A relation between Wiener index and Mostar index for daisy cubes

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Abstract

Daisy cubes form a class of isometric subgraphs of the hypercubes $Q_n$. They include some previously well-known families of graphs like Fibonacci cubes and Lucas cubes. Daisy cubes also appear in chemical graph theory. Two distance invariants, Wiener and Mostar indices, have been introduced in the context of the mathematical chemistry. The Wiener index $W(G)$ is the sum of distance between all unordered pairs of vertices of a graph $G$. The Mostar index $Mo(G)$ is a measure of how far $G$ is from being distance balanced. In this paper, it is proved that the Wiener and Mostar indices of a daisy cube $G$ are linked by the relation $2W(G) - Mo(G) = |V(G)| \cdot |E(G)|$. An expression concerning the Wiener and Mostar indices for daisy cubes is also deduced.

Keywords: daisy cube; Wiener index; Mostar index; Fibonacci cube; partial cube.

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1. Introduction

The Fibonacci cube of dimension $n$, denoted as $\Gamma_n$, is the subgraph of the hypercube $Q_n$ induced by vertices with no consecutive 1’s. This graph was introduced in [6] as an interconnection network. Lucas cubes (see [17]) are the cyclic version of Fibonacci cubes. Structural properties of these graphs have been widely studied (see [10] for a survey). Fibonacci cubes also play a role in mathematical chemistry. Indeed they are precisely the resonance graphs of fibonacenes, an important class of hexagonal chains [15]. Later in [21], a similar connection have been found between Lucas cubes and the resonance graphs of cyclic polyphenanthrenes, which are related to non-cyclic fibonacenes. Fibonacci cubes and Lucas cubes belong to daisy cubes [13], a family of isometric subgraphs of hypercubes. The connection between daisy cubes and resonance graphs of catacondensed even ring systems have been explored in [2].

The Wiener index $W(G)$ of a connected graph $G$ is the sum of distance of all unordered pairs of vertices of $G$. This distance invariant is important in mathematical chemistry. The Wiener index of $\Gamma_n$ and $\Lambda_n$ have been determined in [12]. Recently the Mostar index $Mo(G)$ has been introduced in [3] again in the context of graph chemical theory. It measures how far $G$ is from being distance-balanced. The Mostar index of Fibonacci and Lucas cubes have been determined in [4]. See [1] for a recent survey on Mostar index. In this note we prove that if $G$ is a daisy cube, then the Wiener and the Mostar index are linked by the relation

$$2W(G) - Mo(G) = |V(G)| \cdot |E(G)|.$$ 

In the last section we derive similar expressions for $W(G)$ and $Mo(G)$ from the sequence of the number of edges using the direction $i$ for $i \in [n]$.

2. Preliminaries

In this section, some concepts and notations needed in the rest of this paper are given. We denote by $[n]$ the set of integers $i$ such that $1 \leq i \leq n$. Let $\{F_n\}$ be the Fibonacci numbers: $F_0 = 0$, $F_1 = 1$, $F_n = F_{n-1} + F_{n-2}$ for $n \geq 2$. Let $B = \{0, 1\}$. If will be convenient to identify elements $u = (u_1, \ldots, u_n) \in B^n$ and strings of length $n$ over $B$. We thus briefly write $u$ as $u_1 \ldots u_n$ and call $u_i$ the $i$th coordinate of $u$. We will use the power notation for the concatenation of bits, for instance $0^n = 0 \ldots 0 \in B^n$. We will denote by $\overline{u}$ the binary complement of $u_i$.

The vertex set of $Q_n$, the hypercube of dimension $n$, is the set $B^n$, two vertices being adjacent if and only if they differ in precisely one coordinate. We will say that an edge $uv$ of $Q_n$ uses the direction $i$ if $u$ and $v$ differ in the coordinate $i$.

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The distance between two vertices \( u \) and \( v \) of a graph \( G \) is the number of edges on a shortest shortest \( u, v \)-path. It is immediate that the distance between two vertices of \( Q_n \) is the number of coordinates the strings differ, sometimes called Hamming distance. The Wiener index \( W(G) \) of a connected graph \( G \) is defined as the sum of all distances between pairs of vertices of \( G \). Hence,

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

A Fibonacci string of length \( n \) is a binary string \( b = b_1b_2 \ldots b_n \) with \( b_i \cdot b_{i+1} = 0 \) for \( 1 \leq i < n \). In other words a Fibonacci string is a binary string without 11 as substring. The Fibonacci cube \( Q_n \) is the subgraph of \( Q_n \) induced by \( F_n \) the set of Fibonacci strings of length \( n \). Because of the empty string \( \epsilon \), \( \Gamma_0 = K_1 \). Not that for any integer \( n \), \( |V(\Gamma_n)| = F_{n+2} \). A Fibonacci string \( b \) of length \( n \) is a Lucas string if \( b_1 \cdot b_n \neq 1 \). That is, a Lucas string has no two consecutive 1s including the first and the last elements of the string. The Lucas cube \( \Lambda_n \) is the subgraph of \( Q_n \) induced by the Lucas strings of length \( n \). We have \( \Lambda_0 = \Lambda_1 = K_1 \).

Fibonacci cubes and Lucas cubes where extended to generalized Fibonacci cubes [8] and generalized Lucas cubes [7]. For any arbitrary string \( f \) the generalized Fibonacci cubes \( Q_n[f] \) is the subgraph of \( Q_n \) induced by strings of \( B^n \) which do not contain \( f \) as substring. Similarly the generalized Lucas cubes \( Q_n[f] \) is induced by strings without a circulation containing \( f \) as substring. Classical Fibonacci and Lucas cubes correspond to \( f = 11 \).

If \( u \) and \( v \) are vertices of a graph \( G \), the interval \( I_G(u,v) \) between \( u \) and \( v \) is the set of vertices lying on shortest \( u, v \)-path, that is, \( I_G(u,v) = \{w|d(u,w) = d(u,v) \} \). We will also write \( I(u,v) \) when \( G \) will be clear from the context. A subgraph \( H \) of a graph \( G \) is an isometric subgraph if the distance between any vertices of \( G \) equals the distance between the same vertices in \( H \). Isometric subgraphs of hypercubes are called partial cubes. The dimension of a partial cube \( G \) is the smallest integer \( d \) such that \( G \) is an isometric subgraph of \( Q_d \). Many important classes of graphs are partial cubes, in particular trees, median graphs, benzenoid graphs, phenylenes, grid graphs and bipartite torus graphs. In addition, Fibonacci and Lucas cubes are partial cubes as well, see [9].

If \( G = (V(G), E(G)) \) is a graph and \( X \subseteq V(G) \), then \( (X) \) denotes the subgraph of \( G \) induced by \( X \). Let \( X \subseteq B^n \) be a partial order on \( B^n \) defined with \( u_1 \ldots u_n \leq v_1 \ldots v_n \) if \( u_i \leq v_i \) holds for \( i \in [n] \). For \( X \subseteq B^n \) we define the graph \( Q_n(X) \) as the subgraph of \( Q_n \) with \( Q_n(X) = \langle \{u \in B^n|u \leq x \text{ for some } x \in X\} \rangle \) and say that \( Q_n(X) \) is the daisy cube generated by \( X \). Note that if \( \hat{X} \) is the antichain consisting of the maximal elements of the poset \( (X, \leq) \), then \( Q_n(\hat{X}) = Q_n(X) \). As noticed in the daisy cube introductory paper [13] we can alternatively say that

\[
Q_n(X) = \left\langle \bigcup_{x \in X} I_{Q_n}(x, 0^n) \right \rangle = \left\langle \bigcup_{x \in \hat{X}} I_{Q_n}(x, 0^n) \right \rangle.
\]

Finally we will say that a graph \( G \) is a daisy cube if there exist an isometric embedding of \( G \) in some hypercube \( Q_n \) and a subset \( X \) of \( B^n \) such that \( G \) is the daisy cube generated by \( X \). Such an embedding will be called a proper embedding.

By construction daisy cubes are partial cubes and as noticed in the same paper Fibonacci cubes, Lucas cubes, bipartite wheels, vertex-deleted cubes and hypercubes themselves are daisy cubes. It is easy to see that Pell graphs [16] are also daisy cubes. Furthermore A. Vesel proved [19] that the cube complement of a daisy cube is a daisy cube.

For any fixed integer \( s \geq 2 \) the generalized Fibonacci cubes \( Q_n[1^s] \) and Lucas cubes \( Q_n[\pi^s] \) are also daisy cubes. The Wiener index of these two families of graphs have been studied in [14]. A construction of daisy cubes in terms of expansion procedure is given in [18].

Let a partial cube \( G \) of dimension \( n \) be given together with its isometric embedding into \( Q_n \). Then for \( i = 1, 2, \ldots, n \) and \( \chi = 0,1 \) the semicube \( W_{i,\chi} \) is defined as follows:

\[
W_{i,\chi}(G) = \{u = u_1u_2 \ldots u_n \in V(G) \mid u_i = \chi \}.
\]

For a fixed \( i \), the pair \( W_{i,0}(G), W_{i,1}(G) \) of semicubes is called a complementary pair of semicubes. The Wiener index of partial cubes can be determined using the following result [11].

**Theorem 2.1.** Let \( G \) be a partial cube of dimension \( n \) isometrically embedded into \( Q_n \). Then

\[
W(G) = \sum_{i=1}^{n} |W_{i,0}(G)| \cdot |W_{i,1}(G)|.
\]

Notice that, as expected, this expression is independent of the embedding. Indeed isometric embeddings of \( G \) into \( Q_n \) are unique up to the automorphisms of \( Q_n \), see [20]. These automorphisms are generated by \( \Theta = \{\theta_{i,j}|i, j \in [n] \} \) and
An expression of the Mostar index for partial cubes is given in [5].

### 3. A relation

This section is devoted to the proof of the following theorem.

**Theorem 3.1.** Let $G$ be a daisy cube. Then the Wiener and the Mostar indices of $G$ are linked by the relation

$$2W(G) - Mo(G) = |V(G)| \cdot |E(G)|.$$

Like in [12] where it is applied in particular to Fibonacci cubes and Lucas cubes, Theorem 2.1 will be our starting point for proving the relation. Consider a proper embedding of $G$ in $Q_n$, and thus let $X \subseteq B^n$ such that

$$G = \{ (u, v) \in E G | x \leq x \text{ for some } x \in X \}.$$

For any $i \in [n]$ let $E_i$ be the set of edges of $G$ using the direction $i$.

**Proposition 3.1.** For any $i \in [n]$ we have

$$|W(i,0)(G)| \geq |W(i,1)(G)|.$$

**Proof.** Let $u = u_1u_2\ldots u_n$ in $W(i,1)(G)$ and consider $\theta(u) = u_1 \ldots u_{i-1}0u_{i+1} \ldots u_n$. Note that $\theta(u) \leq u$ and since $u$ is a vertex of $G$ there exists $x \in X$ with $u \leq x$. Therefore $\theta(u) \leq x$ and $\theta(u) \in V(G)$. By this way we construct an injective mapping from $W(i,1)(G)$ to $W(i,0)(G)$.

**Proposition 3.2.** For any $i \in [n]$ we have

$$|E_i| = |W(i,1)(G)|.$$

**Proof.** Indeed let $u = u_1u_2\ldots u_n$ in $W(i,1)(G)$ and let $v = u_1 \ldots u_{i-1}0u_{i+1} \ldots u_n$. Using the same argument as in the previous proof, it is clear that $v$ is a vertex of $G$ and that the edge $uv$ belongs to $E_i$. Reciprocally exactly one of the extremities of a given edge of $E_i$ belongs to $W(i,1)(G)$. We obtain a bijective mapping between $W(i,1)(G)$ and $E_i$.

**Proposition 3.3.** For any edge $uv$ of $E_i$, with $u_i = 0$ we have

$$W(i,0)(G) = \{ w \in V(G) | d(w, u) < d(w, v) \},$$

$$W(i,1)(G) = \{ w \in V(G) | d(w, v) < d(w, u) \}.$$

**Proof.** Since $d(w, u)$ and $d(w, v)$ are the number of coordinates the strings differ and since $u, v$ differ only by the coordinate $i$ it is clear that $d(w, u) = d(w, v) + 1$ if $w \in W(i,1)(G)$ and $d(w, u) = d(w, v) - 1$ otherwise.

**Lemma 3.1.** Let $G$ be a daisy cube of dimension $n$ properly embedded into $Q_n$. Then

$$Mo(G) = \sum_{i=1}^n |W(i,1)(G)|(|W(i,0)(G)| - |W(i,1)(G)|).$$

**Proof.** Let $e = uv$ be an edge of $E_i$ with $u_i = 0$. By Propositions 3.3 and 3.1 we have $n_{u,v} = |W(i,0)(G)| \geq |W(i,1)(G)| = n_{v,u}$. The contribution of the edge $e$ to $\sum_{uv \in E(G)} |n_{u,v} - n_{v,u}|$ is thus $|W(i,0)(G)| - |W(i,1)(G)|$. Therefore

$$Mo(G) = \sum_{i=1}^n \sum_{uv \in E_i} (|W(i,0)(G)| - |W(i,1)(G)|) = \sum_{i=1}^n |E_i||W(i,0)(G)| - |W(i,1)(G)|).$$

The conclusion follows from Proposition 3.2.
We can now proceed to the proof of our relation given in Theorem 3.1. By Theorem 2.1 we obtain
\[ W(G) = \sum_{i=1}^{n} |W(i,0)(G)| \cdot |W(i,1)(G)|. \]
Since \(|W(i,0)(G)| + |W(i,1)(G)| = |V(G)|\) we deduce from Lemma 3.1 that
\[ 2W(G) - Mo(G) = \sum_{i=1}^{n} |W(i,1)(G)| \cdot (2|W(i,0)(G)| - |W(i,0)(G)| + |W(i,1)(G)|) \]
\[ = \sum_{i=1}^{n} |W(i,1)(G)| \cdot |V(G)|. \]
Since \(E(G)\) is the disjoint union \(E(G) = \bigcup_{i=1}^{n} E_i\) we deduce from Proposition 3.2 that \(\sum_{i=1}^{n} |W(i,1)(G)| = |E(G)|\) and the relation follows.

4. Conclusion

The Wiener and Mostar indices of daisy cubes are completely determined by \(|V(G)|\) and the sequence \(|E_i|\) (for \(i \in [n]\)) of the number of edges using the direction \(i\) which is identical to the sequence of \(|W(i,1)(G)|\). Indeed, from Theorem 2.1 and Lemma 3.1 we have the relation
\[ W(G) - Mo(G) = \sum_{i=1}^{n} |W(i,1)(G)|^2. \]
Combining this identity with that of Theorem 3.1 we obtain the following assertion.

**Corollary 4.1.** Let \(G\) be a daisy cube properly embedded into \(Q_n\). For \(i \in [n]\) let \(E_i\) be the set of edges using the direction \(i\). Then the Wiener and the Mostar indices of \(G\) are
\[ W(G) = |V(G)| \cdot |E(G)| - \sum_{i=1}^{n} |E_i|^2, \]
\[ Mo(G) = |V(G)| \cdot |E(G)| - 2 \sum_{i=1}^{n} |E_i|^2. \]

In conclusion of this paper note that it will be interesting to give bijective proofs of Theorem 3.1 and Corollary 4.1.

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