

Graphs with four boundary vertices

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Abstract

A vertex v of a graph G is a *boundary vertex* if there exists a vertex u such that the distance in G from u to v is at least the distance from u to any neighbour of v . We give a full description of all graphs that have exactly four boundary vertices, which answers a question of Hasegawa and Saito. To this end, we introduce the concept of frame of a graph. It allows us to construct, for every positive integer b and every possible “distance-vector” between b points, a graph G with exactly b boundary vertices such that every graph with b boundary vertices and the same distance-vector between them is an induced subgraph of G .

1 Introduction

Let $G = (V, E)$ be a graph. A vertex $v \in V$ is a *boundary vertex* of G if there exists a vertex $u \in V$ such that $d(u, v) \geq d(u, w)$ for all neighbours w of v . Such a vertex u is then called a *witness* for v . The *boundary* of G is the set $\mathcal{B}(G)$ of boundary vertices of G .

The notion of boundary of a graph was introduced by Chartrand et al. [2, 3] and studied further by Cáceres *et al.* [1], Hernando *et al.* [5], and Hasegawa and Saito [4]. In a short note [6], we gave a tight bound (up to a constant factor) of the order of the boundary of a graph in function of its maximum (or minimum) degree, thereby settling a problem suggested by Hasegawa and Saito [4].

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Note that all vertices are boundary vertices in a disconnected graph. Hence we shall restrict attention to connected graphs in the rest of the paper. Any graph with more than one vertex has at least two boundary vertices, namely the endvertices of a longest path. As noted by Hasegawa and Saito [4], a connected graph has exactly two boundary vertices if and only if it is a path. In addition, they described all connected graphs with exactly three boundary vertices.

Theorem 1 (Hasegawa and Saito [4]). *A connected graph G has exactly three boundary vertices if and only if either*

- (i) *G is a subdivision of $K_{1,3}$; or*
- (ii) *G can be obtained from K_3 by attaching paths (possibly of length zero) to its vertices.*

Hasegawa and Saito [4] asked for a characterisation of all graphs with four boundary vertices. The aim of the current paper is to provide such a characterisation. The statement of our main result requires a number of definitions and we therefore postpone it until the next section.

An important tool in our proof is the concept of *frame* of a graph, which is of independent interest. The frame is the vector of all distances between the boundary vertices. In Section 3 we study frames in general. In particular, for every positive integer b and every possible “distance-vector” between b points, we explicitly construct a graph F with exactly b boundary vertices such that every graph with b boundary vertices and the same distance-vector between them is an induced subgraph of F .

Let us note that Hasegawa and Saito [4] proved that any connected graph with exactly four boundary vertices has minimum degree at most 6. Our description shows that the minimum degree is in fact never more than 3.

2 Statement of the main result

Before giving the description of all connected graphs with four boundary vertices, we need to introduce several definitions. The reader may find the next batch of definitions easier to digest by looking at figure 1 below.

Definition 2. Let a and c be two positive integers.

- The $(a \times c)$ -grid is the graph $G_{a \times c}$ with vertex set

$$V_{a \times c}^0 := \{(x, y) \in \mathbf{N}^2 : 0 \leq x \leq a \text{ and } 0 \leq y \leq c\}$$

and an edge between vertices of Euclidean distance 1.

- The graph $N_{a \times c}$ has vertex set $V_{a \times c} := V_{a \times c}^0 \cup V_{a \times c}^1$, where

$$V_{a \times c}^1 := \left\{ \left(x + \frac{1}{2}, y + \frac{1}{2} \right) : (x, y) \in \mathbf{N}^2, \quad 0 \leq x < a \text{ and } 0 \leq y < c \right\}.$$

There is an edge between two vertices if the Euclidean distance is at most 1.

- If $a > 2$ then $X_{a \times c}$ is the subgraph of $N_{(a-1) \times c}$ induced by

$$V_{(a-1) \times c} \setminus \{(x, y) \in \mathbf{N}^2 : 0 < x < a - 1 \text{ and } y \in \{0, c\}\}.$$

If $a = 2$ the $X_{2,c}$ is the subgraph of $N_{1 \times c}$ obtained by removing the edge between the vertices $(0, 0)$ and $(1, 0)$, and the edge between the vertices $(0, c)$ and $(1, c)$. (Note that $X_{a \times c}$ is isomorphic to $X_{c \times a}$ if both a and c are greater than 1.) If $a = 1$ and $c > 1$ then we take the same construction with a and c swapped, i.e. $X_{a,c} := X_{c,a}$. Moreover, we let $X_{1 \times 1}$ be K_4 , the complete graph on four vertices.

- The subgraph of $N_{a \times (c+1)}$ induced by

$$V_{a \times (c+1)} \setminus (\{(x, y) \in \mathbf{N}^2 : x = 0\} \cup \{(x, y) : x < a \text{ and } y \in \{0, c + 1\}\})$$

is $T_{a \times c}$.

- Let $G_{a \times c}^1$ and $G_{a \times c}^2$ be two copies of the $(a \times c)$ -grid with vertex sets $V_1 = \{v_{x,y} : 0 \leq x \leq a, 0 \leq y \leq c\}$ and $V_2 := \{w_{x,y} : 0 \leq x \leq a, 0 \leq y \leq c\}$, respectively. The graph $D_{a \times c}$ is obtained from $G_{a \times c}^1$ and $G_{a \times c}^2$ by identifying $v_{x,y}$ with $w_{x,y}$ for all x and y such that $x \in \{0, a\}$ or $y \in \{0, c\}$; and adding an edge between $v_{x,y}$ and $w_{x,y}$ whenever $0 < x < a$ and $0 < y < c$, and an edge between $w_{x,y+1}$ and $v_{x+1,y}$ whenever $0 \leq x < a$ and $0 \leq y < c$.
- The graph $L_{a \times c}$ is obtained from $D_{a \times c}$ by removing the vertices $w_{x,y}$ for $x \in \{1, 2, \dots, a - 1\}$ and $y \in \{1, 2, \dots, c - 1\}$.

It is straightforward to check that each of the graphs $N_{a \times c}$, $X_{a \times c}$, $T_{a \times c}$, $D_{a \times c}$ and $L_{a \times c}$ has exactly four boundary vertices.

Definition 3. A set $W \subseteq \mathbf{R}^2$ is *axis slice convex* if

- whenever both (x_1, y) and (x_2, y) belong to W and $x_1 < x_2$, then $(x, y) \in W$ for all $x \in \{x_1, x_1 + 1, \dots, x_2\}$; and
- whenever both (x, y_1) and (x, y_2) belong to W and $y_1 < y_2$, then $(x, y) \in W$ for all $y \in \{y_1, y_1 + 1, \dots, y_2\}$.

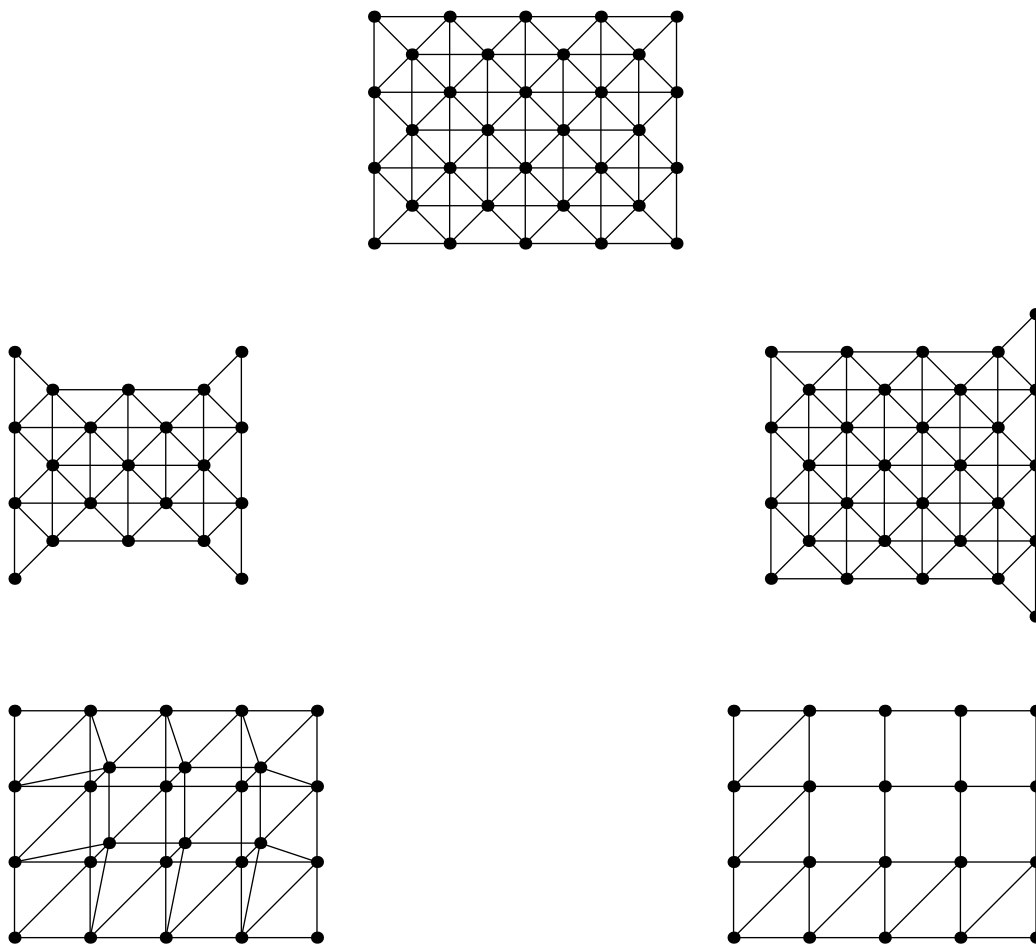


Figure 1: The graphs $N_{4 \times 3}$, $X_{4 \times 3}$, $T_{4 \times 3}$, $D_{4 \times 3}$ and $L_{4 \times 3}$.

We are now in a position to state the characterisation of all connected graphs with four boundary vertices. A path of *arbitrary length* may have length 0. Figure 2 provides examples of graphs from each of the nine families mentioned below.

Theorem 4. *A connected graph G has exactly four boundary vertices if and only if it is either*

- (i) *a subdivision of $K_{1,4}$; or*
- (ii) *a subdivision of the tree with exactly four leaves and two vertices of degree 3; or*
- (iii) *a graph obtained from one of the trees of (ii) by removing a vertex of degree 3 and adding all edges between its three neighbours; or*
- (iv) *the complete graph K_4 on four vertices with arbitrary length paths attached to its vertices; or*
- (v) *a subgraph of $N_{a \times c}$ induced by $V_{a \times c}^0 \cup (W \cap V_{a \times c}^1)$ for some axis slice convex set $W \subseteq \mathbf{R}^2$, with arbitrary length paths attached to its boundary vertices; or*
- (vi) *the graph $X_{a \times c}$ with arbitrary length paths attached to its boundary vertices; or*
- (vii) *a subgraph of $T_{a \times c}$ induced by $V_{a \times (c+1)}^1 \cup (W \cap V_{a \times (c+1)}^0)$ for some axis slice convex set $W \subseteq \mathbf{R}^2$ that contains $\{(a, y) : y = 0, \dots, c + 1\}$ with arbitrary length paths attached to its boundary vertices; or*
- (viii) *the graph $D_{a \times c}$ with arbitrary length paths attached to its boundary vertices; or*
- (ix) *the graph $L_{a \times c}$ with arbitrary length paths attached to its boundary vertices.*

Our main tool in the proof of Theorem 4 is the frame of a graph, which we introduce and study next.

3 The frame of a graph

Definition 5. A *frame* is a metric space (X, d) where X is a finite set and the distance function $d(x, y)$ is an integer for all $x, y \in X$.

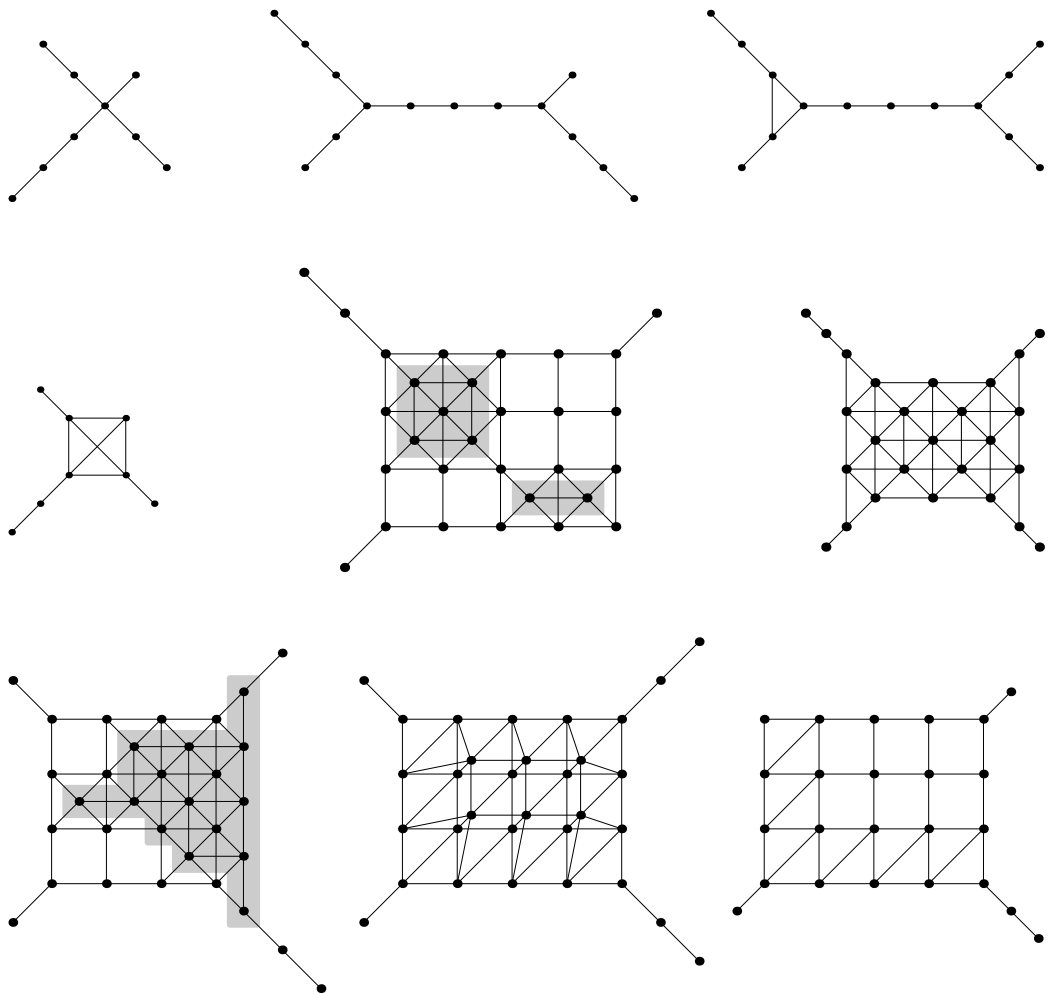


Figure 2: (Examples of) all types of connected graphs with 4 boundary vertices.

Let $G = (V, E)$ be a graph with boundary $\mathcal{B} := \{B_1, \dots, B_b\}$. The pair $\mathcal{F}(G) := (\mathcal{B}, d_G)$, where d_G is the distance in the graph G , is a frame. It is the *frame of the graph G* . For each vertex $v \in V$ we define the *position vector*

$$\varphi(v) := (d_G(v, B_1), \dots, d_G(v, B_b)),$$

that represents its distances from the boundary vertices. For $x, y \in \mathbf{R}^b$, let $d^*(x, y)$ be the L_∞ -distance between x and y , i.e.

$$d^*(x, y) := \max_{1 \leq i \leq b} |x_i - y_i|.$$

Throughout the rest, we make use of the following observation [6, Lemma 3].

Lemma 6. *Each shortest path of G extends to a shortest path between two boundary vertices.*

We now prove that the L_∞ -distance of the position vectors of vertices of a graph is the same as their distance in the graph.

Lemma 7. $d^*(\varphi(u), \varphi(v)) = d_G(u, v)$ for all $u, v \in V(G)$.

Proof of Lemma 7. Let $\mathcal{B} := \{B_1, \dots, B_b\}$ be the boundary of G . Fix two vertices u and v of G . For each $i \in \{1, 2, \dots, b\}$,

$$\varphi(u)_i = d_G(u, B_i) \leq d_G(u, v) + d_G(v, B_i) = d_G(u, v) + \varphi(v)_i.$$

So $d_G(v, u) = d_G(u, v) \geq \varphi(u)_i - \varphi(v)_i$, and hence $d_G(u, v) \geq |\varphi(u)_i - \varphi(v)_i|$. Therefore $d_G(u, v) \geq d^*(u, v)$.

By Lemma 6, any shortest path between v and u extends to a shortest path P between two boundary vertices, say B_i and B_j . If B_i is the endvertex of P closer to u then

$$\varphi(v)_i = d_G(v, B_i) = d_G(v, u) + d_G(u, B_i) = d_G(v, u) + \varphi(u)_i.$$

Consequently, $d_G(v, u) = \varphi(v)_i - \varphi(u)_i \leq d^*(u, v)$, which finishes the proof. ■

The next lemma states two properties of the position vectors.

Lemma 8. *Let $G = (V, E)$ be a graph with boundary $\mathcal{B} := \{B_1, \dots, B_b\}$. For every vertex $u \in V$, the position vector $\varphi(u)$ has the following properties.*

- (i) $\varphi(u)_i + \varphi(u)_j \geq d_G(B_i, B_j)$ for every $i, j \in \{1, \dots, b\}$; and
- (ii) for every $i \in \{1, \dots, b\}$, there exists $j \in \{1, \dots, b\}$ such that $\varphi(u)_i + \varphi(u)_j = d_G(B_i, B_j)$.

Proof. Part **(i)** is a direct consequence of the triangle inequality:

$$\varphi(u)_i + \varphi(u)_j = d_G(u, B_i) + d_G(u, B_j) \geq d_G(B_i, B_j).$$

Part **(ii)** follows from Lemma 6, since for every vertex u and every boundary vertex B_i there exists a shortest path between B_i and B_j containing u , for some index $j \in \{1, 2, \dots, b\}$. \blacksquare

Definition 9. Suppose that $\mathcal{F} = (X, d)$ is a frame with $X = \{B_1, \dots, B_b\}$. We associate a graph $F = F(\mathcal{F})$ with the frame \mathcal{F} , called the *frame-graph* corresponding to \mathcal{F} . The vertex set $V(F)$ consists of the set of b -dimensional integer vectors $x = (x_1, \dots, x_b) \in (\mathbf{Z}^+)^b$ that satisfy

(F1) $x_i + x_j \geq d(B_i, B_j)$ for every $(i, j) \in \{1, 2, \dots, b\}^2$; and

(F2) for every $i \in \{1, 2, \dots, b\}$ there exists $j \in \{1, 2, \dots, b\}$ such that $x_i + x_j = d(B_i, B_j)$.

If $x, y \in V(F)$ then $xy \in E(F)$ if and only if $d^*(x, y) = 1$.

Observe that the vector $\varphi(B_k) = (d(B_k, B_1), \dots, d(B_k, B_b))$ is in $V(F)$ for $k \in \{1, \dots, b\}$.

We state and prove three lemmas. Recall that $d^*(x, y) := \max_i |x_i - y_i|$ is the L_∞ -distance between x and y .

Lemma 10. $d_F(x, y) = d^*(x, y)$ for all $x, y \in V(F)$.

Proof. Let x and y be two vertices of F and set $t := d^*(x, y)$. Since there is a coordinate in which x and y differ by t , it follows from the definition of F that $d_F(x, y) \geq t$.

We now show that $d_F(x, y) \leq d^*(x, y)$ for any two vertices x and y by induction on $t := d^*(x, y) \geq 0$. If $t = 0$ then $x_i = y_i$ for all i , so $x = y$. If $t = 1$ then $xy \in E(F)$ by the definition of F , and hence $d_F(x, y) = 1$. If $t > 1$ then we show that there exists a vector $x' \in V(F)$ such that $xx' \in E(F)$ and $d^*(x', y) < t$. This yields the desired result, because by the induction hypothesis $d_F(x', y) < t$, and therefore $d_F(x, y) \leq t$.

Assume that x'_1, \dots, x'_{i-1} are defined for some integer $i \geq 1$. Let x'_i be the smallest of $x_i - 1, x_i$ and $x_i + 1$ that satisfies $x'_i + x'_j \geq d(B_i, B_j)$ for every $j < i$ and $|x'_i - y_i| < t$.

First, we need to show that at least one of $x_i - 1, x_i$ and $x_i + 1$ satisfies the last two conditions. The choice $x'_i = x_i + 1$ ensures that $x'_i + x'_j \geq (x_i + 1) + (x_j - 1) = x_i + x_j \geq d(B_i, B_j)$ by **(F1)**. If $|x_i + 1 - y_i| < t$ then

$x_i + 1$ is a possible choice. If $|x_i + 1 - y_i| \geq t$ then let $x'_i = y_i + t - 1$. Since $x_i \leq y_i + t$, it follows that $x_i - 1 \leq x'_i \leq x_i$. As $t \geq 2$, for every $j < i$

$$x'_j + x'_i \geq y_j - (t - 1) + y_i + t - 1 = y_j + y_i \geq d(B_i, B_j).$$

Therefore, $y_i + t - 1 \in \{x_i - 1, x_i\}$ is a possible choice.

Now we show that $x' \in V(F)$. By the definition, $x'_i + x'_j \geq d(B_i, B_j)$. If $x'_i = x_i - 1$ then since $x \in V(F)$ there exists j such that $x_i + x_j = d(B_i, B_j)$. So $x'_i + x'_j \leq (x_i - 1) + (x_j + 1) = d(B_i, B_j)$. If $x'_i > x_i - 1$ then $x'_i - 1$ was not a possible choice. Thus, either there exists $j < i$ such that $x'_j + x'_i - 1 < d(B_j, B_i)$ in which case $x'_j + x'_i \leq d(B_i, B_j)$, or $|x'_i - 1 - y_i| \geq t$ in which case $x'_i = y_i - t + 1$. Since $y \in V(F)$, there exists j such that $y_i + y_j = d(B_i, B_j)$. Therefore, since $t \geq 2$,

$$x'_i + x'_j \leq (y_i - t + 1) + (y_j + t - 1) = d(B_i, B_j).$$

This concludes the proof. ■

Note that by Lemma 10 the graph F is connected, since any two vertices have a finite distance.

Lemma 11. *For all $x \in V(F)$ and $i \in \{1, \dots, b\}$, it holds that $x_i = d_F(x, \varphi(B_i))$.*

Proof. By Lemma 10, it suffices to prove that $x_i = d^*(x, \varphi(B_i))$. Since $d^*(x, \varphi(B_i)) = \max_j |x_j - d(B_i, B_j)|$, it follows that $x_i \leq d^*(x, \varphi(B_i))$. We now prove that $x_i \geq |x_j - d(B_i, B_j)|$ for all j , which yields the result.

Fix an index $j \neq i$. Since $x_i + x_j \geq d(B_i, B_j)$, we obtain $x_i \geq d(B_i, B_j) - x_j$. So it only remains to show that $x_i \geq x_j - d(B_i, B_j)$. Since $x \in V(F)$, there exists k such that $x_j + x_k = d(B_j, B_k)$. Therefore

$$\begin{aligned} x_j &= d(B_j, B_k) - x_k \leq d(B_j, B_k) - (d(B_i, B_k) - x_i) \\ &\leq x_i + d(B_i, B_j). \end{aligned}$$

Thus $x_i \geq x_j - d(B_i, B_j)$, which concludes the proof. ■

Lemma 12. *The boundary of F is $\{\varphi(B_1), \dots, \varphi(B_b)\}$.*

Proof. Let x be a boundary vertex of F and y be a witness for x . Set $t := d_F(x, y)$. We first prove that there exists $i \in \{1, \dots, b\}$ such that $y_i = x_i + t$. By Lemma 10, there exists $j \in \{1, \dots, b\}$ such that $t = |x_j - y_j|$. If $y_j = x_j + t$ then we set $i := j$. If $y_j = x_j - t$ then since there exists i such that $x_j + x_i = d(B_i, B_j)$ by **(F2)**, we obtain $x_i = d(B_i, B_j) - x_j = d(B_i, B_j) - y_j - t \leq y_i - t$ using **(F1)**. As $y_i \leq x_i + t$, it follows that $y_i = x_i + t$.

Since $d_F(\varphi(B_i), y) = y_i = x_i + t = d_F(\varphi(B_i), x) + d_F(x, y)$, there is a shortest path between $\varphi(B_i)$ and y that contains x . Since y is a witness for x , we infer that $x = \varphi(B_i)$. Thus, $\mathcal{B}(F) \subseteq \{\varphi(B_1), \dots, \varphi(B_b)\}$.

To finish the proof, we need to show that $\varphi(B_i)$ is a boundary vertex of F for each $i \in \{1, 2, \dots, b\}$. Pick an arbitrary i , and let j be such that B_j is a witness for B_i in G (such a j exists by Lemma 6). We show that $\varphi(B_j)$ is also a witness for $\varphi(B_i)$ in F . Let $x \in V(F)$ be a neighbour of $\varphi(B_i)$, and suppose that $d_F(x, \varphi(B_j)) > d_F(\varphi(B_i), \varphi(B_j))$. Then there exists a $\varphi(B_j)x$ -path of length $d_F(x, \varphi(B_j))$ that goes through $\varphi(B_i)$. We already know that $\mathcal{B}(F) \subseteq \{\varphi(B_1), \dots, \varphi(B_b)\}$, so that this path must extend to a shortest $\varphi(B_i)\varphi(B_k)$ -path for some k by Lemma 6. Hence, $d_G(B_j, B_i) + d_G(B_i, B_k) = d_F(\varphi(B_j), \varphi(B_i)) + d_F(\varphi(B_i), \varphi(B_k)) = d_F(\varphi(B_j), \varphi(B_k)) = d_G(B_j, B_k)$. So in G there must also be a path of length $d_G(B_j, B_k)$ going through B_i . But this implies B_i has a neighbour v with $d_G(v, B_j) = d_G(B_i, B_j) + 1$, which contradicts the assumption that B_j is a witness for B_i in G .

Hence, $\varphi(B_i)$ is a boundary vertex of F for all $i \in \{1, 2, \dots, b\}$. This concludes the proof. \blacksquare

The next theorem summarizes the previous study.

Theorem 13. *Let \mathcal{F} be a frame on the points B_1, \dots, B_b , and suppose that the graph G has frame \mathcal{F} . Set $F := F(\mathcal{F})$. Then the map*

$$\begin{aligned} \varphi : V(G) &\longrightarrow V(F) \\ v &\longmapsto \varphi(v) = (d_G(v, B_1), \dots, d_G(v, B_b)) \end{aligned}$$

is an embedding of G into F as an induced subgraph. Moreover, the set $\{\varphi(B_1), \dots, \varphi(B_b)\}$ is precisely the boundary of F and $d_G(u, v) = d_F(\varphi(u), \varphi(v))$ for all vertices $u, v \in V(G)$.

Note that the theorem in particular implies that F has frame \mathcal{F} (if we identify $\varphi(B_i)$ with B_i).

Proof of Theorem 13. That φ is an embedding, and G is an induced subgraph of F follows directly from Lemma 7, Lemma 8 and the definition of F . By Lemma 10 and Lemma 7 it follows that $d_G(u, v) = d^*(\varphi(u), \varphi(v)) = d_F(\varphi(u), \varphi(v))$. By Lemma 12 the boundary of F is $\{\varphi(B_1), \dots, \varphi(B_b)\}$. \blacksquare

4 The frame of a graph with four boundary vertices and minimum degree at least 2

In this section we study the graph F corresponding to (the frame of) a connected graph G with four boundary vertices and minimum degree at least 2 (vertices of degree 1 are dealt with later on). In view of Theorem 13, we identify $v \in V(G)$ with $\varphi(v) \in V(F)$ for the ease of exposition.

Let B_1, B_2, B_3 and B_4 be the boundary vertices of F and G . By assumption, each of them has degree at least 2.

Lemma 14. *Let G be a graph with minimum degree at least 2. For every $B \in \mathcal{B}(G)$, there exist two distinct vertices A_1 and A_2 in $\mathcal{B}(G) \setminus \{B\}$, such that the shortest BA_1 -path and the shortest BA_2 -path in G are unique, and these two paths only have the vertex B in common.*

Proof. We consider two cases.

Case 1: *There exists a shortest path between two boundary vertices A_1 and A_2 containing B .* We claim that the path A_1B is unique. Assume on the contrary that there is another shortest path between A_1 and B . Observe that there exist two distinct vertices x and y that are at the same distance from B , and at the same distance from A_1 . They also are at the same distance from A_2 . Therefore, the endvertices of an extension of a shortest path between x and y must be distinct from A_1, A_2 and B . But these endvertices are boundary vertices, which is a contradiction since there are four boundary vertices in total. Similarly, the path BA_2 is unique as well.

Note that the A_1B -path and the BA_2 -path can only have the vertex B in common, since their lengths sum up to the distance between A_1 and A_2 .

Case 2: *The vertex B is not contained in any shortest path between two boundary vertices distinct from B .* In this case, the neighbourhood of B induces a clique. Indeed, if u and v are two non-adjacent neighbours of B then extending the shortest path uBv shows that B belongs to a shortest path between two other boundary vertices, a contradiction. Let u and v be two neighbours of B . Let P be the extension of the path uv with endvertices A_1 and A_2 , where A_1 is closer to u .

Let $U := \{s \in N(B) : d(A_1, s) + 1 = d(A_1, B)\}$. Note that $u \in U$. We claim that $U = \{u\}$. To show this, it suffices to prove that every vertex in U has the same distance to A_1, B and A_2 as well (this is because if w is such that $d(w, A_1) = d(u, A_1), d(w, A_2) = d(u, A_2)$ and $d(w, B) = d(u, B)$ then extending a shortest uw -path show that there are at least 5 boundary vertices, a contradiction). Indeed, for A_2 , suppose that $w \in U$. It holds

that $d(w, A_2) \leq d(u, A_2)$, since $N(B)$ induces a clique, and thus $uv \in E$. If the inequality is strict, then there is a path between A_1 and A_2 of length $d(A_1, w) + d(w, A_2)$, which contradicts that P is a shortest A_1A_2 -path.

Now, the shortest path between u and A_1 is unique, for otherwise there exist two vertices that are at the same distance from B, A_1 and A_2 , a contradiction. Consequently, the path BA_1 is unique as well. By symmetry, the path BA_2 is unique. Again, the paths cannot have any vertex other than B in common. ■

Lemma 15. *Let G be a graph with minimum degree at least 2 and exactly 4 boundary vertices B_1, B_2, B_3, B_4 . Without loss of generality, we can assume that the shortest B_1B_2 -, B_2B_3 -, B_3B_4 - and B_1B_4 -paths are unique, and that among these paths, those that share an endvertex do not share any other vertex.*

Proof. The sought conclusion holds if $\text{diam}(G) = 1$, in which case G is K_4 . So we assume throughout the rest of the proof that $\text{diam}(G) \geq 2$. Note that if two vertices are at distance $\text{diam}(G)$ of each other, then they are boundary vertices. We split the analysis into two cases.

Suppose first that whenever two vertices are at distance $\text{diam}(G)$ of each other, then there is a unique shortest path between them. Up to relabelling the boundary vertices, we may assume that $d(B_1, B_2) = \text{diam}(G)$. Let P be the unique shortest path between B_1 and B_2 . Any neighbour of B_1 that is not on P is at distance at least $\text{diam}(G)$ from B_2 . Thus, any such neighbour is a boundary vertex of G (with witness B_2). Since B_1 has degree at least 2, we deduce that there is an edge between B_1 and, say, B_4 . Note that necessarily $d(B_2, B_4) = \text{diam}(G)$. Similarly, there is an edge between B_2 and B_3 (note that B_2 is not adjacent to B_4 since $\text{diam}(G) \geq 2$) and $d(B_4, B_3) = \text{diam}(G)$. This concludes the proof in the case where any two vertices at distance $\text{diam}(G)$ have a unique shortest path between them.

Assume now that there are two vertices of G at distance $\text{diam}(G)$ of each other with at least two distinct shortest paths between them. Up to relabelling the boundary vertices, we may assume that those two vertices are B_1 and B_3 . By applying Lemma 14 to B_1 and B_3 , we infer that the shortest paths between B_1, B_2 , between B_2, B_3 , between B_3, B_4 and between B_4, B_1 are all unique. If there are at least two distinct shortest paths between B_2 and B_4 , then applying Lemma 14 to each boundary vertex yields the desired conclusion. So we may assume that there is a unique shortest path P between B_2 and B_4 . Now, the aforementioned unique shortest paths satisfy the statement of the theorem unless they intersect. Assume that the unique shortest paths P_{12} between B_1 and B_2 , and P_{23} between B_2 and B_3 intersect. Since those paths are unique, the neighbour of B_2 on P_{12} also belongs to

P_{23} . There is another neighbour X of B_2 , since G has minimum degree at least 2. Let $x := d(B_1, B_2)$, $y := d(B_3, B_2)$ and $z := d(B_4, B_2)$. By Theorem 13 and the fact that $\text{diam}(G) = d(B_1, B_3) \leq x + y - 2$, the position vector of X is $(x, 1, y, z - 1)$. Further, we conclude that $d(B_1, B_4) = x + z - 1$ and $d(B_3, B_4) = y + z - 1$. The path P intersects a shortest path between B_1 and B_3 at some vertex T . Indeed, since the shortest B_1B_3 -path is not unique, there are two vertices T and T' such that $d(T, B_1) = d(T', B_1)$ and $d(T, B_3) = d(T', B_3)$. Thus, a shortest TT' -path extends to a shortest path between B_2 and B_4 , which must be P (since the shortest B_2B_4 -path is unique). Let $t := d(B_4, T) < z$. Now, $x + z - 1 = d(B_1, B_4) \leq d(B_1, T) + t$ and $y + z - 1 = d(B_3, B_4) \leq d(B_3, T) + t$. So

$$x + y - 2 + 2z \leq d(B_1, T) + d(B_3, T) + 2t = d(B_1, B_3) + 2t \leq x + y - 2 + 2t.$$

This is a contradiction since $t < z$. ■

In the remainder of this section we let P_{ij} be the unique shortest B_iB_j -path. Let us set

$$\begin{aligned} a &:= d(B_1, B_2), & b &:= d(B_1, B_3), & c &:= d(B_1, B_4), \\ a' &:= d(B_3, B_4), & b' &:= d(B_2, B_4), & c' &:= d(B_2, B_3). \end{aligned}$$

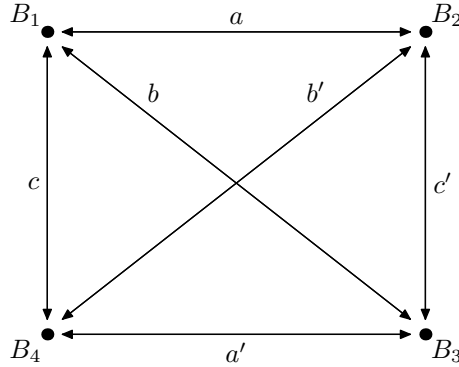


Figure 3: Notations of the distances between the boundary vertices.

Lemma 16. *Without loss of generality, we may assume that one of the following holds:*

- (i) $a = a'$, $c = c'$, and $b = b' = a + c$;
- (ii) $a = a'$, $c = c'$, and $b = b' = a + c - 1$;

(iii) $a = a', c = c', b = a + c$, and $b' = a + c - 1$;

(iv) $a = a', c' = c + 1$, and $b = b' = a + c$.

Proof. Note that the lemma is true if $\text{diam}(G) = 1$. So we assume that $\text{diam}(G) \geq 2$.

First, we show that $b' \in \{a + c - 1, a + c\}$. If B_1 and B_2 are adjacent, i.e. if $a = 1$, then the triangle inequality ensures that $b' \in \{c - 1, c, c + 1\}$. Moreover, $b' \neq c - 1$ for otherwise P_{14} and P_{12} would share the vertex B_2 , thereby contradicting Lemma 15. The situation is analogous if B_1 and B_4 are adjacent, i.e. if $c = 1$. So, assume that both a and c are greater than 1. Let v_{ij} be the neighbour of B_i on P_{ij} . Extending the shortest path between v_{14} and v_{12} (note that they are distinct by the proof of Lemma 14), we obtain a shortest path between B_2 and B_4 . Indeed, B_1 cannot be involved since it is adjacent to both v_{14} and v_{12} . Further, if B_3 were involved then for $v = B_2$ or $v = B_4$ it would follow that the unique shortest vB_1 -path and the unique shortest vB_3 -path share a vertex different from v . This would contradict Lemma 15. This shows that $b' \in \{a + c, a + c - 1\}$.

Similarly, by considering a', c' , and v_{34}, v_{32} , we deduce that $b' \in \{a' + c', a' + c' - 1\}$. Thus one of the following holds.

(b'.1) $a + c = a' + c'$;

(b'.2) $a + c = a' + c' - 1 = b'$;

(b'.3) $a + c - 1 = a' + c' = b'$.

Proceeding analogously with B_1 and B_4 yields that $b \in \{a' + c, a' + c - 1\}$ and $b \in \{a + c', a + c' - 1\}$. Consequently, one of the following holds.

(b.1) $a + c' = a' + c$;

(b.2) $a + c' = a' + c - 1 = b$;

(b.3) $a + c' - 1 = a' + c = b$.

Both one of (b'.1), (b'.2), (b'.3) and one of (b.1), (b.2), (b.3) hold.

Suppose first that (b'.1) holds. Then, $a - a' = c' - c$. If (b.1) holds then $a - a' = c - c'$. So $c - c' = -(c - c')$, giving that $c = c'$ and $a = a'$. Thus, up to switching of the accents, we are in situation (i), (ii) or (iii). If (b.2) holds then $a - a' = c - c' - 1$. So, $2(c - c') = 1$, i.e. $c = c' + 1/2$. But this cannot be since both c and c' are integers. The situation when (b.3) holds is similar.

Assume now that **(b'.2)** holds. Thus, $a - a' = c' - c - 1$. If **(b.1)** holds then $a - a' = c - c'$. So $2(c - c') = 1$, a contradiction. If **(b.2)** holds then $a - a' = c - c' - 1$. So $c' = c$ and $a' = a + 1$, and hence up to relabelling we are in situation **(iv)**. Last, if **(b.3)** holds then $a - a' = c - c' + 1$. So $c' = c + 1$ and $a = a'$, and hence we are in situation **(iv)**.

Finally, the situation when **(b'.3)** holds is completely analogous to the situation when **(b'.2)** holds. \blacksquare

Theorem 17. *Let G be a graph with minimum degree at least 2 and exactly four boundary vertices. Let F be the graph corresponding to its frame as constructed in Definition 9. Then F is isomorphic to either $N_{a \times c}$, $X_{a \times c}$, $T_{a \times c}$ or $D_{a \times c}$.*

For convenience we split the theorem into several lemmas.

Lemma 18.

- (i) *If $a = a'$, $c = c'$, and $b = b' = a + c$ then F is isomorphic to $N_{a \times c}$.*
- (ii) *If $a = a'$, $c' = c + 1$, and $b = b' = a + c$ then F is isomorphic to $T_{a \times c}$.*

Proof. For non-negative integers x and y let us set

$$\begin{aligned} v_{x,y} &:= (x + y, a - x + y, a + c - x - y, c + x - y) \quad \text{and} \\ w_{x,y} &:= (x + y + 1, a - x + y, a + c - 1 - x - y, c + x - y). \end{aligned}$$

(i). Observe that $v_{x,y}$ is the position vector for the vertex (x, y) in $N_{a \times c}$ for every $x \in \{0, 1, \dots, a\}$ and every $y \in \{0, 1, \dots, c\}$. Further, $w_{x,y}$ is the position vector of $(x + \frac{1}{2}, y + \frac{1}{2})$ in $N_{a \times c}$ if $x \in \{0, 1, \dots, a - 1\}$ and $y \in \{0, 1, \dots, c - 1\}$. Therefore these vectors satisfy the requirements **(F1)** and **(F2)**, so that they form the vertices of an induced copy of $N_{a \times c}$ inside F .

Now pick $u = (u_1, u_2, u_3, u_4) \in V(F)$. We wish to show that $u \in V(N_{a \times c})$, which will give that F indeed coincides with $N_{a \times c}$. We know that $u_1 + u_2 \geq a$. First suppose that $u_1 + u_2 = a$. Then u lies on a $B_1 B_2$ -path of length a . Since there is only one such path (by Lemma 15), namely $P_{12} = v_{0,0} v_{1,0} \dots v_{a,0}$, we deduce that $u \in V(N_{a \times c})$. Let us thus assume that $u_1 + u_2 > a$. Similarly, we can suppose that $u_2 + u_3 > c$, $u_3 + u_4 > a$, and $u_1 + u_4 > c$. Observe that, by **(F2)**,

$$u_1 + u_3 = u_2 + u_4 = a + c. \quad (1)$$

Now assume that $u_1 + u_2 - a$ is even, and set $y := (u_1 + u_2 - a)/2$ and $x := u_1 - y$. Hence, $u_1 = x + y$ and $u_2 = a - x + y$, so that by (1) we deduce

that $u_3 = a + c - x - y$ and $u_4 = c + x - y$. Because $c + 2x = u_1 + u_4 > c$ and $2a + c - 2x = u_2 + u_3 > c$, it follows that $0 < x < a$. Similarly, we obtain $0 < y < c$ since $a + 2y = u_1 + u_2 > a$ and $a + 2c - 2y = u_3 + u_4 > a$. Consequently, $u = v_{x,y} \in V(N_{a \times c})$ if $u_1 + u_2 - a$ is even.

Let us assume now that $u_1 + u_2 - a$ is odd. We set $y := (u_1 + u_2 - a - 1)/2$ and $x := u_1 - y - 1$. Thus, $u_1 = x + y + 1$ and $u_2 = a - x + y$. In addition, (1) implies that $u_3 = a + c - 1 - x - y$ and $u_4 = c + x - y$. Because $c + 2x + 1 = u_1 + u_4 > c$ and $2a + c - 1 - 2x = u_2 + u_3 > c$, we obtain $0 \leq x < a$. And because $a + 2y + 1 = u_1 + u_2 > a$ and $a + 2c - 1 - 2y = u_3 + u_4 > a$, we obtain $0 \leq y < c$. Hence, $u = w_{x,y} \in V(N_{a \times c})$ when $u_1 + u_2 - a$ is odd.

So F and $N_{a \times c}$ indeed coincide.

(ii). The points in

$$\begin{aligned} W := & \{v_{x,y} : 0 \leq x < a \text{ and } 0 \leq y \leq c\} \\ & \cup \{w_{x,y} : 0 \leq x < a \text{ and } 0 \leq y < c\} \\ & \cup \{(a - 1 + i, i, c + 1 - i, a + c - i) : 0 < i \leq c\} \\ & \cup \{(a, 0, c + 1, a + c), (a + c, c + 1, 0, a)\} \end{aligned}$$

satisfy the requirements **(F1)** and **(F2)**. So $W \subseteq V(F)$. Also note that W is precisely the set of position vectors of $T_{a \times c}$, so that $T_{a \times c}$ is an induced subgraph of F .

Now pick $u \in V(F)$. Analogously as before, we may assume that $u_1 + u_2 > a$, $u_2 + u_3 > c + 1$, $u_3 + u_4 > a$, and $u_1 + u_4 > c$. Moreover, $u_1 + u_3 = u_2 + u_4 = a + c$. Suppose that $u_1 + u_2 - a$ is even. Set $y := (u_1 + u_2 - a)/2$ and $x := u_1 - y$. Then $u_1 = x + y$ and $u_2 = a - x + y$. It thus follows that $u = v_{x,y}$. In addition, since $u_1 + u_2 > a$, $u_2 + u_3 > c + 1$, $u_3 + u_4 > a$, and $u_1 + u_4 > c$, it follows that $0 < x < a$ and $0 < y < c$. Hence, $u \in V(T_{a \times c})$ if $u_1 + u_2 - a$ is even.

Now suppose that $u_1 + u_2 - a$ is odd. Set $y := (u_1 + u_2 - a - 1)/2$ and $x := u_1 - y$. Analogously to before, we infer that $u = w_{x,y}$ with $0 \leq x < a$ and $0 \leq y < c$ if $u_1 + u_2 - a$ is odd.

Thus F coincides with $T_{a \times c}$ as required. ■

Lemma 19. *If $a = a'$, $c = c'$, $b = a + c$, and $b' = a + c - 1$ then F is isomorphic to $D_{a \times c}$.*

Proof. Recall that $B_1 = (0, a, a + c, c)$, $B_2 = (a, 0, c, a + c - 1)$, $B_3 = (a + c, c, 0, a)$, and $B_4 = (c, a + c - 1, a, 0)$. For $x \in \{1, 2, \dots, a\}$ and $y \in \{0, 1, \dots, c - 1\}$ let us set

$$v_{x,y} := (x + y, a - x + y, a + c - (x + y), c - 1 + x - y).$$

For $x \in \{0, 1, \dots, a-1\}$ and $y \in \{1, 2, \dots, c\}$ let us set

$$w_{x,y} := (x+y, a-1-x+y, a+c-(x+y), c+x-y).$$

First, note that $B_2 = v_{a,0}$ and $B_4 = w_{0,c}$ but neither B_1 nor B_3 corresponds to any of the points $v_{x,y}$ or $w_{x,y}$. Observe also that the points $v_{x,y}$ and $w_{x,y}$ satisfy the criteria **(F1)** and **(F2)**, and that they are the position vectors of the vertices of $D_{a \times c}$ other than B_1 and B_3 . Hence, together with B_1 and B_3 , they form an induced copy of $D_{a \times c}$ inside F .

Now let $u = (u_1, u_2, u_3, u_4) \in V(F)$ be arbitrary. First, suppose that $u_1 + u_2 = a$. Then, u is on the unique shortest path P_{12} between B_1 and B_2 . Notice that $B_1 v_{1,0} \dots v_{a-1,0} B_2$ is a $B_1 B_2$ -path of length a . Hence it equals P_{12} . It follows that $u \in D_{a \times c}$. Thus, we can suppose that $u_1 + u_2 > a$. Similarly, we may assume $u_1 + u_4 > c$, $u_2 + u_3 > c$, and $u_3 + u_4 > a$. Notice that

$$u_1 + u_3 = a + c, \quad u_2 + u_4 = a + c - 1, \quad (2)$$

by **(F2)**.

Suppose that $u_1 + u_2 - a$ is even. Let us write $y = (u_1 + u_2 - a)/2$ and $x = u_1 - y$. Then, $u_1 = x + y$ and $u_2 = a - x + y$. Further, using (2), we infer that u is in fact of the same form as $v_{x,y}$ for some x and y . It remains to be checked that $0 < x < a$ and $0 \leq y < c$. Since $u_2 + u_3 = 2a + c - 2x > c$ and $u_1 + u_4 = c - 1 + 2x > c$, it follows that $0 < x < a$. Since $u_1 + u_2 = a + 2y > a$ and $u_3 + u_4 = a + 2c - 1 + 2y > a$, it follows that $0 < y < c$. Thus, $u \in V(D_{a \times c})$ if $u_1 + u_2 - a$ is even.

Now suppose that $u_1 + u_2 - a$ is odd. Set $y := (u_1 + u_2 - a + 1)/2$ and $x := u_1 - y$. Note that $u_1 = x + y$, $u_2 = a - 1 - x + y$, so that by (2) the vertex u is of the same form as $w_{x,y}$ for this choice of x and y . Again it remains to be seen that $0 < x < a$ and $0 < y < c$. Since $u_2 + u_3 = 2a + c - 1 - 2x > c$ and $u_1 + u_4 = c + 2x > c$, it follows that indeed $0 < x < a$. Further, $0 < y < c$ because $u_1 + u_2 = a - 1 + 2y > a$ and $u_3 + u_4 = a + 2c + 2y > a$. Thus, we conclude that $u \in V(D_{a \times c})$ if $u_1 + u_2 - a$ is odd.

Therefore, F coincides with $D_{a \times c}$. ■

Lemma 20. *If $a = a'$, $c = c'$, and $b = b' = a + c - 1$ then F is isomorphic to $X_{a \times c}$.*

Proof. By the symmetry of the roles played by a and c , we may assume that $a \geq c$ (recall that $X_{a \times c} = X_{c \times a}$). First, note that if $a = c = 1$ then F and G are necessarily isomorphic to $K_4 = X_{1 \times 1}$. Thus, suppose that $a \geq 2$. This time set

$$v_{x,y} := (x+y, a-1-x+y, a+c-1-x-y, c+x-y)$$

for $0 \leq x \leq a - 1$ and $1 \leq y \leq c - 1$, and

$$w_{x,y} := (x + y + 1, a - 1 - x + y, a + c - 2 - x - y, c + x - y)$$

for $0 \leq x \leq a - 2$ and $0 \leq y \leq c - 1$. Then $v_{x,y}$ satisfies **(F1)** and **(F2)** if $0 \leq x \leq a - 1$ and $1 \leq y \leq c - 1$. Furthermore, $w_{x,y}$ satisfies **(F1)** and **(F2)** if $0 \leq x \leq a - 2$ and $0 \leq y \leq c - 1$. In addition, together with B_1, B_2, B_3 , and B_4 , these vertices induce a copy of $X_{a \times c}$ in F .

Now pick $u \in V(F)$. We can again assume that $u_1 + u_2 > a$, $u_1 + u_4 > c$, $u_2 + u_3 > c$, and $u_3 + u_4 > a$. Consequently, $u_1 + u_3 = u_2 + u_4 = a + c - 1$.

If $u_1 + u_2 - a + 1$ is even, then set $y := (u_1 + u_2 - a + 1)/2$ and $x := u_1 - y$. So $u = v_{x,y}$ for some $x \in \{1, 2, \dots, a - 2\}$ and $y \in \{1, 2, \dots, c - 1\}$. If $u_1 + u_2 - a + 1$ is odd, then we set $y := (u_1 + u_2 - a)/2$ and $x := u_1 - y$. So $u = w_{x,y}$ for some $x \in \{0, 1, \dots, a - 2\}$ and $y \in \{1, 2, \dots, c - 2\}$.

Thus $F = X_{a \times c}$ as required. ■

5 The proof of Theorem 4

Notice that if $N(v) = \{u\}$ in G then $v \in \mathcal{B}(G)$ and

$$\mathcal{B}(G) \setminus \{v\} \subseteq \mathcal{B}(G \setminus \{v\}) \subseteq (\mathcal{B}(G) \cup \{u\}) \setminus \{v\}.$$

Thus, if we remove a vertex of degree 1 from a graph with four boundary vertices then we either end up with graph with exactly three boundary vertices, or with another graph with four boundary vertices. Let G be an arbitrary graph with four boundary vertices. By repeatedly removing vertices of degree 1, we infer that G is either obtained from a graph with three boundary vertices by attaching a path to a non-boundary vertex, or from a graph with four boundary vertices and minimum degree at least 2 by attaching paths to the boundary vertices. By Theorem 1, the first case corresponds precisely to parts **(i)**, **(ii)** and **(iii)** of Theorem 4.

In the rest of the proof we therefore assume that G has four boundary vertices and minimum degree at least 2. Let F be the frame-graph of G . By Theorem 17, we know that F is isomorphic to either $N_{a \times c}, X_{a \times c}, T_{a \times c}$ or $D_{a \times c}$ for some integers a and c .

The following observation follows immediately from Theorem 13, which implies that $d_F(u, v) = d_G(u, v)$ for all $u, v \in V(G)$.

Corollary 21. *Let $u, v \in V(G)$ and let F be the frame-graph of G . If there is a unique shortest path P in F between u and v , then $P \subseteq G$.*

Repeated applications of Corollary 21 yield the following.

- If $F = X_{a \times c}$ then $G = F$;
- if $F = D_{a \times c}$ then either $G = D_{a \times c}$ or $G = L_{a \times c}$;
- if $F = N_{a \times c}$ then $V_{a \times c}^0 \subseteq V(G)$ and $V_{a \times c}^1 \cap V(G)$ is axis slice convex; and
- if $F = T_{a \times c}$ then $P_{23}, V_{a \times (c+1)}^1 \subseteq V(G)$ and $V(G) \cap V_{a \times (c+1)}^0$ is axis slice convex.

Suppose that $F = N_{a \times c}$ and $V(G) = V_{a \times c}^0 \cup (W \cap V_{a \times c}^1)$ for some axis slice convex set W . Then a vertex $v \in V(G) \setminus \{B_1, B_2, B_3, B_4\}$ is not a boundary vertex of G , since there is a shortest path to any vertex $u \in V(G)$ (that is also a shortest path in F), and the path can be extended to a path between B_i and B_j for some i and j .

The case where $F = T_{a \times c}$ can be dealt with similarly. This concludes the proof of Theorem 4. ■

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