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 $k$, $\lambda$ 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 $G$, $W_{\lambda+1}(G) = |F| W_{\lambda}(G) - \sum_{F \in \mathcal{F}} W_{\lambda}(G \setminus F)$, where $\mathcal{F}$ is the partition of $E(G)$ induced by the Djoković–Winkler relation $\Theta$. This result extends a previously known result for trees and implies several relations for distance-based topological indices.

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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. 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 $W(G) = \sum_{k \geq 1} d(G,k) k^\lambda$. 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 $\lambda$ is some real (or complex) number. Several particular instances of the invariant $W_\lambda$ have been previously studied. For instance, $W_{-2}$, $W_{-1}$, $\frac{1}{2} W_2 + \frac{1}{2} W_1$, and $\frac{1}{6} W_3 + \frac{1}{2} W_2 + \frac{1}{2} W_1$ 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 $W_\lambda$ were examined [10,11,15].

Let $T$ be a tree; then in [12] the following recursive formula for $W_\lambda$ has been obtained:

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

(1)

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

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

(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 $\Theta$ 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 $\Theta$ 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, $\Theta$ is transitive precisely for partial cubes; hence $\Theta$ partitions the edge set of a partial cube. Let $\bar{G}$ be a partial cube and $\mathcal{F} = \{F_1, F_2, \ldots, F_r\}$ the partition of its edge set induced by the relation $\Theta$. Then we say that $\mathcal{F}$ is the $\Theta$-partition of $G$.

For the proof of our main theorem we need the following facts about $\Theta$; 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 $\Theta$.

(ii) Let $F$ be a class of the $\Theta$-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 $\Theta$-partition. Then for any real (or complex) number $\lambda$,

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

**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 \( d(u, v) = k, 1 \leq k \leq s \). 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,

\[
X = \sum_{k=1}^{r} (r - k)d(G, k)k^\lambda \\
= r \sum_{k=1}^{s} d(G, k)k^\lambda - \sum_{k=1}^{s} d(G, k)k^{\lambda + 1} \\
= r W_\lambda(G) - W_{\lambda + 1}(G). \quad \square
\]

If \( F \) is a \( \Theta \)-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 \( \Theta \)-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 \( \Theta \)-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:

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

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 \( \Theta \)-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 \( n_{1\ell}(F, F') \neq 0 \) 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 $\Theta$-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, $W_2(G) = rW(G) - \sum_{i=1}^r W(G \setminus F_i)$. On the other hand, $WW(G) = W(G)/2 + W_2(G)/2$. Combining these two equalities we get

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

By Corollary 3 we have

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

while on the other hand

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

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

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

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

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

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) $(n_{11} + n_{12})n_{22} + n_{11}(n_{12} + n_{22}) - (n_{11}n_{12} + n_{12}n_{22}) = 2n_{11}n_{22}$,
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. \( \square \)

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