A theorem on Wiener-type invariants for isometric subgraphs of hypercubes

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Abstract

Let $d(G,k)$ be the number of pairs of vertices of a graph G that are at distance k, λ a real (or complex) number, and $W_\lambda(G) = \sum_{k\geq 1} d(G,k)\, k^\lambda$. It is proved that for a partial cube G, $W_{\lambda+1}(G) = |\mathcal{F}|\, W_\lambda(G) - \sum_{F\in\mathcal{F}} W_\lambda(G\setminus F)$, where $\mathcal{F}$ is the partition of $E(G)$ induced by the Djoković-Winkler relation Θ. This result extends previously known result for trees and implies several relations for distance-based topological indices.

Key words: graph distance, hypercube, partial cube, Wiener number, hyper-Wiener index.

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1 Introduction

The *Wiener number* (or *Wiener index*) $W(G)$ of a connected graph G is the sum of distances between all pairs of vertices of G, that is,

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

In the case of trees the Wiener number was introduced back in 1947 by Wiener in [25], hence the name of this graph invariant. Until today, it has been extensively investigated, above all in mathematical chemistry, see special issues of journal devoted to the topic [13, 14], recent surveys [5, 6], and recent papers [7, 8, 9].

The Wiener number can be extended to disconnected graphs as follows [12]. Denote by $d(G,k)$ the number of pairs of vertices of G that are at distance k. Note that $d(G,0)$ and $d(G,1)$ represent the number of vertices and edges, respectively. Then W can be extended to disconnected graphs as $W(G) = \sum_{k\geq 1} d(G,k)\,k$. Moreover, this definition can be further generalized in the following natural way [11, 12]:

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

where λ is some real (or complex) number. Several particular instances of the invariant W_λ have been previously studied. For instance, 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 the so-called Harary index, reciprocal Wiener index, hyper–Wiener index, and Tratch-Stankevich-Zefirov index, cf. [12] and references therein. In the chemical literature also $W_{1/2}$ [27] as well as the general case W_λ were examined [10, 11, 15].

Let T be a tree, then in [12] the following recursive formula for W_λ has been obtained:

$$W_{\lambda+1}(T) = (n-1)\,W_\lambda(T) - \sum_{e\in E(T)} W_\lambda(T-e)\,. \tag{1}$$

In this note we prove that if G is a partial cube and $\mathcal{F}$ the partition of $E(G)$ induced by the Djoković-Winkler relation Θ, then

$$W_{\lambda+1}(G) = |\mathcal{F}|\,W_\lambda(G) - \sum_{F\in\mathcal{F}} W_\lambda(G\setminus F)\,. \tag{2}$$

Since trees are partial cubes in which the partition $\mathcal{F}$ is trivial, that is, every edge of a tree forms a class of the partition, (1) immediately follows from (2). In addition we will demonstrate that some known relations between distance-based topological indices follow from formula (2).

2 The main result

For $u,v \in V(G)$, let $d_G(u,v)$ denote the length of a shortest path (also called *geodesic*) in G from u to v. A subgraph H of a graph G is called *isometric* if $d_H(u,v) = d_G(u,v)$ for all $u,v \in V(H)$. Isometric subgraphs of hypercubes are called *partial cubes*. Clearly, hypercubes are partial cubes, as well as are trees and median graphs. Partial cubes form a well studied class of graphs, we refer to classical references [1, 4, 26], book [16], recent paper [20] and references therein. For applications of partial cubes to mathematical chemistry see [3, 17, 18, 19, 21].

The *Djoković-Winkler relation* Θ is defined on the edge set of a graph in the following way [4, 26]. Edges $e = xy$ and $f = uv$ of a graph G are in relation Θ if

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

Winkler [26] proved that among bipartite graphs, Θ is transitive precisely for partial cubes, hence Θ partitions the edge set of a partial cube. Let G be a partial cube and $\mathcal{F} = \{F_1, F_2, \ldots, F_r\}$ the partition of its edge set induced by the relation Θ. Then we say that $\mathcal{F}$ is the Θ-*partition* of G.

For the proof of our main theorem we need the following facts about Θ, cf. [16, 20].

Lemma 1 *Let G be a partial cube.*

(i) A path P in G is a geodesic if and only if no two different edges of P are in relation Θ.

(ii) Let F be a class of the Θ-partition *of G. Then $G \setminus F_i$ consists of two connected components.*

We are now ready for our main result.

Theorem 2 *Let G be a partial cube and $\mathcal{F}$ its Θ-partition. Then for any real (or complex) number λ,*

$$W_{\lambda+1}(G) = |\mathcal{F}|\, W_\lambda(G) - \sum_{F\in\mathcal{F}} W_\lambda(G \setminus F)\,.$$

Proof. Let s be the diameter of G, then

$$W_\lambda(G) = \sum_{k=1}^{s} d(G,k)\, k^\lambda\,.$$

Let $\mathcal{F} = \{F_1, F_2, \ldots, F_r\}$ and set

$$X = \sum_{i=1}^{r} W_\lambda(G \setminus F_i)\,.$$

Let u and v be arbitrary vertices of G, where $d(u,v) = k$, $1 \le k \le s$. Let P be a u,v-geodesic. By Lemma 1 (i), the edges of P belong to pairwise different classes of $\mathcal{F}$. We may assume without loss of generality that they belong to $F_1, F_2, \ldots, F_k$. By Lemma 1 (ii), u and v belong to different connected components of $G \setminus F_i$ for $i = 1, \ldots, k$. On the other hand, u and v are in the same connected component of $G \setminus F_i$ for $i = k+1, \ldots, r$. Clearly, in the latter case, $d_{G\setminus F_i}(u,v) = k$. It follows that the pair $\{u,v\}$ contributes $(r-k)$-times to X. Thus,

$$\begin{aligned} X &= \sum_{k=1}^{s} (r-k)\, d(G,k)\, k^\lambda \\ &= r\sum_{k=1}^{s} d(G,k)\, k^\lambda - \sum_{k=1}^{s} d(G,k)\, k^{\lambda+1} \\ &= r\, W_\lambda(G) - W_{\lambda+1}(G)\,. \end{aligned}$$

□

If F is a Θ-class of the hypercube Q_n, then $Q_n \setminus F$ consists of two disjoint copies of Q_{n-1}. Thus, by Theorem 2, $W_{\lambda+1}(Q_n) = nW_\lambda(Q_n) - 2nW_\lambda(Q_{n-1})$. By this recurrence relation it follows that $W_\lambda(Q_n) = p_\lambda(n)4^n$, where $p_\lambda(n)$ is a polynomial. This can also be seen from the formula $W_\lambda(Q_n) = 2^{n-1}\sum_{k=1}^{n}\binom{n}{k}k^\lambda$.

3 Applications

In this section we give two applications of Theorem 2. The first one is the following result for the Wiener number, first given in [19], and extended to the so-called L_1-graphs in [2].

Let G be a partial cube, $\mathcal{F}$ its Θ-partition, and $F \in \mathcal{F}$. Then we will denote the connected components of $G \setminus F$ by $G_1(F)$ and $G_2(F)$. Set $n_1(F) = |G_1(F)|$ and $n_2(F) = |G_2(F)|$.

Corollary 3 *Let G be a partial cube and $\mathcal{F}$ its Θ-partition. Then*

$$W_1(G) = W(G) = \sum_{F \in \mathcal{F}} n_1(F)\, n_2(F)\,.$$

Proof. Let $n = |V(G)|$, then for any $F \in \mathcal{F}$, $n_1(F) + n_2(F) = n$. Using Theorem 2 we can compute as follows.

$$\begin{aligned}
W_1(G) &= |\mathcal{F}|\, W_0(G) - \sum_{F \in \mathcal{F}} W_0(G \setminus F) \\
&= |\mathcal{F}| \binom{n}{2} - \sum_{F \in \mathcal{F}} \left[\binom{n_1(F)}{2} + \binom{n_2(F)}{2}\right] \\
&= |\mathcal{F}| \binom{n}{2} - \frac{1}{2}\sum_{F \in \mathcal{F}} \left[n^2 - n - 2\, n_1(F)\, n_2(F)\right] \\
&= |\mathcal{F}| \binom{n}{2} - \frac{1}{2}\sum_{F \in \mathcal{F}} (n^2 - n) + \sum_{F \in \mathcal{F}} n_1(F)\, n_2(F) \\
&= \sum_{F \in \mathcal{F}} n_1(F)\, n_2(F)\,.
\end{aligned}$$

□

For the second application some more concepts are needed. The hyper-Wiener index WW is a topological index proposed by Randić [24] for trees and extended to all graphs by Klein, Lukovits, and Gutman [22] as

$$WW(G) = \frac{1}{2}W_1(G) + \frac{1}{2}W_2(G)\,.$$

Let G be a partial cube, $\mathcal{F}$ its Θ-partition, and $F, F' \in \mathcal{F}, F \neq F'$. Then we will denote $n_{11}(F, F') = |G_1(F) \cap G_1(F')|$, $n_{12}(F, F') = |G_1(F) \cap G_2(F')|$, $n_{21}(F, F') = |G_2(F) \cap G_1(F')|$, and $n_{22}(F, F') = |G_2(F) \cap G_2(F')|$. We say that the classes F and F' *cross* if $n_{k\ell}(F, F') \neq 0$ for $1 \leq k, \ell \leq 2$, and write $F \# F'$ to denote the fact that F and F' cross, see [20, 23]. Now we can deduce from Theorem 2 the following result given in [17].

Corollary 4 *Let G be a partial cube and $\mathcal{F} = \{F_1, F_2, \ldots, F_r\}$ its Θ-partition. Then*

$$WW(G) = W(G) + \sum_{i<j} [n_{11}(F_i, F_j)\, n_{22}(F_i, F_j) + n_{12}(F_i, F_j)\, n_{21}(F_i, F_j)] \,.$$

Proof. By Theorem 2, $W_2(G) = r\, W(G) - \sum_{i=1}^{r} W(G \setminus F_i)$. On the other hand, $WW(G) = W(G)/2 + W_2(G)/2$. Combining these two equalities we get

$$WW(G) \quad = \quad W(G) + \frac{1}{2}\left[(r-1)W(G) - \sum_{i=1}^{r} W(G \setminus F_i)\right] . \tag{3}$$

By Corollary 3 we have

$$(r-1)W(G) = \sum_{j=1}^{r-1}\sum_{i=1}^{r} n_1(F_i)\, n_2(F_i) = \sum_{i=1}^{r}\sum_{j=1}^{r-1} n_1(F_i)\, n_2(F_i) \,, \tag{4}$$

while on the other hand

$$\sum_{i=1}^{r} W(G \setminus F_i) \quad = \quad \sum_{i=1}^{r}\Big[W(G_1(F_i)) + W(G_2(F_i))\Big] . \tag{5}$$

Combining (4) and (5) with (3) we obtain:

$$WW(G) \quad = \quad W(G) + \frac{1}{2}\sum_{i=1}^{r}\left[\sum_{j=1}^{r-1} n_1(F_i)\, n_2(F_i) - W(G_1(F_i)) - W(G_2(F_i))\right] . \tag{6}$$

Having in mind Corollary 3 we now consider the contribution of a fixed pair of classes F_i and F_j to the right-hand side sum in (6). For the rest of the proof let n_{11}, n_{12}, n_{21}, and n_{22} denote $n_{11}(F_i, F_j)$, $n_{12}(F_i, F_j)$, $n_{21}(F_i, F_j)$, and $n_{22}(F_i, F_j)$, respectively.

Suppose first that F_i and F_j cross. Then the contribution of the pair F_i, F_j is

$$\Big[(n_{11} + n_{12})(n_{21} + n_{22}) + (n_{11} + n_{21})(n_{12} + n_{22})\Big] - \Big[(n_{11}n_{12} + n_{21}n_{22})$$
$$+ (n_{11}n_{21} + n_{12}n_{22})\Big] = 2n_{11}n_{22} + 2n_{12}n_{21} \,.$$

If F_i, F_j do not cross, then there are four possibilities of how F_i and F_j are related, the possibilities are shown in Fig. 1.

Then the contributions of the classes F_i and F_j are, respectively:

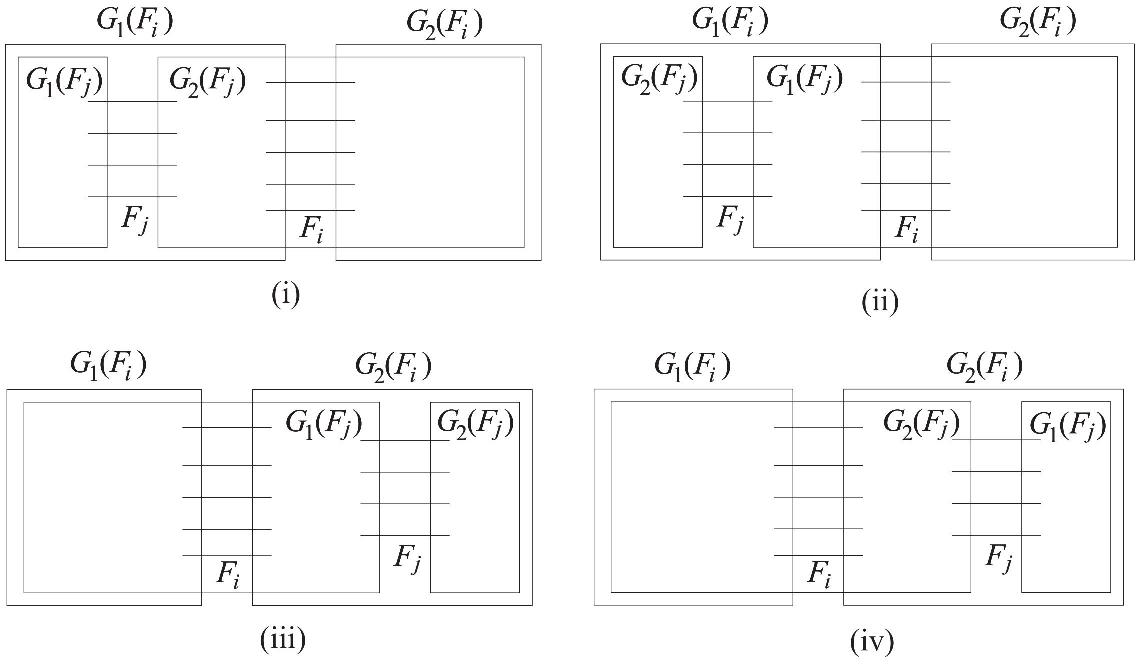

Figure 1: Non-crossing classes F_i and F_j

$$
\begin{array}{rl}
\text{(i)} & (n_{11}+n_{12})n_{22}+n_{11}(n_{12}+n_{22})-(n_{11}n_{12}+n_{12}n_{22}) = 2n_{11}n_{22}\,, \\
\text{(ii)} & (n_{11}+n_{12})n_{21}+n_{12}(n_{11}+n_{21})-(n_{12}n_{11}+n_{11}n_{21}) = 2n_{12}n_{21}\,, \\
\text{(iii)} & (n_{21}+n_{22})n_{11}+n_{22}(n_{11}+n_{21})-(n_{21}n_{22}+n_{21}n_{11}) = 2n_{11}n_{22}\,, \\
\text{(iv)} & (n_{21}+n_{22})n_{12}+n_{21}(n_{12}+n_{22})-(n_{21}n_{22}+n_{22}n_{21}) = 2n_{12}n_{21}\,.
\end{array}
$$

Since in cases (i), (ii), (iii), and (iv) we have $n_{21}=0$, $n_{22}=0$, $n_{12}=0$, and $n_{11}=0$, respectively, in all cases the contribution of F_i and F_j to the right-hand side sum in (6) can be written as

$$2n_{11}n_{22}+2n_{12}n_{21}$$

which completes the argument. □

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References

[1] V. Chepoi, *d*-Convexity and isometric subgraphs of Hamming graphs, Cybernetics 1 (1988) 6–9.

[2] V. Chepoi, M. Deza, and V. Grishukhin, Clin d'oeil on L_1-embeddable planar graphs, Discrete Appl. Math. 80 (1997) 3–19.

[3] V. Chepoi and S. Klavžar, The Wiener index and the Szeged index of benzenoid systems in linear time, J. Chem. Inf. Comput. Sci. 37 (1997) 752–755.

[4] D. Djoković, Distance preserving subgraphs of hypercubes, J. Combin. Theory Ser. B 14 (1973) 263–267.

[5] A.A. Dobrynin, R. Entringer, and I. Gutman, Wiener index of trees: theory and applications, Acta Appl. Math. 66 (2001) 211–249.

[6] A.A. Dobrynin, I. Gutman, S. Klavžar, and P. Žigert, Wiener index of hexagonal systems, Acta Appl. Math. 72 (2002) 247–294.

[7] A.A. Dobrynin and L.S. Mel'nikov, Trees and their quadratic line graphs having the same Wiener index, MATCH Commun. Math. Comput. Chem. 50 (2004) 146-164.

[8] A.A. Dobrynin and L.S. Mel'nikov, Wiener index, line graphs and the cyclomatic number, MATCH Commun. Math. Comput. Chem. 53 (2005) 209-214.

[9] A.A. Dobrynin and L.S. Mel'nikov, Wiener index for graphs and their line graphs with arbitrary large cyclomatic numbers, Appl. Math. Lett. 18 (2005) 307–312.

[10] B. Furtula, I. Gutman, Ž. Tomović, A. Vesel, and I. Pesek, Wiener-type topological indices of phenylenes, Indian J. Chem. 41A (2002) 1767–1772.

[11] I. Gutman, A property of the Wiener number and its modifications, Indian J. Chem. 36A (1997) 128–132.

[12] I. Gutman, A.A. Dobrynin, S. Klavžar, and L. Pavlović, Wiener-type invariants of trees and their relation, Bull. Inst. Combin. Appl. 40 (2004) 23–30.

[13] I. Gutman, S. Klavžar, and B. Mohar (eds.), Fifty Years of the Wiener Index, MATCH Commun. Math. Comput. Chem. 35 (1997) 1–259.

[14] I. Gutman, S. Klavžar, and B. Mohar (eds.), Fiftieth Anniversary of the Wiener Index, Discrete Appl. Math. 80(1) (1997) 1–113.

[15] I. Gutman, D. Vidović, and L. Popović, On graph representation of organic molecules – Cayley's plerograms vs. his kenograms, J. Chem. Soc. Faraday Trans. 94 (1998) 857–860.

[16] W. Imrich and S. Klavžar, Product Graphs: Structure and Recognition (John Wiley & Sons, New York, 2000).

[17] S. Klavžar, Applications of isometric embeddings to chemical graphs, DIMACS Ser. Discrete Math. Theo. Comput. Sci. 51 (2000) 249–259.

[18] S. Klavžar and I. Gutman, Wiener number of vertex-weighted graphs and a chemical application, Discrete Appl. Math. 80 (1997) 73–81.

[19] S. Klavžar, I. Gutman, and B. Mohar, Labeling of benzenoid systems which reflects the vertex-distance relations, J. Chem. Inf. Comput. Sci. 35 (1995) 590–593.

[20] S. Klavžar and H.M. Mulder, Partial cubes and crossing graphs, SIAM J. Discrete Math. 15 (2002) 235–251.

[21] S. Klavžar, A. Vesel, P. Žigert, and I. Gutman, Binary coding of Kekulé structures of catacondensed benzenoid hydrocarbons, Comput. & Chem. 25 (2001) 569–575.

[22] D.J. Klein, I. Lukovits, and I. Gutman, On the definition of the hyper-Wiener index for cycle-containing structures. J. Chem. Inf. Comput. Sci. 35 (1995) 50–52.

[23] F.R. McMorris, H.M. Mulder, and F.R. Roberts, The median procedure on median graphs, Discrete Appl. Math. 84 (1998) 165–181.

[24] M. Randić, Novel molecular descriptor for structure-property studies, Chem. Phys. Lett. 211 (1993) 478–483.

[25] H. Wiener, Structural determination of paraffin boiling points, J. Amer. Chem. Soc. 69 (1947) 17–20.

[26] P. Winkler, Isometric embeddings in products of complete graphs, Discrete Appl. Math. 7 (1984) 221–225.

[27] H.Y. Zhu, D.J. Klein, and I. Lukovits, Extensions of the Wiener number, J. Chem. Inf. Comput. Sci. 36 (1996) 420–428.