On the Wiener index of generalized Fibonacci cubes and Lucas cubes

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Abstract

The generalized Fibonacci cube $Q_d(f)$ is the graph obtained from the *d*-cube Q_d by removing all vertices that contain a given binary word f as a factor; the generalized Lucas cube $Q_d(\overline{f})$ is obtained from Q_d by removing all the vertices that have a circulation containing f as a factor. In this paper the Wiener index of $Q_d(1^s)$ and the Wiener index of $Q_d(\overline{1^s})$ are expressed as functions of the order of the generalized Fibonacci cubes. For the case $Q_d(111)$ a closed expression is given in terms of Tribonacci numbers. On the negative side, it is proved that if for some d, the graph $Q_d(f)$ (or $Q_d(\overline{f})$) is not isometric in Q_d , then for any positive integer k, for almost all dimensions d' the distance in $Q_{d'}(f)$ (resp. $Q_{d'}(\overline{f})$) can exceed the Hamming distance by k.

Key words: hypercube; generalized Fibonacci cube; generalized Lucas cube; isometric embedding, Wiener index.

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1 Introduction

The Wiener index of a graph is one of the most studied graph invariants, the main reason for this fact is its vast applicability in theoretical chemistry, cf. the comprehensive surveys [2, 3] on the Wiener index of rather specific classes of graphs—trees and hexagonal systems. But this index is also extensively investigated elsewhere, [12, 17, 21, 23] is just a selection of recent papers that indicates a wide variety of topics studied with respect to the Wiener index. Moreover, it is an intrinsic indicator of a potential applicability of (interconnection) networks. In this respect the average distance [1] is more relevant, however the studies of the Wiener index and the average distance are equivalent because for a given graph G, these invariants differ only by the factor $\binom{|V(G)|}{2}$.

In [15] it was demonstrated that each of the Wiener index of Fibonacci cubes and Lucas cubes can be expressed in a closed form. The first of these classes of graphs was introduced as a model for interconnection network [7] and received a lot of attention afterwards, see the survey [11]. Lucas cubes [19] can be considered as a symmetrization of Fibonacci cubes and have found their role in theoretical chemistry [24].

Fibonacci cubes and Lucas cubes were extended to generalized Fibonacci cubes [9] and to generalized Lucas cubes [10], respectively. (We note that the term "generalized Fibonacci cubes" was used in [8] (see also [18, 22]) for a restricted family of the graphs from [9].) The main goal of this paper is to extend the results from [15] on the Wiener index of Fibonacci (Lucas) cubes to those for generalized Fibonacci (Lucas) cubes that admit isometric embeddings into hypercubes. Such potential classes were identified in [9, 10].

We proceed as follows. In the rest of this section we formally introduce the concepts needed in this paper. In the following section the Wiener index of $Q_d(1^s)$ (Theorem 2.3) and the Wiener index of $Q_d(\overline{1^s})$ (Theorem 2.5) are expressed as sums involving $|V(Q_{d'}(1^s))|$ for some d'. In the case of $Q_d(111)$ it is shown how a closed expression for its Wiener index can be obtained. In the final section we show that if $Q_d(f)$ or $Q_d(\overline{f})$ is not isometric in Q_d , then in almost all dimensions the distance function is arbitrarily larger than the corresponding Hamming distance.

Graph considered here are finite, simple, and connected. For a (connected) graph G, the distance $d_G(u, v)$ (or d(u, v) if G is clear from the context) between vertices u and v is the usual shortest path distance. A subgraph H of a graph G is *isometric* if $d_H(u, v) = d_G(u, v)$ holds for all $u, v \in V(H)$. The Wiener index, W(G), of a graph G is defined as $\sum d(u, v)$, where the summation runs over all unordered pairs $\{u, v\}$ of vertices of G.

Let $B = \{0, 1\}$ and call the elements of B bits. An element of B^d is called a *(binary)* word of length d. We will use the product notation for words meaning concatenation. For example, $1^{s}0^{t}$ is the word of length s + t whose first s bits are 1 and last t bits are 0. A word f is a factor of a word u if u = vfw for some words v and w.

The *d*-cube Q_d is the graph whose vertices are all the binary words of length *d*, two vertices are adjacent if they differ in exactly one bit. The Hamming distance H(u, v)between binary words *u* and *v* (of equal length) is the number of bits in which they differ. It is well-known that $d_{Q_d}(u, v) = H(u, v)$ holds for any $u, v \in V(Q_d)$. If *f* is an arbitrary binary word and *d* is a positive integer, then the generalized Fibonacci cube $Q_d(f)$ is the graph obtained from Q_d by removing all the vertices that contain *f* as a factor. Similarly, the generalized Lucas cube $Q_d(f)$ is the graph obtained from Q_d by removing all the vertices that have a circulation containing *f* as a factor. The Fibonacci cube Γ_d is the graph $Q_d(11)$ and the Lucas cube Λ_d is $Q_d(\overline{11})$.

If $b = b_1 \dots b_d$ is a binary word, then let \overline{b} denote its binary complement and let $b^R = b_d \dots b_1$ be the reverse of b. It is easy to see (cf. [9, 10]) that if f is an arbitrary binary word, then $Q_d(f) \cong Q_d(\overline{f}) \cong Q_d(f^R)$ and $Q_d(\overline{f}) \cong Q_d(\overline{f}) \cong Q_d(\overline{f^R})$, where \cong stands for graph isomorphism. We will implicitly use these facts when considering all possible words.

2 The Wiener index of $Q_d(1^s)$ and $Q_d(\overline{1^s})$

In this section we extend results from [15] on the Wiener index of $Q_d(11)$ and $Q_d(\overline{11})$ to $Q_d(1^s)$ and $Q_d(\overline{1^s})$, respectively. For this sake we will apply the following result from [14] (see also [13] for its wide generalization). If G is a subgraph of Q_d , then set $W_{(i,\chi)}(G) = \{u = u_1 \dots u_d \in V(G) \mid u_i = \chi\}$ for $1 \le i \le d, 0 \le \chi \le 1$.

Theorem 2.1 [14] If G is an isometric subgraphs of Q_d , then

$$W(G) = \sum_{i=1}^{d} |W_{(i,0)}(G)| \cdot |W_{(i,1)}(G)|$$

If $d \ge 1$ and $s \ge 2$, then let $x_d^{(s)} = |V(Q_d(1^s))|$. For any $s \ge 2$ we also set $x_0^{(s)} = 1$ and $x_{-1}^{(s)} = 1$.

Lemma 2.2 Let $d \ge 1$ and $s \ge 2$. Then $x_d^{(s)} = 2^d$ for $1 \le d \le s - 1$, $x_s^{(s)} = 2^s - 1$, and $x_d^{(s)} = x_{d-1}^{(s)} + x_{d-2}^{(s)} + \dots + x_{d-s}^{(s)}$ for $d \ge s + 1$.

Proof. If $d \leq s - 1$, then $Q_d(1^s) = Q_d$, hence the first assertion follows. $Q_d(1^s)$ is obtained from Q_d by deleting the vertex 1^s , therefore $x_s^{(s)} = 2^s - 1$. Let now $d \geq s + 1$. Then there are $x_{d-1}^{(s)}$ vertices u of $Q_d(1^s)$ with $u_1 = 0$. The other vertices can be partitioned into those starting with 10 and with 11, respectively. The number of the former ones is $x_{d-2}^{(s)}$, while the other vertices can be partitioned into those starting with 10 and with 11, respectively. The number of the 110 and with 111, respectively. Continuing in this manner, and having in mind that 1^s is not a factor of a vertex of $Q_d(1^s)$, the last assertion follows.

Theorem 2.3 For any $d \ge 1$ and any $s \ge 2$,

$$W(Q_d(1^s)) = \sum_{i=1}^d \left(x_{i-1}^{(s)} x_{d-i}^{(s)} \left(\sum_{j=2}^s x_{i-j}^{(s)} \left(\sum_{k=(d-i-1)-(s-j)}^{d-i-1} x_k^{(s)} \right) \right) \right).$$

Proof. From [9, Proposition 3.1] we know that $Q_d(1^s)$ is an isometric subgraph of Q_d , hence Theorem 2.1 applies to $Q_d(1^s)$.

We first observe that $|W_{(i,0)}(Q_d(1^s))| = x_{i-1}^{(s)} x_{d-i}^{(s)}$ because the factors before and after the *i*-th bit are arbitrary. This assertion also holds for i = 1 and for i = d since we have set $x_0^{(s)} = 1$. Consider now the set of vertices $W_{(i,1)}(Q_d(1^s))$ and let *u* be an arbitrary vertex with $u_i = 1$. Suppose that u_i is preceded with *r* ones, where $0 \le r \le s-2$, so that $u_{i-r-1} = 0$. Then the first i - r - 2 bits are arbitrary, that is, there are $x_{i-r-2}^{(s)}$ such factors for $0 \le r \le s-2$. For a fixed *r*, there can be *t* ones succeeding u_i , where $0 \le t \le s - r - 2$. Then the following bit to the right is 0, while the last d - i - t - 1 bits are arbitrary. Putting these observations together and checking the initial conditions, the result follows. If s = 2, then Theorem 2.3 reduces to

$$W(Q_d(11)) = \sum_{i=1}^{d} x_{i-1}^{(s)} x_{d-i}^{(s)} x_{i-2}^{(s)} x_{d-i-1}^{(s)}$$

which is [15, Theorem 3.1] after observing that $x_i^{(2)} = F_{i+2}$, where F_n are the Fibonacci numbers.

We next have a closer look at the case where s = 3. In the following, let us simplify the notation $x_i^{(3)}$ to x_i . Theorem 2.3 gives us

$$W(Q_d(111)) = \sum_{i=1}^d \left(x_{i-1} \, x_{d-i} \left(x_{i-2} \, x_{d-i-1} + x_{i-2} \, x_{d-i-2} + x_{i-3} \, x_{d-i-1} \right) \right) \,.$$

This expression can be rewritten as

$$W(Q_d(111)) = \sum_{i=1}^d x_{i-2} x_{i-1} x_{d-i-1} x_{d-i}$$

+
$$\sum_{i=1}^d x_{i-2} x_{i-1} x_{d-i-2} x_{d-i}$$

+
$$\sum_{i=1}^d x_{i-3} x_{i-1} x_{d-i-1} x_{d-i}.$$

To obtain a closed expression for each of the above three sums, we invoke the fascinating theory developed by Greene and Wilf in [4]. They have proved that if each of the sequences $\{G_i(d)\}$ satisfies a linear recurrence, then

$$\sum_{j=0}^{d-1} G_1(a_1d + b_1j + c_1)G_2(a_2d + b_2j + c_2)\cdots G_k(a_kd + b_kj + c_k)$$

can be expresses in a closed form. Using the Mathematica package CFSum.nb [5] we have obtained:

$$W(Q_d(111)) = \frac{1}{484} \left((268 + 67d) x_d^2 - (118 + 4d) x_d x_{d+1} - (50 - 14d) x_d x_{d+2} - (66 + 7d) x_{d+1}^2 + (90 + 16d) x_{d+1} x_{d+2} - (18 + 6d) x_{d+2}^2 \right).$$

Denoting with T_n the Tribonacci numbers [20, Sequence A000073] and noting that $x_d = T_{d+3}$, we have arrived at:

Theorem 2.4 For any $d \ge 0$,

$$W(Q_d(111)) = \frac{1}{484} \left((268 + 67d) T_{d+3}^2 - (118 + 4d) T_{d+3} T_{d+4} - (50 - 14d) T_{d+3} T_{d+5} - (66 + 7d) T_{d+4}^2 + (90 + 16d) T_{d+4} T_{d+5} - (18 + 6d) T_{d+5}^2 \right).$$

The first values of the sequence $\{W(Q_d(111))\}_{d\geq 0}$ are 0, 1, 8, 36, 164, 694, 2792, 11008, 42484, 161395.

Parallel to the above, it is possible to make a derivation of a closed expression for $W(Q_d(1^s))$ for any $s \ge 4$. However, the results are too long to be written down.

We now turn to the generalized Lucas cubes $Q_d(\overline{1^s})$ for which the derivation is simpler than the above derivation for $Q_d(1^s)$. Recalling that $x_{-1}^{(s)} = x_0^{(s)} = 1$, $s \ge 2$, and $x_d^{(s)} = |V(Q_d(1^s))|, d \ge 1, s \ge 2$, we have:

Theorem 2.5 For any $d \ge 1$ and any $s \ge 2$,

$$W(Q_d(\overline{1^s})) = \begin{cases} d2^{2d-2}; & d < s, \\ dx_{d-1}^{(s)} \sum_{j=1}^{s-1} j x_{d-j-2}^{(s)}; & d \ge s. \end{cases}$$

Proof. If d < s then $Q_d(\overline{1^s})$ is isomorphic to Q_d and it is well-known that $W(Q_d) = d2^{2d-2}$, see [6, Exercise 19.3].

Invoking [10, Proposition 2] which asserts that $Q_d(\overline{1^s})$ is isometric in Q_d , we can again make use of Theorem 2.1. To simplify the notation set $G_d^s = Q_d(\overline{1^s})$. If d = s, then $x_s^{(s)} = 2^s - 1$, $|W_{(1,0)}(G_s^s)| = 2^{s-1}$, and $|W_{(1,1)}(G_s^s)| = 2^{s-1} - 1$, hence the theorem holds in this case.

Assume $d \ge s + 1$. For a fixed $\chi \in B$, the number of vertices in $W_{(i,\chi)}(G_d^s)$ is independent of the selection of *i*. Therefore, $W(Q_d(G_d^s)) = d \cdot |W_{(1,0)}(G_d^s)| \cdot |W_{(1,1)}(G_d^s)|$. Clearly, $|W_{(1,0)}(G_d^s)| = x_{d-1}^{(s)}$. Consider next the set $W_{(1,1)}(G_d^s)$ and suppose that a word *u* from it starts with $1^r 0$, where $1 \le r \le s - 1$. Then *u* ends with 01^p , where $r + p \le s - 1$, that is, $0 \le p \le s - r - 1$. Hence, for a fixed *r*, there are $x_{d-r-2}^{(s)} + x_{d-r-3}^{(s)} + \cdots + x_{d-s-1}^{(s)}$ such words. Summing over all *r* we get that

$$|W_{(1,1)}(G_d^s)| = x_{d-3}^{(s)} + 2x_{d-4}^{(s)} + 3x_{d-5}^{(s)} + \dots + (s-1)x_{d-s-1}^{(s)},$$

hence the result.

If s = 2, then Theorem 2.5 reduces to $W(Q_d(\overline{11})) = dx_{d-1}^{(2)}x_{d-3}^{(2)}$. Recalling that $x_i^{(2)} = F_{i+2}$, where F_n are the Fibonacci numbers, we get $W(Q_d(\overline{11})) = dF_{d+1}F_{d-1}$, which is [15, Theorem 3.4].

In Theorem 2.5, the values for $W(Q_d(\overline{1^s}))$ in the two cases appear much different. The following result shows that this is actually not the case because $d2^{2d-2}$ can be expressed as a sum of the values $x_i^{(s)}$ as follows:

Proposition 2.6 If $d \ge 1$, $s \ge 2$, and d < s, then

$$d2^{2d-2} = d x_{d-1}^{(s)} \left(\sum_{j=1}^{s-1} j x_{d-j-2}^{(s)} + 1 \right).$$

Proof. We know that $x_{d-1}^{(s)} = 2^{d-1}$ as $x_k^{(s)} = 2^k$ for all k < s. Considering that $x_k^{(s)} = 0$ for k < -1 and $x_{-1}^{(s)} = 1$, we get

$$\sum_{j=1}^{s-1} j x_{d-j-2}^{(s)} + 1 = \sum_{j=1}^{d-1} j x_{d-j-2}^{(s)} + 1 = \sum_{j=1}^{d-2} j x_{d-j-2}^{(s)} + (d-1)x_{-1}^{(s)} + 1$$
$$= \sum_{j=1}^{d-2} j x_{d-j-2}^{(s)} + d.$$

Set $A = \sum_{j=1}^{d-2} j x_{d-j-2}^{(s)}$. Then as $x_k^{(s)} = 2^k$ for all k < s,

$$A = \sum_{j=1}^{d-2} j \, 2^{d-j-2}.$$

Hence

$$2A = \sum_{j=1}^{d-2} j \, 2^{d-j-1} = \sum_{j=0}^{d-3} (j+1) \, 2^{d-j-2}$$

and therefore

$$2A - A = \sum_{j=0}^{d-3} 2^{d-j-2} - (d-2) = 2(2^{d-2} - 1) - (d-2) = 2^{d-1} - d.$$

Thus

$$\sum_{j=1}^{s-1} j x_{d-j-2}^{(s)} + 1 = A + d = 2^{d-1}$$

and the result is proved.

3 On distances in non-isometric families

We say that a binary word f is good if $Q_d(f)$ is an isometric subgraph in Q_d for all d. The word f is bad if it is not good. These concepts were introduced in [16], where it was proved that if \mathcal{G}_n is the set of words f of length n that are good, then $\lim_{n\to\infty} |\mathcal{G}_n|/2^n$ exists and that it is close to 0.08. In other words, about eight percent of all binary words are good.

Completely analogously we now also introduce good and bad words with respect to the generalized Lucas cubes. In the following two results it will be clear from the context whether we are talking about bad words w.r.t. generalized Fibonacci cubes or generalized Lucas cubes, hence in both cases we will simply speak about bad words.

Theorem 3.1 Let f be a bad word. Then for any positive integer k there exist a positive integer d and words $x, y \in Q_d(f)$ such that $d_{Q_\delta(f)}(x, y) > H(x, y) + k$ holds for any $\delta \ge d$.

Proof. Note first that $Q_d(1) = K_1$, $Q_d(11) = \Gamma_d$, and $Q_d(10) = P_{d+1}$. If follows that all words f of length at most two are good. Hence by the theorem's assumption, $|f| \ge 3$. Since f is bad, there exist a dimension d' and words $u, v \in Q_{d'}(f)$ such that $d_{Q_{d'}(f)}(u,v) \ge H(u,v)+1$. (Actually $d_{Q_{d'}(f)}(u,v)$ is at least H(u,v)+2, but H(u,v)+1suffices and makes the presentation simpler.) Let z be a fixed word (to be explicitly defined in each of the cases considered below) and set $x = u(zu)^k$ and $y = v(zv)^k$. Hence x and y are words of length d = k|z| + (k+1)d'. The word z is defined as follows.

Case 1. If $f = 1^{s}0^{t}$, $s, t \ge 1$, $s + t \ge 3$, then let $z = 1^{s+1}010^{t+1}$. **Case 2.** If $f \ne 1^{s}0^{t}$, $f = 1 \dots 0$, then let $z = 1^{|f|+1}0^{|f|+1}$. **Case 3.** If $f \ne 1^{s}0^{t}$, $f = 0 \dots 1$, then let $z = 0^{|f|+1}1^{|f|+1}$. **Case 4.** If $f \ne 1^{s}0^{t}$, $f = 1 \dots 1$, then let $z = 0^{|f|+1}$. **Case 5.** If $f \ne 1^{s}0^{t}$, $f = 0 \dots 0$, then let $z = 1^{|f|+1}$.

We claim that in each of the cases $x, y \in V(Q_d(f))$.

Consider Case 1. By [9, Theorem 3.3], the word $1^{s}0$ is good for any $s \ge 1$, hence so is 10^{s} . Thus we can assume $s, t \ge 2$. Suppose on the contrary that f is a factor of x or y, say of x. Since $u \in V(Q_{d'}(f))$ and since f is not a factor of z, f must be a factor of uz or a factor of zu. In the first case f must actually be a factor of u because f ends with the bit 0. Similarly, in the second case f must also be a factor of u because fstarts with the bit 1. Since this is not possible, the claim is proved in Case 1.

For Case 2 note that since f starts with 1, ends with 0, and is not of the form $1^{s}0^{t}$, it must necessarily contain 01 as a factor. Therefore, if f is a factor of x, then the first bit of f cannot be in any factor of z. It follows that then the first bit of f must start in some u and, as f is not a factor of u, it must end in z. But this is not possible since f ends with 0 and z starts with $1^{|f|+1}$.

Arguments in the remaining three cases are similar to the ones just given for Case 2 and are left to the reader. This proves the claim.

Hence in any case we have $x, y \in V(Q_d(f))$. Therefore, since x and y contain k + 1 copies of u and v respectively, and since to get from one factor u in x to the corresponding factor v in y at least H(u, v) + 1 changes of bits are required, we get

$$d_{Q_d(f)}(x,y) \ge (k+1)d_{Q_{d'}(f)}(u,v) \ge (k+1)(H(u,v)+1) \ge H(x,y) + k + 1.$$

Let now $\delta > d$. If the first bit of f is 1, set $x' = 0^{\delta - d}x$ and $y' = 0^{\delta - d}y$, otherwise (that is, if the first bit of f is 0), set $x' = 1^{\delta - d}x$ and $y' = 1^{\delta - d}y$. Then $x', y' \in V(Q_{\delta}(f))$ and we have $d_{Q_{\delta}(f)}(x', y') \ge H(x', y') + k + 1$.

Theorem 3.2 Let f be a bad word. Then for any positive integer k there exist a positive integer d and words $x, y \in Q_d(\overline{f})$ such that $d_{Q_{\delta}(\overline{f})}(x, y) > H(x, y) + k$ holds for any $\delta \geq d$.

Proof. Words 1^s are good by [10, Proposition 2]. Note also that $Q_d(\overline{1^{s}0})$ contains an isolated vertex 1^d (cf. [10, Proposition 10]). Hence 1^s_0 are bad words and the assertion

of the theorem clearly holds (provided the distance function is naturally extended with $d_G(x, y) = \infty$ for vertices x and y from different components of G). Hence we can assume in the rest that $|f| \ge 3$. This part of the proof is parallel to the proof of Theorem 3.1, hence we just give a sketch of it.

Since f is bad, there exists a dimension d' and words $u, v \in Q_{d'}(\overline{f})$ such that $d_{Q_{d'}(\overline{f})}(u,v) \ge H(u,v) + 1$. Let z be defined as in Theorem 3.1 and set $x = (zu)^{k+1}$ and $y = (zv)^{k+1}$. Hence x and y are words of length d = (k+1)(|z|+d').

Using [10, Proposition 10]) again, in Case 1 (it refers to the first case from the proof of Theorem 3.1) we can assume $s, t \ge 2$. As proved in Theorem 3.1, x and y are in $Q_d(f)$ and we get

$$d_{Q_d(f)}(x,y) \ge (k+1)d_{Q_{d'}(f)}(u,v) \ge (k+1)(H(u,v)+1) \ge H(x,y) + (k+1).$$

Let now $\delta > d$. If the last bit of f is 1, set $x' = 0^{\delta-d}x$ and $y' = 0^{\delta-d}y$, otherwise, set $x' = 1^{\delta-d}x$ and $y' = 1^{\delta-d}y$. Then $x', y' \in V(Q_{\delta}(f))$ and we have $d_{Q_{\delta}(f)}(x', y') \ge H(x', y') + k + 1$.

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