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Cut method and its applications in benzenoid graph

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Abstract: *A general description of the cut method is presented and an overview of its applications in a benzenoid graph is given. The Wiener index, the Szeged index and the hyper-Wiener index of a benzenoid graph is calculated based on the consideration of the elementary cuts and the pair of elementary cuts of the corresponding benzenoid graph.*
Keywords: *Benzenoid graph, cut method, hyper-Wiener index, Szeged index, Wiener index.*

I. Introduction

Cut method is defined in the following general form. For a given (molecular) graph G,

1. Partition the edge set of G into classes $F_1, F_2, \dots\dots\dots, F_k$, call them cuts, such that each of the graphs $G - F_i, i = 1,2, \dots\dots k$, consists of two (or more) connected components; and
2. Use properties (of the components) of the graphs $G - F_i$ to derive a required property of G.

The cut method can hardly be studied in the above generality; instead we are interested in classes of (chemical) graphs that allow applicable partitions into cuts and in relevant properties. Often a property of G, that we are interested in, is some graph invariant, for instance the Wiener index. We could be interested to obtain expressions for such invariants for certain (chemically) important classes of graphs or to develop fast algorithms for computing them.

The cut method turned out to be especially useful when if comes to metric properties of graphs. The key idea how the graphs $G - F_i$ can be used to obtain such properties of G is to find an isometric embedding $f: G \rightarrow H$, where H is a properly selected target graph and to use the image f(G) to obtain distance properties of G. The key subidea is then to select H to be a Cartesian product graph. We introduce and explain the concepts mentioned in this paragraph in Section 2.

The most prominent class of chemical graphs for which the cut method turned out to be extremely fruitful is the class of benzenoid graphs. In fact, the 1995 paper [1] and the elaboration of its method for the computation of the Wiener index of benzenoid graphs (and, more generally, of partial cubes) from [2] can be considered as the starting point of the cut method. We explain the method and its consequences in Section 3.

A similar approach that works for the Wiener index can be applied to the Szeged index as well. This is presented in Section 4. We continue with a section on the hyper-Wiener index. Again, the cut method is applicable; however, in this case it is slightly more involved than the corresponding methods for the Wiener and the Szeged index because the computation of the hyper-Wiener index requires not only graph distance but also squares of graphs distances.

II. Preliminaries

Let $G = (V, E)$ be a connected graph and $u, v \in V$. Then the distance $d_G(u, v)$ between u and v is the number of edges on a shortest u, v-path.

The Cartesian product G□H of graphs Gand H is probably the most important graph product and is defined in the following way:

1. $V(G\square H) = V(G) \times V(H)$;
2. $E(G\square H)$ Consists of pairs $(g, h)(g', h')$ where either $g = g'$ and $hh' \in E(H)$, or $gg' \in E(G)$ and $h = h'$.

The graphs Gand H are called factors of G□H. The Cartesian product is commutative and associative. The latter property implies that products of several factors are well-defined. The fundamental metric property of the Cartesian product is that the distance function is additive:

$$d_{G\square H}\Big((g,h),(g',h')\Big) = d_G(g,g') + d_H(h,h')$$

This property has been independently discovered several times.

The simplest Cartesian products are products in which all factors are the complete graph on two vertices K_2. These graphs are known as hypercubes. More precisely, the n-cube Q_n is the Cartesian product of n factors K_2, that is,$Q_n = \square_{i=1}^{n} K_2$. It is important to observe that the n-cube Q_n can be equivalently described as the graph whose vertex set consists of all n-tuples $b_1 b_2 \dots\dots b_n$ with $b_i \in \{0,1\}$, where two vertices are adjacent if the corresponding tuples differ in precisely one position.

A subgraph H of a graph G is isometric if for any vertices u and v of H,

$$d_H(u,v) = d_G(u,v)$$

The class of graphs that consists of all isometric subgraphs of hypercubes turns out to be very important and has got the name partial cubes. We point out that hypercubes; even cycles, trees, median graphs, benzenoid graphs, and Cartesian products of partial cubes are all partial cubes.

III. Wiener index

The Wiener index $W(G)$ of a graph $G = (V, E)$ is defined with

$$W(G) = \frac{1}{2}\sum_{u\in U}\sum_{v\in V} d_G(u,v)$$

As we have already mentioned, the cut method was first implemented for a calculation of the Wiener index of benzenoid graphs. In fact, the method works for any partial cube as the next theorem asserts. For its formulation we need the following concepts.

Let G be a connected graph. Then $e = xy$ and $f = uv$ are in the Djokovic-Winkler relation Θ [3, 4] if

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

The relation Θ is always reflexive and symmetric, and is transitive on partial cubes. Therefore, Θ partitions the edge set of a partial cube G into equivalence classes, called Θ-classes.

3.1. Theorem

[1] Let G be a partial cube and let $F_1, \ldots\ldots F_k$ be its Θ-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

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

Let G be a partial cube isometrically embedded into Q_k. (Note that the number of Θ-classes is equal to the dimension of the hypercube into G is embedded.) Then a vertex u of G can be considered as a binary k-tuple $u = u_1u_2 \ldots\ldots\ldots u_k$, and the distance between two vertices is the number of positions in which they differ. For $b, b' \in \{0,1\}$, let $\delta(b,b') = 0$ if $b = b'$, and $\delta(b,b') = 1$ if $b \neq b'$. Having this in mind we can compute as follows:

$$\begin{aligned} W(G) &= \frac{1}{2}\sum_{u\in V}\sum_{v\in V} d_G(u,v) \\ &= \frac{1}{2}\sum_{u\in V}\sum_{v\in V} d_{Q_k}(u,v) \\ &= \frac{1}{2}\sum_{u\in V}\sum_{v\in V}\sum_{i=1}^{k} \delta(u_i,v_i) \\ &= \sum_{i=1}^{k}\left(\frac{1}{2}\sum_{u\in V}\sum_{v\in V}\delta(u_i,v_i)\right) \\ &= \sum_{i=1}^{k} n_1(F_i)\ .\, n_2(F_i) \end{aligned}$$

In benzenoid graphs the Θ-classes are precisely their orthogonal cuts. Hence if $\mathcal{C}$ is the set of orthogonal cuts of a benzenoid graph B, and for $C\epsilon\mathcal{C}$ we let $n_1(C)$ and $n_2(C)$ be the number of vertices in the two components of $G - C$, respectively, then Theorem 3.1 specializes as follows [1,2]:

$$W(B) = \sum_{C\epsilon\mathcal{C}} n_1(C)\ .\, n_2(C)$$

We illustrate the use of the above equation in the ovalene H_2, see Fig.1.

The Ovalene H_2 has three horizontal cuts, two of them being symmetric. Each of these two cuts contribute 7.25 to $W(H_2)$, while contribution of the remaining cut is 16.16. Hence horizontal cuts contribute 2.7.25+16.16=606. Clearly, there are two more groups of elementary cuts which contributes 2.5.27+2.12.20=750. Hence we conclude that $W(H_2) = 606 + 2\ .750 = 2106$.

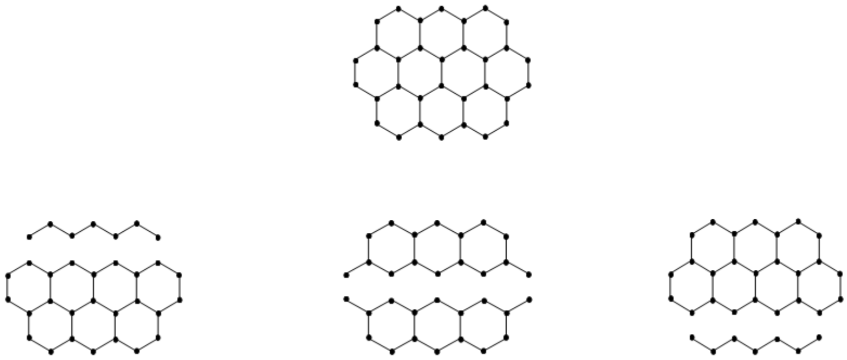


Figure 1: Ovalene H_2 and three of its cuts

IV. Szeged index

For an edge $e = uv$ of a connected graph G let $W_{uv} = \{x \in V(G) | d_G(x,u) < d_G(x,v)\}$. The set W_{vu} is defined analogously. Then the Szeged index of G is defined as:

$$Sz(G) = \sum_{uv \in E(G)} |W_{uv}| . |W_{vu}|$$

Now, let uv be an edge of a partial cube G and suppose that it belongs to the Θ-class. Then it follows easily from definitions that W_{uv} and W_{vu} induce the connected components of $G - F$. Therefore, Theorem 3.1 has its variant for the Szeged index:

4.1. Theorem

Let G be a partial cube and let $F_1, \dots\dots\dots, F_k$ be its Θ-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

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

Theorem 4.1 was elaborated in [5] for benzenoid graphs. Since the Θ-classes of a benzenoid graph are its cuts, the result specializes to:

4.2. Corollary

[5] Let B be a benzenoid graph and $\mathcal{C}$ the set of its orthogonal cuts. For $C \in \mathcal{C}$ let $n_1(C)$ and $n_2(C)$ be the number of vertices in the two components of $G - C$, respectively. Then

$$Sz(B) = \sum_{C \epsilon \mathcal{C}} |C| . n_1(C) . n_2(C)$$

Consider again the ovalene H_2 from Fig.1. The computation of $Sz(H_2)$ goes along the same lines as the computation of $W(H_2)$, except that now we need to multiply each contribution with the size of the corresponding cut. Therefore,

$$Sz(H_2) = \{(4.2.7.25) + (5.16.16)\} + 2\{(3.2.5.27) + (4.2.12.20)\} = 8140.$$

5. Hyper-Wiener index

The hyper-Wiener index WW was proposed by Randic in [6]. His definition was originally given only for trees and was extended to all connected graphs $G = (V, E)$ by Klein, Lukovits and Gutman [7] as follows:

$$WW(G) = \frac{1}{4} \sum_{u \in V} \sum_{v \in V} d_G(u,v) + \frac{1}{4} \sum_{u \in V} \sum_{v \in V} d_G(u,v)^2 \qquad (1)$$

Note that the first term is one half of the Wiener index, while in the second we need to compute the squares of distances. The cut method is applicable also in this case, but because squares of distances are involved, the method, that we describe next, becomes slightly more involved.

Let G be a partial cube and let $F_1, \dots\dots\dots, F_k$ be its Θ-classes. For each Θ-class F_i let $u_i v_i$ be a representative of F_i. Then for any $1 \le i < q$ let

$$n_{11}(F_i, F_j) = \left| W_{u_i v_i} \cap W_{u_j v_j} \right|, \qquad n_{22}(F_i, F_j) = \left| W_{v_i u_i} \cap W_{v_j u_j} \right|,$$

and

$$n_{12}(F_i, F_j) = \left| W_{u_i v_i} \cap W_{v_j u_j} \right|, \qquad n_{21}(F_i, F_j) = \left| W_{v_i u_i} \cap W_{u_j v_j} \right|$$

Now consider the following theorem.

5.1. Theorem

[8] Let G be a partial cube with Θ-classes $F_1, \dots\dots\dots, F_k$ and representatives $u_i v_i \in F_i, 1 \le i \le k$. Then

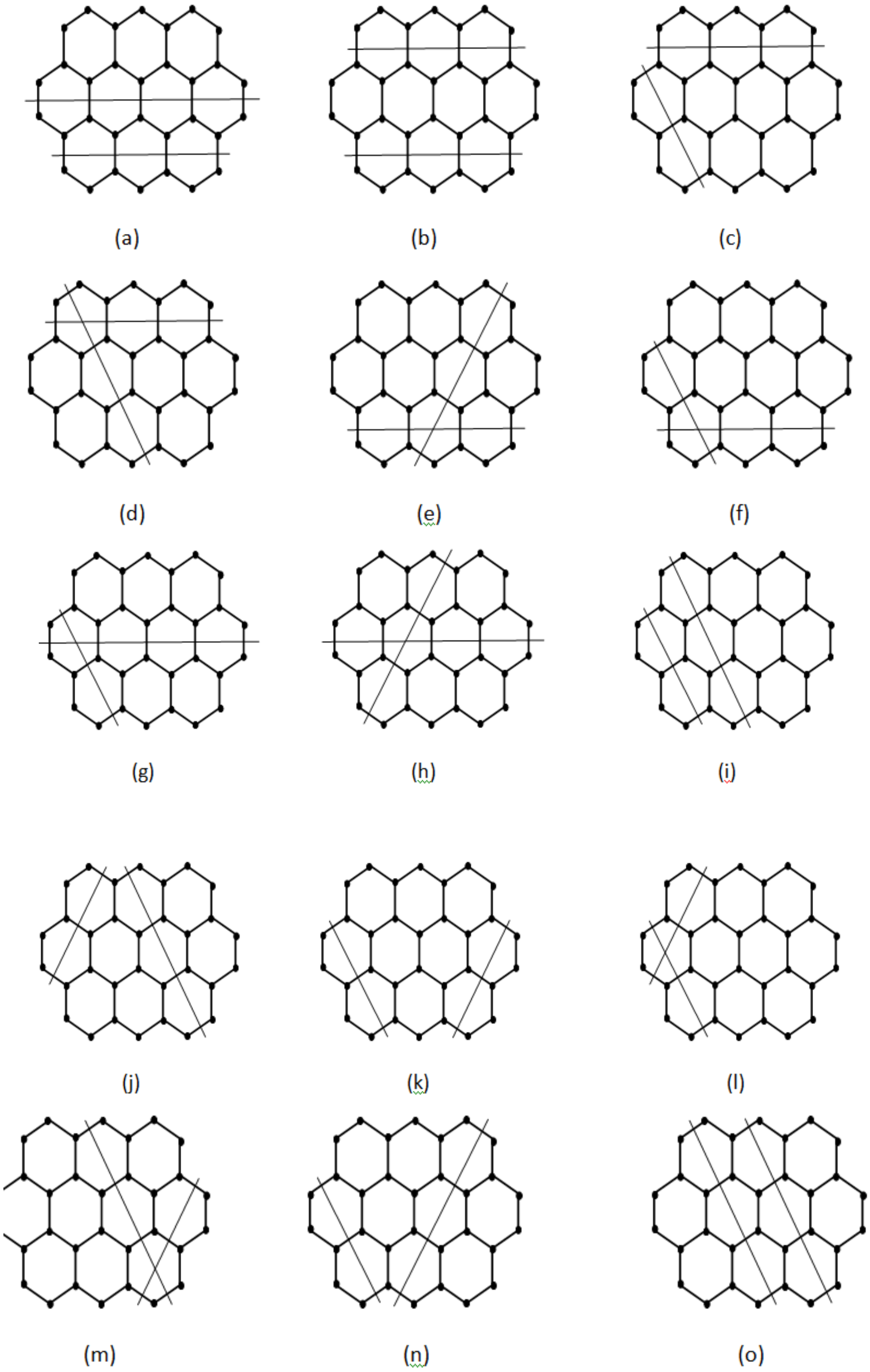
$$WW(G) = W(G) + \sum_{i=1}^{k} \sum_{j=i+1}^{k} \left(n_{11}(F_i, F_j) \,.\, n_{22}(F_i, F_j) + n_{12}(F_i, F_j) \,.\, n_{21}(F_i, F_j) \right) \quad (2)$$

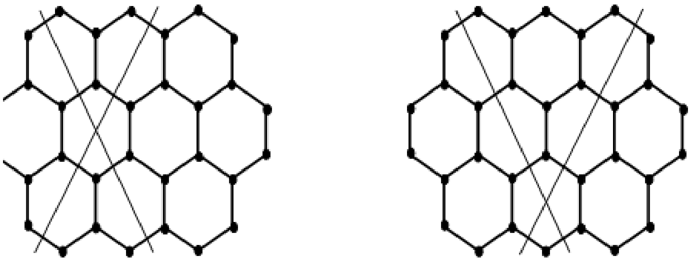
The key step in proving Theorem 5.1 is to show that

$$\sum_{u \in V} \sum_{v \in V} d_G(u,v)^2 = 2W(G) + 4 \sum_{i=1}^{k} \sum_{j=i+1}^{k} \left(n_{11}(F_i, F_j) \,.\, n_{22}(F_i, F_j) + n_{12}(F_i, F_j) \,.\, n_{21}(F_i, F_j) \right)$$

The result then follows immediately by plugging the last equality into (2).

For an example consider again the ovalene.





(p) (q)

Figure 2: Types of pairs of cuts in the ovalene

It contains 11 cuts, hence there are $\binom{11}{2} = 55$ pairs of cuts to be considered. These cuts can be grouped into 17 types that are shown in Fig.2.

There are 2, 1, 4, 4, 4, 4, 4, 4, 4, 7, 4, 2, 4, 1, 2, 2, 2 pairs of cuts in the cases (a), (b), (c), (d), (e), (f), (g), (h), (i), (j), (k), (l), (m), (n), (o), (p), (q) respectively. Hence the second term of Theorem 5.1 gives

$$2(7.16 + 0.9) + (7.7 + 0.18) + 4(0.20 + 7.5) + 4(1.14 + 6.11) + 4(3.8 + 4.17) + 4(5.3 + 2.22) + 4(1.12 + 15.4) + 4(4.8 + 12.8) + 4(5.20 + 0.7) + 7(5.12 + 0.15) + 4(5.5 + 0.22) + 2(2.24 + 3.3) + 4(4.19 + 1.8) + (5.12 + 0.14) + 2(12.12 + 0.8) + 2(8.16 + 4.4) + 2(11.11 + 9.1) = 4403.$$

Since $\mathrm{W}(\mathrm{H}_2) = 2106$ we conclude by Theorem 5.1 that $\mathrm{WW}(\mathrm{H}_2) = 6509$.

V. Conclusion

The cut method is applied in ovalene (a benzenoid graph) and the Wiener index, the Szeged index and the hyper-Wiener index has been calculated.

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