left(C^{(i_2)}_{j_2}\right) \cap \cdots \cap V\left(C^{(i_p)}_{j_p}\right) \right|.$$
This notation is schematically illustrated in Fig. 5. The graph in question has four \( \Theta \)-classes, the components of each of the \( G - F_i \) are indicated. Then \( n^{1,3,4}_{2,1,2} \) is the order of the intersection of the gray parts.

![Figure 5: Partitions of \( G - F_i \), \( 1 \leq i \leq 4 \), into connected components, and the parts corresponding to \( n^{1,3,4}_{2,1,2} \)](image)

We now set

\[
N_{i_1,i_2,\ldots,i_p} = \sum_{\forall r: j_r \neq j'_r} n_{j_1,j_2,\ldots,j_p} n_{j'_1,j'_2,\ldots,j'_p},
\]

where the summation runs over all admissible indices \( j_1, j_2, \ldots, j_p \) and \( j'_1, j'_2, \ldots, j'_p \), and where, as indicated, \( j_r \neq j'_r \) for \( r = 1, 2, \ldots, k \).

**Theorem 4.5** [89, Theorem 2.1]. Let \( G \) be a graph with transitive \( \Theta \) and let \( s \) be a positive integer. Then with the above notation,

\[
W_s(G) = \sum_{t_{i_1}, t_{i_2}, \ldots, t_{i_p} > 0} \left( \frac{s}{t_{i_1} + t_{i_2} + \cdots + t_{i_p}} \right) N_{i_1,i_2,\ldots,i_p}.
\]

Having in mind that (i) numerous topological indices can be expressed with the corresponding distance moments and that (ii) graphs with transitive \( \Theta \) in particular include partial cubes as a proper subclass, Theorem 4.5 is a quite general result. To justify this statement, we next list several corollaries of it from earlier papers.

The already mentioned hyper-Wiener index \( WW \) was proposed by Randić [15] for the case of trees, while Klein, Lukovits and Gutman [14] extended the definition to all connected graphs \( G \) as follows:

\[
WW(G) = \frac{1}{4} \sum_{u \in V} \sum_{v \in V} d_G(u,v) + \frac{1}{4} \sum_{u \in V} \sum_{v \in V} d_G(u,v)^2.
\]
It is hence clear that \( WW(G) = \frac{1}{2} W_2(G) + \frac{1}{2} W_1(G) = \frac{1}{2} W_2(G) + \frac{1}{2} W(G) \) and therefore a two-fold application of Theorem 4.5 applies to the hyper-Wiener index. Let now \( G \) be a partial cube and let \( F_1, \ldots, F_k \) be its \( \Theta \)-classes (= \( \Theta^* \)-classes). Then as we already know, \( G - F_i \) consists of exactly two connected components \( C_1^{(i)} \) and \( C_2^{(i)} \) (that is, in the above notation, \( C_3^{(i)} = \emptyset \)) and Theorem 4.5 reduces to:

**Corollary 4.6** [90, Theorem 2.1] Let \( G \) be a partial cube with \( \Theta \)-classes \( F_1, \ldots, F_k \) and for \( i = 1, \ldots, k \) let \( C_1^{(i)} \) and \( C_2^{(i)} \) be the connected components of \( G - F_i \). Then

\[
WW(G) = W(G) + \sum_{i < j} \left( |C_1^{(i)} \cap C_1^{(j)}| \cdot |C_2^{(i)} \cap C_2^{(j)}| + |C_1^{(i)} \cap C_2^{(j)}| \cdot |C_2^{(i)} \cap C_1^{(j)}| \right).
\]

An application of Corollary 4.6 to the coronene/circumcoronene homologous series \( H_k, k \geq 1 \), yields [91]:

\[
WW(H_k) = \frac{548}{15} k^6 + \frac{82}{5} k^5 - \frac{55}{6} k^4 - 3k^3 + \frac{17}{15} k^2 + \frac{1}{10} k.
\] (4)

Similarly, using the approach parallel to the one from [34] that yielded (1), the hyper-Wiener index of one-pentagonal carbon nanocones was determined in [92]:

\[
WW(G[n]) = 21n^6 + \frac{409}{3} n^5 + \frac{8575}{24} n^4 + \frac{5795}{12} n^3 + \frac{8501}{24} n^2 + \frac{533}{4} n + 20.
\]

Theorem 4.5 thus applies to distance moments \( W_s \) where \( s \) is a positive integer. To present a result that applies to all real number, we first extend the definition of the Wiener index to disconnected graphs as follows. Denote by \( d(G, k) \) the number of pairs of vertices of \( G \) that are at distance \( k \). In particular, \( d(G, 0) \) and \( d(G, 1) \) are the number of vertices and edges of \( G \), respectively. Then the Wiener index can be extended to disconnected graphs as \( W(G) = \sum_{k \geq 1} d(G, k) k \). Moreover, for any real (or complex) number \( \lambda \) we also set [19, 93]:

\[
W_\lambda(G) = \sum_{k \geq 1} d(G, k) k^\lambda.
\]

Now we can state:

**Theorem 4.7** [94, Theorem 2] Let \( G \) be a partial cube and \( F_1, \ldots, F_k \) its \( \Theta \)-partition. Then for any real (or complex) number \( \lambda \),

\[
W_{\lambda+1}(G) = kW_\lambda(G) - \sum_{j=1}^{k} W_\lambda(G - F_j).
\]

In [94], the hyper-Wiener index of \( H_k \) as given in Eq. (4) was deduced as a consequence of Theorem 4.7. The latter theorem was later independently proved also in [34, Theorem 4]. Moreover, Theorem 4.7 also implies:
Corollary 4.8 [80] Let $B$ be a benzenoid graph and let $F_1, \ldots, F_k$ be its $\Theta$-partition (i.e., its orthogonal cuts). Then
\[
WW(B) = \frac{k + 1}{2} W(B) - \frac{1}{2} \sum_{j=1}^{k} W(B - F_j).
\]

4.5 COLORED WIENER INDEX IN GRAPHS

A concept of Wiener-type indices of graphs was recently introduced in [95] as follows. Let $G$ be a (connected) graph and let $X \subseteq V(G)$. Then the relative Wiener index of $X$ in $G$ is
\[
W_X(G) = \sum_{\{u,v\} \subseteq X} d_G(u,v).
\]
Clearly, $W_{V(G)}(G) = W(G)$. Moreover, if $X_k, k \geq 1,$ is the set of vertices of $G$ of degree $k$, then $W_{X_k}(G)$ is equal to the generalized terminal Wiener index $TW_k(G)$.

Very recently, Nadjafi-Arani, Das, and Slater [96] extended this definition to colored graphs. More precisely, let $G$ be a graph of order $n$ and size $m$, and for $H \subseteq V(G)$ let $W(H)$ denote the sum of distances between each pair of vertices of $H$. Assume that $n_1 + n_2 + \cdots + n_r = n = |V(G)|$ and $S = \{n_2, n_3, \ldots, n_r\}$. An $S$-coloring $P = \{S_2, S_3, \ldots, S_r\}$ is a partition of $V(G) - S_1$ with $|S_i| = n_i$, moreover, we consider $S_1$ corresponding to uncolored vertices. The colored Wiener index of $CW_P(G)$ is the sum of the distances between vertices of the same color. Note that we do not consider uncolored vertices in $CW_P(G)$. If we wish to color all vertices, then we set $S_1 = \emptyset$ and $n_1 = 0$. One can easily see that, if we color $X \subseteq V(G)$ by one color, then we have $CW_P(G) = W_X(G)$. Actually, Dankelmann, Goddard, and Slater [97] considered graphs $G$ in which all the vertices are colored. They defined the colored distance of $G$ as the sum of the distances between all unordered pairs of vertices having different colors.

In [96] the cut method was applied for computing the colored Wiener index in general graphs. This approach leads to generalizations of Theorems 4.2 and 4.3 and reads as follows. Let $G$ be a (connected) graph with an $S$-coloring $P = \{S_2, S_3, \ldots, S_r\}$. Also let $\{F_1, \ldots, F_k\}$ be the $\Theta^*$-partition of $G$ and let $G/F_j$ be the corresponding quotient graphs as described in Section 4.2. But now, instead of the vertex weighted graphs $(G/F_j, w_j)$, consider the vertex weighted graphs $(G/F_j, w'_{ij})$, where $w'_{ij} : V(G/F_j) \to \mathbb{R}^+$ is the function that assigns to a vertex $C$ (that is, to a connected component) the number of vertices of color $i$ in $C$, $2 \leq i \leq r$, that is, $|C \cap S_i|$. Then we have:

Theorem 4.9 [96] For any connected graph $G$ with an $S$-coloring $P$,
\[
CW_P(G) = \sum_{j=1}^{k} \sum_{i=2}^{r} W(G/F_j, w'_{ij}).
\]
Moreover, similarly as Theorem 4.2 generalizes to Theorem 4.3, one can generalize Theorem 4.9 in two directions, to arbitrary vertex weighted graphs and to any coarser partition of the $\Theta^*$-partition:

**Theorem 4.10** [96] Let $(G, w)$ be a connected, vertex weighted graph, with an $S$-coloring $P$. Also let $E = \{E_1, \ldots, E_t\}$ be a partition of $E(G)$ coarser than the $\Theta^*$-partition. Then

$$CW_P(G, w) = \sum_{j=1}^{t} \sum_{r=2}^{r} W(G/E_j, w'_{ij}),$$

where $w'_{ij} : V(G/E_j) \rightarrow \mathbb{R}^+$ is defined by $w'_{ij}(C) = \sum_{x \in C \cap S_i} w(x)$, for all connected components $C$ of $G \setminus E_j$.

To conclude the paper we emphasize that Putz et al. [9, 10] used the colored Wiener index to describe the total parabolic energy combines information on the molecular connectivity network (conveyed by the Wiener index) and the chemical reactivity (expressed by electronegativity and chemical hardness of the colored atoms) and exhibits a correlation to the chemical reactivity. They mentioned the ability of axial coloring (some special vertex coloring in chemical graphs) to describe the electronic properties of the carbon atoms constituting a PAH molecule. In general, the reactive-parabolic colored Wiener index better correlates the structural properties for both topological efficiency indices and below of the classical Wiener index with respect to the eccentric connectivity in molecules. For the physical-chemical parameters, the reactive-parabolic colored Wiener index correlates the retention indices and molecular weight better than the classical Wiener index.

## 5 CONCLUDING REMARKS

In this survey paper we have presented state of the art on the cut method and listed its applications in chemistry. It should be clear from the paper that the method turned out to be very useful for different purposes and for numerous classes of chemical graphs. On the other hand, we believe that many additional possible instances and applications of the method are waiting to be discovered. One direction would be to apply the existing methods to additional families of (chemical) graphs. We have already mentioned that the existing cut method for the Wiener index of $\ell_1$-graphs has until now been applied only in some particular cases. Moreover, it would certainly be interesting to extend the other cut methods to $\ell_1$-graphs as well. Finally, the possible power of the cut method for invariants that are not distance-based is in most cases yet to be explored.
ACKNOWLEDGEMENTS

We are grateful to one of the reviewers for a very careful reading of the manuscript and for numerous useful suggestions. This work has been financed by ARRS Slovenia under the grant P1-0297.

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