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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 a previously known result for trees and implies several relations for distance-based topological indices.

Keywords: Graph distance; Hypercube; Partial cube; Wiener number; Hyper-Wiener index

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. Right up to today, it has been extensively investigated, above all in mathematical chemistry; see special issues of journals devoted to the topic [13,14], recent surveys [5,6], and recent papers [7–9].

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]:

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

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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 a *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 trees and median graphs. Partial cubes form a well studied class of graphs; we refer the reader to classical references [1,4,26], the book [16], the recent paper [20] and references therein. For applications of partial cubes to mathematical chemistry see [3,17–19,21].

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 $G \backslash F_i$ for $i = 1, \ldots, k$. On the other hand, u and v are in the same connected component of $G \backslash F_i$ for $i = k+1, \ldots, r$. Clearly, in the latter case, $d_{G\backslash F_i}(u, v) = k$. It follows that the pair $\{u, v\}$ contributes $(r-k)$ times to X. Thus,

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

If F is a Θ-class of the hypercube Q_n, then $Q_n \backslash F$ consists of two disjoint copies of Q_{n-1}. Thus, by Theorem 2, $W_{\lambda+1}(Q_n) = n W_{\lambda}(Q_n) - 2n W_{\lambda}(Q_{n-1})$. 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 $G \backslash F$ 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:

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

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 et al. [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 define $n_{11}(F, F') = |G_1(F) \cap G_1(F')|$, $n_{12}(F, F') = |G_1(F) \cap G_2(F')|$, $n_{21}(F, F') = |G_2(F) \cap G_1(F')|$, 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 $1 \le k, \ell \le 2$, 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].

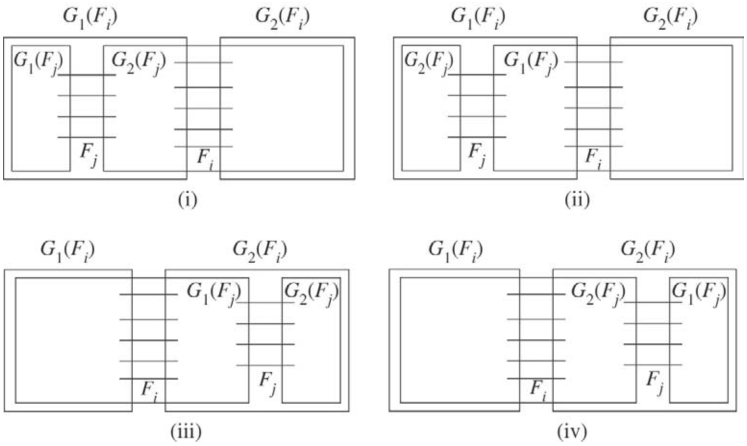

Fig. 1. Non-crossing classes F_i and F_j.

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

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

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

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

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

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

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

$$\begin{aligned}&[(n_{11}+n_{12})(n_{21}+n_{22}) + (n_{11}+n_{21})(n_{12}+n_{22})] - [(n_{11}n_{12}+n_{21}n_{22}) + (n_{11}n_{21}+n_{12}n_{22})]\\ &\quad = 2n_{11}n_{22} + 2n_{12}n_{21}.\end{aligned}$$

If F_i, F_j do not cross, then there are four possibilities for 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,

(i) $(n_{11}+n_{12})n_{22} + n_{11}(n_{12}+n_{22}) - (n_{11}n_{12}+n_{12}n_{22}) = 2n_{11}n_{22}$,

(ii) $(n_{11}+n_{12})n_{21}+n_{12}(n_{11}+n_{21})-(n_{12}n_{11}+n_{11}n_{21})=2n_{12}n_{21}$,
(iii) $(n_{21}+n_{22})n_{11}+n_{22}(n_{11}+n_{21})-(n_{21}n_{22}+n_{21}n_{11})=2n_{11}n_{22}$,
(iv) $(n_{21}+n_{22})n_{12}+n_{21}(n_{12}+n_{22})-(n_{21}n_{22}+n_{22}n_{21})=2n_{12}n_{21}$.

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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