An Extremal Graph Problem on a Grid and an Isoperimetric Problem for Polyominoes

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Submitted: Jun 13, 2023; Accepted: Mar 18, 2024; Published: Apr 5, 2024

Abstract

Let G denote the infinite grid graph with vertex set $\{(a, b) \ : \ a, b \in \mathbb{Z}\}$ and edge set $\big\{\{u, v\} : |u-v| = 1 \text{ or } |u-v| = \sqrt{2}\big\}$. A question in landscape ecology, restated in graph theoretic terms, asks the following. What is the maximum number of edges in an induced subgraph of G of order n? It was conjectured by Taliceo and Fleron [19] that the maximum is $4n - \lceil \sqrt{28n - 12}\, \rceil$. We prove the conjecture by formulating and solving a discrete version of the classical isoperimeteric problem.

Mathematics Subject Classifications: 05C10, 05C30, 05B50, 52B60

1 Introduction - an Extremal Problem for a Graph on a Grid

Denote by G_1 the infinite graph with vertex set $L = \{(a, b) \ : \ a, b \in \mathbb{Z}\}$ and edge set

$$E_1 := \big\{\{u, v\} : |u - v| = 1\big\}.$$

Let G_2 denote the infinite graph with vertex set L and edge set

$$E_2 := \big\{\{u, v\} : |u - v| = 1 \text{ or } |u - v| = \sqrt{2}\big\}.$$

The graph G_1 is a grid and G_2 is a grid with the diagonals of the unit squares added.

The paper [19] poses a question in landscape ecology. It involves a widely used aggregation index for measuring landscape compactness, measuring how many pixels representing land are edge-connected to others in a satelite image. In graph theoretic terms, the question can be restated as follows.

Question 1. Given a positive integer $n \geqslant 1$, what is the maximum number $M(n)$ of edges in an induced subgraph of G_2 with n vertices?

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 https://doi.org/10.37236/12133

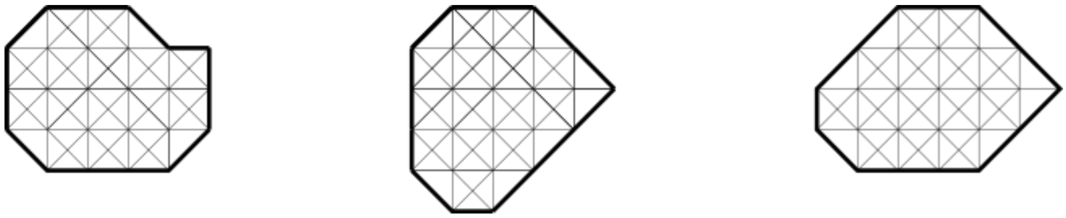

Figure 1: Optimal graphs for Question 1 with $n = 25$. The graphs are those induced in G_2 by the vertices which are inside and on the polygon.

The solution to Question 1 may not be unique. Figure 1 shows three graphs that achieve the maximum for $n = 25$. The vertex sets of these graphs are all the vertices of the grid inside and on the polygon. The edges are all the induced edges in G_2. Note that the polygon need not be convex for an optimum graph.

Taliceo and Fleron [19] give the bounds

$$4n - \left\lceil \sqrt{28n - 12}\, \right\rceil \leqslant M(n) \leqslant 4n - 2\left\lceil \sqrt{4n}\, \right\rceil. \tag{1}$$

They state that these bounds are "sufficient for use in landscape ecology", but make the following conjecture.

Conjecture 2.

$$M(n) = 4n - \left\lceil \sqrt{28n - 12}\, \right\rceil.$$

In Section 4 (Theorem 18) we prove Conjecture 2. It is a consequence of the proof, and also noted in [19], that the convex hull in G_2 of an optimum graph is, very loosely, almost a regular octagon.

Remark 3. Question 1 is a particular instance of a more general topic in graph theory, edge isoperimetric problems. Given a graph $G = (V, E)$ and a finite subset $W \subset V$, define $\Phi(W) = \{\{u, v\} \in E : u \in W, v \notin W\}$, which can be regarded as a "boundary" of W. The *edge isoperimetric problem* is, for each positive integer n, to find $\min \big\{ |\Phi(W)| : |W| = n \big\}$ and a set of vertices that realizes this minimum. The edge isoperimetric problem for the d-dimensional cube graph dates back to Harper's 1960's work [10]. A substantial literature on the edge isoperimetric problem has since evolved; see for example [1, 2, 4, 5, 6, 10, 11, 17, 20] and references therein. Let $m(W)$ denote the number of edges in the subgraph of G induced by W. If G is regular, say of degree r, then $2m(W) + |\Phi(W)| = nr$. Therefore, the edge isoperimetric problem is equivalent to finding the maximum number of edges in an induced subgraph of G of order n. Question 1 is exactly this problem for the case of the infinite graph $G = G_2$, a case not previously solved.

Our approach to Question 1 differs from the methods used in the references above. Detailed in Section 2 and encapsulated by Question 6 in that section, it transforms Question 1 into new discrete polyomino analog of the classical isoperimetric problem.

2 An Isoperimetric Problem for Polyominoes

Polyominoes have been used in puzzles since at least 1907, but the name was only coined in 1953 by S. Golomb [8]. In addition to problems involving tiling regions in the plane by polyominoes, polyominoes come into play in a number of areas, for example in combinatoirics [3], in geometric and topological extremal problems [13], and in commutative algebra [16]. There is no known explicit formula for the number of polyominoes with a given number of squares, but growth rate asymptotics is an active subject and has connections to statistical mechanics [7, 12, 21].

Definition 4 (Polyomino)**.** A *polyomino* is a nonempty finite subset of the set of all closed unit squares in the grid G_1. For a polyomino P let $|P|$ denote the number of squares in P, which is the area of the union of the squares in P. For ease of exposition, unless confusion arises, we will use the same term "polyomino" for both the set of squares and the union of the squares. An *edge* of a polyomino P is an edge of some square of P and a *vertex* is a vertex of some square of P. The *boundary* ∂P of a polyomino P is the union of all edges of P that are contained in exactly one square. The *perimeter* p is the number of edges on ∂P.

A polyomino P will be called *simple* if ∂P is a simply polygon - no self crossings. The polyominoes in Figure 2, for example, are not simple. Equivalently, a polyomino is simple if it is connected, simple connected (the polyomino on the right in Figure 2 is not), and has no cut point as in the polyomino on the left in Figure 2.

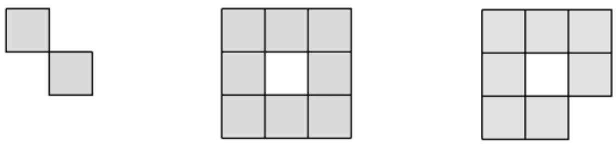

Figure 2: Polyominoes that are not simple.

Definition 5 ($\widehat{\boldsymbol{f}}$-perimeter)**.** The set $V(\partial P)$ of vertices on the boundary of a simple polyomino P consists of the vertices of P that lie on ∂P, *even if the internal angle is* π. Therefore, the set A of possible internal angles of a simple polyomino P at a vertex of its boundary is

$$A = \{\pi/2,\, \pi,\, 3\pi/2\}.$$

That the sum of the internal angles is $(p-2)\pi$ implies that there are exactly 4 more internal angles $\pi/2$ than angles $3\pi/2$.

Let $\alpha(v)$ denote the internal angle of a simple polyomino P at vertex $v \in \partial P$. Given a function $\widehat{f} : A \to \mathbb{R}$, define a function f on the set of all simple polyominoes by

$$f(P) = \sum_{v \in V(\partial P)} \widehat{f}\big(\alpha(v)\big).$$

Both $\widehat{f}$ and f will be referred to as *isoperimetric functions.* The number $f(P)$ will be referred to as the *$\widehat{f}$-perimeter of P.* We pose the following discrete isoperimetric problem, which we call the *polyomino isoperimetric problem* for the the isoperimetric function $\widehat{f}$.

Question 6. For a given isoperimetric function $\widehat{f} : A \to \mathbb{R}$, what is the minimum $\widehat{f}$-perimeter of a polyomino of area n?

The classical isoperimetric problem in the plane asks for the geometric figure of maximum area for a given perimeter, equivalently the geometric figure of minimum perimeter for a given area. The solution is a disk. For the isoperimetric function $\widehat{f}$ defined for all $\alpha \in A$ by $\widehat{f}(\alpha) = 1$, the $\widehat{f}$-perimeter is the ordinary perimeter of P. So, for this particular isomperimetric function, Question 6 is the classic isoperimetric problem, but for polyominoes. The solution, in this case, can be easily obtained using a result of Harary and Harborth [9].

Theorem 7. *The minimum perimeter over all simple polyominoes of area n is $2\lceil 2\sqrt{n}\,\rceil$.*

Proof. Let $e(P)$ denote the total number of edges of P, $e(\partial P)$ the number of edges on ∂P, i.e., the perimeter of P, and $e(P^o)$ the number of edges of P not on the boundary. Let $n = |P|$. Summing the four edges of each square of P results in the equality

$$4n = 2\,e(P^o) + e(\partial P) = 2e(P) - e(\partial P).$$

The first equality in the following equation is from [9, Theorem 2]:

$$2n + \lceil 2\sqrt{n}\,\rceil = \min\{e(P) : |P| = n\} = \frac{1}{2}\big(4n + \min\{e(\partial P) : |P| = n\}\big).$$

Therefore

$$\min\{e(\partial P) : |P| = n\} = 2\,\lceil 2\sqrt{n}\,\rceil. \qquad \square$$

Remark 8. There is usually not a unique optimum polyomino in Theorem 7. For example, Figure 3 shows four optima for $n = 7$. In general it can be shown that all optimum solutions for a given n are contained in a rectangular portion of the grid G_1 with dimensions either $m \times m$, $m \times (m-1)$, or $(m-1) \times (m+1)$, where $m = \lceil \sqrt{n}\,\rceil$. So, an optimum polyomino is, very loosely, almost a square.

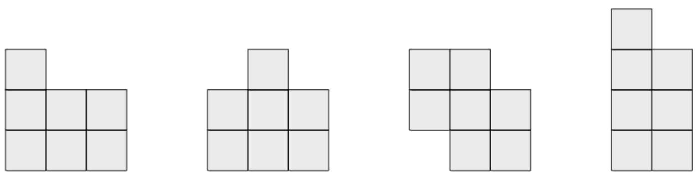

Figure 3: Optimal polyominoes for Question 6 with $n = 7$.

Remark 9. Discrete isoperimetric problems on the grid date back at least to the previously mentioned 1976 paper [9]. The authors of that paper refer to a finite set of regular polygons of the regular square, triangular or hexagonal tilings of the plane as an "animal", and their results concern certain"extremal animals". The tiling of *type* (p, q), $(p-2)(q-2) \geqslant 4$, is the regular tiling by p-gons, q incident at each vertex, of the Euclidean or hyperbolic plane. Recently G. Malen, E Roldán, and R. Toalá-Enríquez have investigated extremal (p, q)-animals [14]. In particular, they find for each such (p, q) an animal that minimizes the perimeter for a given number of tiles. An explicit formula for the minimum perimeter, as a function of the number of tiles in the animal, appears in [18]. This generalizes Theorem 7 to the hyperbolic case.

For a given isoperimetric function $\widehat{f}$ and a given natural number n, denote the minimum $\widehat{f}$-perimeter over all polyominoes of area n by

$$m_{\widehat{f}}(n) := \min\{f(P) : |P| = n\}.$$

Theorem 7 can be restated as follows. If the isoperimetric function $\widehat{f} : A \to \mathbb{R}$ is defined by $\widehat{f}(\alpha) = 1$ for all $\alpha \in A$, then $m_{\widehat{f}}(n) = 2\lceil 2\sqrt{n}\,\rceil$. The following corollary is broader than Theorem 7 in that it applies to a certain infinite family of isoperimetric functions. Although it does not seem immediately to generalize, it would be worth pursuing similar results for other infinite families of isoperimetric functions.

Corollary 10. *If the isoperimetric function* $\widehat{f} : A \to \mathbb{R}$ *is*

$$\widehat{f}(\pi/2) = a, \quad \widehat{f}(\pi) = b, \quad \textit{and} \quad \widehat{f}(3\pi/2) = c, \tag{2}$$

where (a, b, c) *is any point on the plane* $x - 2y + z = 0$ *in* $\mathbb{R}^3$*, then*

$$m_{\widehat{f}}(n) = 2b\lceil 2\sqrt{n}\,\rceil + 4(a-b).$$

Proof. Define functions $\widehat{f_1} : A \to \mathbb{R}$ and $\widehat{f_2} : A \to \mathbb{R}$ as follows. Let $\widehat{f_1}(\alpha) = 1$ for all $\alpha \in A$, and let $\widehat{f_2}(\alpha) = i$ where $\alpha = i\pi/2$, $i = 1, 2, 3$. Let P by a polyomino and let p denote the perimeter of P. Because the sum of the internal angles of P is $(p-2)\pi$, we have $f_1(P) = p$. Also, if P has c_i internal angles of size $i\pi/2$, $i = 1, 2, 3$, then $c_1\pi/2 + c_2\pi + c_3 3\pi/2 = (p-2)\pi$, i.e., $f_2(P) = c_1 + 2c_2 + 3c_3 = 2(p-2)$. The plane $x - 2y + z = 0$ is spanned by the vectors $(1, 1, 1)$ and $(1, 2, 3)$. Hence $(a, b, c) = r(1, 1, 1) + s(1, 2, 3)$ for some r, s. Therefore $f = rf_1 + sf_2$ and consequently

$$f(P) = rf_1(P) + sf_2(P) = rp + 2s(p-2) = (r+2s)p - 4s = bp + 4(a-b).$$

Therefore, if $b \neq 0$ then $f(P)$ is minimized if only if p is minimized. According to Theorem 7, that minimum is $p = 2\lceil 2\sqrt{n}\,\rceil$. Therefore, whether or not $b = 0$, we have $m_{\widehat{f}}(n) = 2b\lceil 2\sqrt{n}\,\rceil + 4(a-b)$. □

Theorem 11 below gives the relationship between the graph theoretic Question 1 and the polyomino isoperimetric Question 6 - in other words between $M(n)$, the maximum number of edges in an induced subgraph of G_2 of order n, and $m_{\widehat{f}}(n)$, the minimum $\widehat{f}$-perimeter of a simple polyomino of area n for an appropriate isoperimetric function $\widehat{f}$.

Theorem 11. *If the isoperimetric function* $\widehat{f} : A \to \mathbb{R}$ *is defined by*

$$\widehat{f}(3\pi/2) = 1, \qquad \widehat{f}(\pi/2) = \widehat{f}(\pi) = 3, \tag{3}$$

then

$$M(n) = 4n - \frac{1}{2}m_{\widehat{f}}(n) + 2.$$

The proof of Theorem 11 appears in Section 3. Theorem 11, in turn, will be used in Section 4 to prove Conjecture 2. Some open problems appear in Section 5.

3 Proof of Theorem 11

Definition 12 (Dual Polyomino)**.** Let H be the induced subgraph of a set of n vertices of the grid G_2. The *dual polyomino* $P := P(H)$ of H is obtained by replacing each vertex $u \in V(H)$ by a unit square centered at u. Translating by $\sqrt{2}/2$ along the diagonal, $P(H)$ can be considered as a finite subset of squares of the grid G_1. Note that $|P(H)| = n$. Figure 4 is an example of a graph H and its dual. The dual polyomino $P(H)$ may not be simple, but it will be shown in Lemma 13 that if H realizes the maximum in Question 1, then $P(H)$ must be simple.

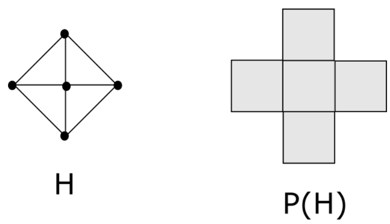

Figure 4: A graph H and its dual $P(H)$.

The mapping $H \mapsto P(H)$ has an inverse $P \mapsto H(P)$. Given a polyomino P, the vertex set of $H(P)$ is the set of centers of the squares in P (shifted to coincide with vertices of G_2), and $H(P)$ is the induced subgraph of G_2 with respect to this vertex set. This provides a bijection between the induced subgraphs of G_2 of order n and the set of polyonimoes in G_1 of area n.

For a graph G denote the number of edges by $e(G)$. Define an induced subgraph H of G_2 of order n as a *maximizing graph* if $e(H') \leqslant e(H)$ for all subgraphs H' of G_2 of order n.

Lemma 13. *For every n, there is a maximizing graph H such that $P(H)$ is a simple polyomino.*

Proof. For a given n, assume that H is a maximizing graph. Referring to Definition 4 and Figure 2, if $P := P(H)$ is not simple than either

1. P is disconnected,

2. P is not simply connected, or

3. P has a cut point.

We will show that, in each case, H is not maximizing.

Concerning condition (1), assume that $P := P(H)$ is not connected and let P_1 be a connected component and $P_2 = P \setminus P_1$. Let e_1 be an edge of ∂P_1 with the smallest y-coordinate, and e_2 an edge of ∂P_2 with the largest y-coordinate. Translate P_1 so that e_1 coincides with e_2. Let P_1' denote the translated P_1; let $P' = P_1' \cup P_2$; and let $H' = H(P')$. Then $e(H') > e(H)$, contradicting that H is a maximizing graph.

Concerning condition (2) in Definition 4, if $n \geqslant 3$, then it is easy to see that a maximizing graph H has no vertices of degree 1. Let K be any maximal 2-connected subgraph of H. As a planar graph, K has an outer face whose boundary is a simple (no self-intersection) polygon $Q(K)$. If, for all maximal 2-connected subgraphs K of H, all vertices of G_2 inside $Q(K)$ are contained in K, then $P(H)$ is simply connected. So assume that there is a maximal 2-connected subgraph K of H and $\overline{K}$ is the subgraph of G_2 induced by the nonempty set of vertices of G_2 that lie inside $Q(K)$ but do not lie in K. Let $e(K)$ denote the number of edges in K, $e(\overline{K})$ the number of edges in $\overline{K}$, $e(K, \overline{K})$ the number of edges from a vertex in K to a vertex in $\overline{K}$, and $e(\widehat{K})$ the number of edges in the subgraph $\widehat{K}$ of G_2 induced by all the vertices on or inside $Q(K)$. Similarly, let $n(K)$, $n(\overline{K})$, and $n(\widehat{K})$ denote the number of vertices in these subgraphs of G_2. Then

$$n(K) = n(\widehat{K}) - n(\overline{K}) \qquad \text{and} \qquad e(K) = e(\widehat{K}) - e(\overline{K}) - e(K, \overline{K}). \tag{4}$$

In G_2 consider a translation of $\overline{K}$ by a vector (a, b), $a, b \in \mathbb{Z}$, such that all vertices of the translated subgraph $\overline{K}'$ remain on or inside $Q(K)$ and at least one vertex of $\overline{K}'$ lies on $Q(K)$. Let K' be the subgraph of G_2 induced by the vertices of $\widehat{K} - \overline{K}'$. According to Equation 4,

$$n(K') = n(\widehat{K}) - n(\overline{K}') = n(\widehat{K}) - n(\overline{K}) = n(K)$$

and

$$\begin{aligned} e(K') &= e(\widehat{K}) - e(\overline{K}') - e(K', \overline{K}') = e(\widehat{K}) - e(\overline{K}) - e(K', \overline{K}') \\ &> e(\widehat{K}) - e(\overline{K}) - e(K, \overline{K}) = e(K). \end{aligned}$$

The inequality in the formula above is because there is at least one edge included in $e(K, \overline{K})$ that is not edges included in $e(K', \overline{K}')$; hence $e(K, \overline{K}) > e(K', \overline{K}')$. Replacing K by K' in H results in a graph H' that contradicts the maximality of H. Therefore $P(H)$ is simply connected.

Concerning condition (3) assume, by way of contradiction, there are two distinct squares s, s' whose intersection is a single vertex v. Since we have already proved that $P(H)$ is simply connected, the vertex v must be a cutpoint of $P(H)$. Now an argument like that used to prove condition (1) shows that H is not maximum, a contradiction. □

Because of Lemma 13 and for simplicity of exposition, from here the term polyomino will mean simple polyomino.

Proof of Theorem 11. In the proof the isoperimetric function $\widehat{f}: A \to \mathbb{R}$ will be as in Equation (3). For an induced subgraph H of G_2, let $e(H)$ denote the number of edges in H and $e_d(H)$ the number of diagonal edges in H. Let $P := P(H)$ be the dual polyomino. The order of H is n, which is also the number of squares in $P(H)$. Let $e(P)$ denote the number of edges of P, and $e(\partial P)$ the number of edges on the boundary of P. Let $s(\partial P)$ be the number of vertices on the boundary of P subtending an internal angle of $3\pi/2$ and let $t(P)$ be the number of vertices of P not on its boundary, i.e., internal vertices. We have

$$e_d(H) = 2t(P) + s(\partial P), \tag{5}$$

because there is a diagonal edge in H if and only if there is a corresponding boundary vertex of P with internal angle $3\pi/2$ or a corresponding internal vertex of P where two diagonal edges of H cross,

$$e(H) - e_d(H) = e(P) - e(\partial P), \tag{6}$$

because for each horizontal (vertical) edge e of H there is a corresponding vertical (horizontal) internal edge of P that crosses e, and

$$4n = 2e(P) - e(\partial P). \tag{7}$$

Pick's theorem for the area of a polygon [15] gives

$$n = t(P) + \frac{1}{2}\, e(\partial P) - 1. \tag{8}$$

Equations 5 and 8 imply

$$e_d(H) = 2n + 2 - e(\partial P) + s(\partial P). \tag{9}$$

Equations 6 and 9 imply

$$e(H) = e(P) - 2e(\partial P) + 2n + s(\partial P) + 2. \tag{10}$$

Equations 7 and 10 imply

$$\begin{aligned} e(H) &= 4n - \frac{3}{2}e(\partial P) + s(\partial P) + 2 = 4n - \frac{1}{2}\big(3\, e(\partial P) - 2\, s(\partial P)\big) + 2 \\ &= 4n - \frac{1}{2}\Big(\big(3\, e(\partial P) - 3\, s(\partial P)\big) + s(\partial P)\Big) + 2 = 4n - \frac{1}{2}\, f(P) + 2. \end{aligned}$$

Now

$$\begin{aligned} M(n) &= \max\{e(H) : |V(H)| = n\} = \max\{4n - \frac{1}{2}\, f(P(H)) + 2 : |P(H)| = n\} \\ &= 4n - \frac{1}{2}\, \min\{f(P(H)) : |V(H)| = n\} + 2 = 4n - \frac{1}{2}\, \min\{f(P) : |P| = n\} + 2 \\ &= 4n - \frac{1}{2}\, m_{\widehat{f}}(n) + 2. \end{aligned}$$

The second to last equality is a consequence of Lemma 13 and the fact that duality is bijective. ☐

4 Proof of Conjecture 2

The possible internal angles at a vertex of the boundary of a polyomino P are $\pi/2, \pi$, or $3\pi/2$. Traversing the vertices of the boundary of P clockwise let $C = (\alpha_0, \alpha_1, \ldots, \alpha_k = \alpha_0)$ be the circular sequence of angles $\pi/2$ and $3\pi/2$ - ignoring those of angle π.

In this section the isoperimetric function $\widehat{f} : A \to \mathbb{R}$ will always be as in Equation (3).

Lemma 14. *For every (simple) polyomino P of area $n \geqslant 1$ that minimizes the $\widehat{f}$-perimeter, the circular sequence C defined above contains no two consecutive terms $3\pi/2$.*

Proof. Let P be a polyomino that minimizes $\{f(Q) : |Q| = n\}$, i.e., minimizes the $\widehat{f}$-perimeter. For each pair u, v of vertices on ∂P corresponding to two consecutive $3\pi/2$ angles in the circular sequence C, call the line segment of length say j, along ∂P joining u and v a *gap* of size j. Denote sum of all gap sizes in P by $g(P)$. Let e_u be the edge on ∂P incident to u, not on the gap, and e_v the edge on ∂P, not on the gap, incident to v. Call these two edges the *walls* of the gap. On the left in Figure 5, P has a single gap of size 2. The gap and its two walls are shown by thick lines in the figure.

Let W be the dual of P in the graph theoretic sense (not Definition 12). Specifically, there is a vertex of W at the center of each square of P and two vertices of W are joined by a edge (straight line segment) if the two corresponding squares share an edge. Thus W can be considered as a subgraph of the grid G_1. Figure 6 shows a polyhedron P and below in red the graph W. We claim that W contains no vertex of degree 1. Otherwise, let w be such a vertex and s_w the corresponding square of P. Remove s_w from P and add a square to P, formerly not in P, at a position where a gap meets one of its walls. (Note that, even if removing s_w eliminates a wall, the other wall remains.) The resulting polyomino P' remains simple and it is easy to check that $f(P') < f(P)$, contradicting the minimality of P. In Figure 5 any one of the three gray squares can serve as s_w. If the leftmost gray square is chosen as s_w, then P' is shown in the middle figure. If the top left gray square is chosen as s_w, then P' is shown in the right figure.

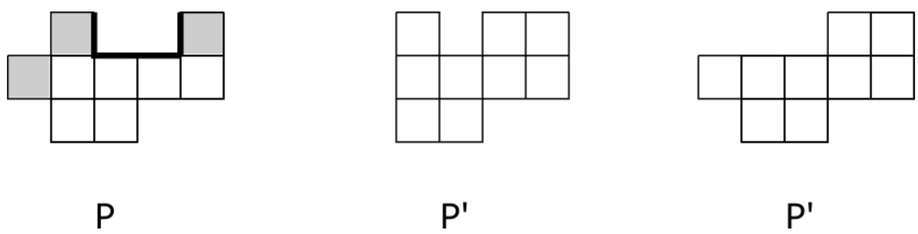

Figure 5: Illustration for the proof of Lemma 14.

Let B be an end block (a block containing at most one cut vertex of W) of the graph W. Since W has no vertex of degree 1, the block B does not consist of just a single edge. Since B is a plane graph and has no cut vertex, its outer boundary ∂B is a simple cycle γ. In Figure 6, W, shown in red, has two end blocks, both 4-cycles. All the vertices of G_1 inside γ are vertices of B; otherwise P is not simply connected, in particular, not simple.

Now consider the set Q of squares of P corresponding to the vertices of B. Then Q must be a simple polyomino, and the consecutive edges of ∂Q, except possibly one, say e, are consecutive edges of ∂P. Moreover, there is no square of Q that has all four of its vertices on ∂P, as is the case, for example, with the gray square in Figure 6. Because there are four more internal angles $\pi/2$ than angles $3\pi/2$ in Q, there must be two consecutive $\pi/2$ angles, not including the angles at the two vertices of B incident with edge e. Thus there are two consecutive $\pi/2$ internal angles of P. Let v be a vertex corresponding to one of the $\pi/2$ angles of such a pair, and let s_v be the square of P containing v. In Figure 6, for example, the red square is such a square.

We must show that if C has two consecutive $3\pi/2$ terms, then P does not minimize the $\widehat{f}$-perimeter. We will prove this by induction on $g(P)$. If $g(P) = 1$, then remove square s_v from P and add a square to P, formerly not in P, at a position where a gap meets one of its walls. The resulting polyomino P' remains simple. This is a consequence of the fact proved in the preceeding paragraph - that there is no square of Q that has all four of its vertices on ∂P. The technical aspects of the proof in the paragraph above is simply to insure that such a square, like the gray one in Figure 6, is not the one removed from P. If the gray square is removed, then the resulting polyomino would not simple because the top left vertex of the gray square would be a cut point of the polyomino P. In Figure 6 the square s_v is in red and P' is shown on the right. Now it is easy to check that either

1. $f(P') < f(P)$, or
2. $f(P') = f(P)$ and $g(P') < g(P)$.

In the first case we are done because P does not minimize the $\widehat{f}$-perimeter. In the second case, by the induction hypothesis, P' and thus also P, does not minimize the $\widehat{f}$-perimeter. $\square$

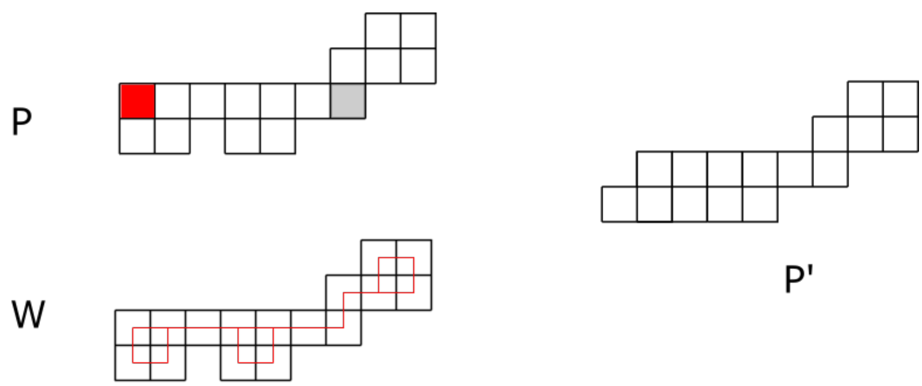

Figure 6: Illustration for the proof of Lemma 14.

Corollary 15. *Let P be a polyomino of area $n \geqslant 1$ that minimizes the $\widehat{f}$-perimeter. In the circular sequence C there are exactly four consecutive pairs $(\pi/2, \pi/2)$; all other consecutive pairs are $(\pi/2, 3\pi/2)$ or $(3\pi/2, \pi/2)$.*

Proof. Let a denote the number of $\pi/2$ angles and b the number of $3\pi/2$ angles. The formula for the sum of the angles of a polygon yields $a\pi/2 + 3b\pi/2 = (a + b - 2)\pi$, equivalently $a = b+4$. This implies that there are exactly four consecutive pairs $(\pi/2, \pi/2)$ in C.

The second statement follows immediately from the first and from Lemma 14. □

Corollary 15 provides the following information about a polyomino P that, for a given n, realizes the minimum of the $\widehat{f}$-perimeter. There is a smallest bounding rectangle R with horizontal and vertical sides that contains P. There are vertices l_1, l_2 of ∂P that lie on the left side of R and vertices r_1, r_2 and the right side. Likewise, there are vertices b_1, b_2 on the bottom and t_1, t_2 on the top. Traversing the boundary of R clockwise, the points $l_1, l_2, t_1, t_2, r_1, r_2, b_1, b_2$ satisfy the following properties:

1. The intersection of P with the left side of R is the line segment $\overline{l_1\, l_2}$; the intersection of P with the right side of R is the line segment $\overline{r_1\, r_2}$. The intersection of P with the bottom side of R is the line segment $\overline{b_1\, b_2}$. The intersection of P with the top side of R is the line segment $\overline{t_1\, t_2}$.

2. The part of ∂P joining l_2 and t_1, joining t_2 and r_1, joining r_2 and joining b_1, and joining b_2 and l_1 will be called the four *diagonal sections* of ∂P. The angles of P on a diagonal portion, ignoring angles π, alternate between $\pi/2$ and $3\pi/2$. (It may occur that $l_2 = t_1$.) Similarly for the diagonal sections of ∂P joining t_2 and r_1, joining r_2 and b_1, and joining b_2 and l_1. If the angles at the vertices of ∂P in a diagonal section alternate between $\pi/2$ and $3\pi/2$ with no angles π, then that diagonal section will be called a *staircase*.

Figure 7 shows a typical case. The diagonal section at the lower left is a staircase.

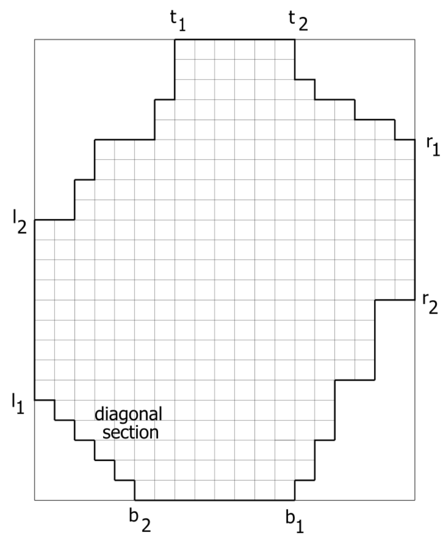

Figure 7: A polyomino satisfying the properties of Lemma 14 and Corollary 15.

Consider any diagonal section, say the one at the lower left, and position P so that the lower left corner of the bounding rectangle R is located at the origin. Let c be the least integer such $W =: L \cap \partial P \neq \emptyset$, where L is the line $x + y = c$. The set O of squares of P that have a vertex on L will be called the *outer layer* of P in the diagonal section. If every vertex of G_1 that lies on L is a vertex of O, then that diagonal section is a staircase. If there is a vertex of G_1 that lies on L that is not a vertex of O, then O will be called an *incomplete outer layer*. Define a *vacant space* in the diagonal section as a square not in P that has its upper right vertex on ∂P. In Figure 8 the dark squares are the outer layer, the one on the left complete and the one on the right incomplete with two vacant spaces. We have used the lower left diagonal section as an example, but the same concepts hold for all four diagonal sections.

It is shown in the next two lemmas that there exists a polyomino P that realizes the minimum $\widehat{f}$-perimeter and that satisfies various geometric properties.

Lemma 16. *For any $n \geqslant 1$ there is a polyomino P of area n that realizes the minimum $\widehat{f}$-perimeter and has the following properties.*

1. *Every diagonal section of ∂P, except possibly one, is a staircase.*
2. *On the one possible exception, if the incomplete outer layer O of squares is removed, then the boundary of the resulting polyomino in that diagonal section is a staircase.*
3. *On the one possible exception, the incomplete outer layer O is a connected set.*

Proof. We again use the lower left diagonal section for ease of explanation, but the following holds for all four diagonal sections.

Let L_i be the line $x + y = c + i$, $i \geqslant 0$. A vertex on ∂P that lies on the line L_i will be referred to as *type* i. The maximum type of a vertex on ∂P will be called the *type* of the diagonal section. Of all polyominoes that realizes the minimum $m_{\widehat{f}}(n)$ of the isoperimetric function $\widehat{f}$, consider one that minimizes the type of the diagonal section. And of all those that minimize the type, consider one that minimizes the number of verticies on ∂P of that type. Let P be such a polyomino. We claim that every vertex of ∂P lies on $L = L_0, L_1$ or L_2. That would also imply statement (2) of the lemma. The lines L, L_1, L_2 are shown in red in Figure 8.

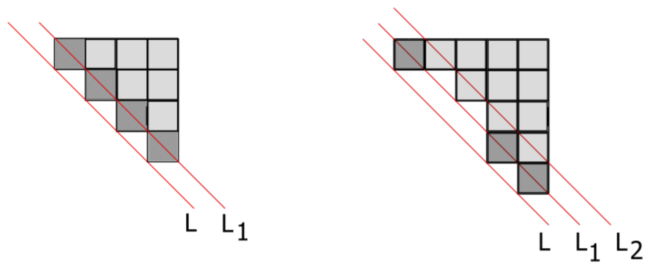

Figure 8: Complete and incomplete outer layers (dark gray) for the lower left diagonal section.

To prove the claim, call a vertex on ∂P with angle $\pi/2$ or $3\pi/2$ *improper* if at least one of the vertices on ∂P adjacent to it has angle π. Let v be a vertex of ∂P of largest type, and assume by way of contradiction that v has type at least 3. There must be such a vertex that is improper and it must have internal angle $3\pi/2$. There also must be an improper vertex u of ∂P on L. Let s be the square in P with vertex u. Remove s from P and add a square to P at the vacant space incident to v. Call the resulting polyomino P'. This is illustrated in the left column of Figure 9. The gray square at vertex u (top figure) is removed and a square is placed at the vacant space at v as shown in the bottom figure. It is easy to check that $f(P') \leqslant f(P)$, contradicting either the minimality of $m_{\widehat{f}}(n)$ or contradicting the minimality of the type. This proves the claim.

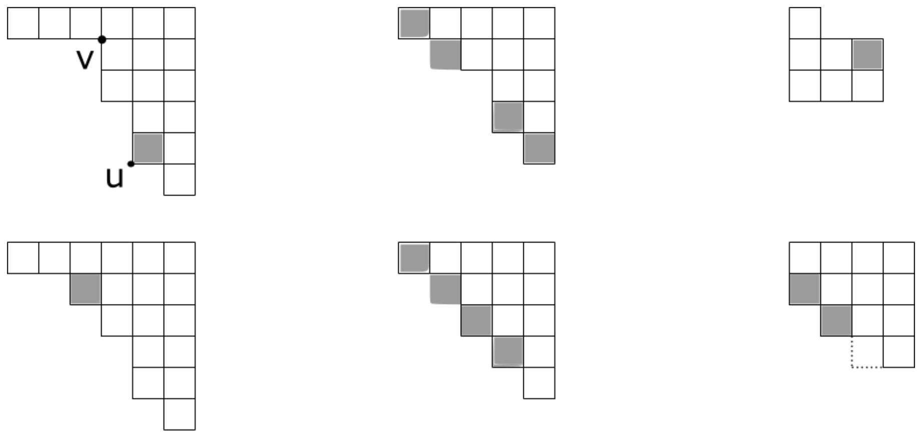

Figure 9: Illustrating the steps in the proof of Lemma 16.

Concerning statement (3) of the lemma, let O be an incomplete outer layer of squares in a diagonal section. By way of contradiction, assume that O_1 and O_2 are nonempyty sets of squares in two connected components of O, with no other connected component of O between them along the diagonal. Label consecutive vertices of G_1 on L (from bottom to top) by $x_1, x_2, \ldots, x_m$ so that $x_1, x_2, \ldots, x_i$ are all the vertices of squares in O_1 and $x_{j+1}, x_{j+2}, \ldots, x_m$ are all the vertices of O_2 with $1 \leqslant i < j \leqslant m$. Now remove O_1 from P and add an equal number of outer layer squares at vacant spaces incident with vertices at $x_{j-i+1}, x_{j-i+2}, \ldots, x_j$. In other words, shift O_1 along the diagonal so that the union of these shifted squares and O_2 is connected. This is illustrated in the middle column of Figure 9. If P' is the resulting polyomino, then it is routine to check that $f(P') < f(P)$, which contradicts the minimality of the $\widehat{f}$-perimeter. In the top figure the incomplete outer layer is disconnected. Two squares are shifted up to form a connected outer layer as shown in the bottom figure.

Concerning statement (1) of the lemma, for a polyomino P that satisfies statements (2) and (3) in the lemma, of the four possible outer layers, let O be an outer layer with the least number of squares. If the outer layers in the other diagonal sections are staircases, then statement (1) is true. Otherwise, consider another diagonal section with an incomplete layer O'. The squares in O form a connected chain. Remove from P a square of O that is at the end of the chain. Add a square to P at a vacant space of the diagonal section containing O' and incident with a square of O'. This is illustrated in the right column of Figure 9. In the top figure the incomplete outer layer O of the upper right diagonal section consists of a single gray square. The square is removed and a square is placed at the vacant space in the lower left diagonal section indicated by the dotted lines in the bottom figure. The added square becomes part of the outer layer of the lower left diagonal section. A routine calculation shows that the resulting polyomino P' is such that $f(P') = f(P)$, contradicting the minimality of O. $\square$

Define the *length* of a diagonal section of ∂P as the number of $3\pi/2$ angles on the staircase after the incomplete outer layer, if there is one, is removed. Denote these lengths by d_1, d_2, d_3, d_4. Note that $d_i = 0$ is possible.

In Figure 10 both polyominoes satisfy the properties in Lemma 16. The polyomino on the left has no incomplete outer layer of squares; all four diagonal sections of the boundary are staircases. In the polyomino on the right, the sole connected incomplete outer layer is shown in red. In the right polyomino all four diagonal sections have length 3. In the left polyomino, the lengths are $0, 1, 2, 2$.

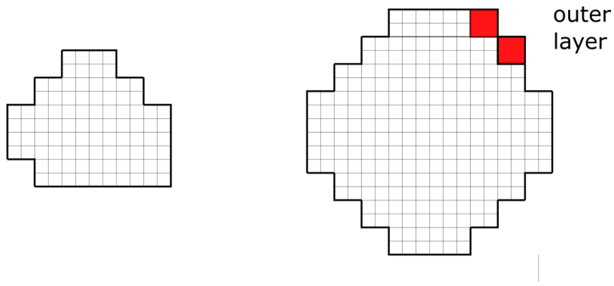

Figure 10: Polyominoes that satisfy the properties in Lemma 16

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Lemma 17. *There is a polyomino P that realizes the minimum $m_{\widehat{f}}(n)$ of the isoperimetric function f and has the following properties in addition to those in Lemma 16.*

1. *There is an integer D such that $d_i = D$ or $d_i = D + 1$ for $i = 1, 2, 3, 4$.*

2. *The number of squares in the incomplete outer layer, if it exists, is at most D.*

Proof. Statement (2) follows from statement (1). Concerning statement (1), among the polyominoes that realize the minimum of the $\widehat{f}$-perimeter and satisty the properties in Lemma 16, choose one that minimizes the difference $d := \max\{d_1, d_2, d_3, d_4\} - \min\{d_1, d_2, d_3, d_4\}$ and of those choose one that mnimizes the number of diagonal sections with smallest length. Call such a polyomino P_0.

Let d_i and d_j be the smallest and largest, respectively, of the lengths of the diagonal sections of P_0, and call the corresponding diagonal sections the i and j diagonal sections. If there is an incomplete outer layer O in P_0 and it is not in diagonal section j, then remove O from P_0 and add an equal number of squares to P_0 at consecutive vacant spaces in the diagonal section j. Call the resulting polynomino P. It is easy to check that this can be done so that $f(P) = f(P_0)$. If there is an incomplete outer layer in P, it is now in a diagonal section of greatest length.

If $d < 2$, then statement (1) is true. Otherwise, remove from P all squares of the outer layer O of complete diagonal section i; let m be the number of squares of O. Now add squares, at most m, to as many vacant spaces of diagonal section j as possible insuring that the new outer layer of diagonal section j is connected. If m is greater than the number m' of vacant spaces, then add $m - m'$ squares to consecutive vacant spaces of the diagonal section that now has largest length. Call the resulting polyomino P'. Note that $|P'| = |P|$. If O contains a square with three edges on ∂P, then it is easy to verify that $f(P') < f(P)$, contradicting the minimality of the $\widehat{f}$-perimeter. Since O contains no square with three edges on ∂P, removing O from P does not change the length of the other three diagonal sections. For the case where O contains no square with three edges on ∂P it is easy to check that $f(P') = f(P)$. Let d'_i, $i = 1, 2, 3, 4$, be the lengths of the corresponding diagonal sections of P'. Note that $d'_i = d_i + 1$, contradicting the minimality of d or the minimality of the number of diagonal sections with smallest length. □

Theorem 18. *If $M(n)$ is the maximum number of edges in an induced subgraph of G_2 of order n, then*

$$M(n) = 4n - \left\lceil \sqrt{28n - 12}\, \right\rceil.$$

Proof. Assume that P is a polyomino that minimizes $f(Q)$ over all polyominoes with $|Q| = n$. Recall that P has the properties stated in Lemmas 16 and 17. Let q be the number of squares in the single incomplete outer layer, if there is one. Let A and B be the length and width of the bounding rectangle of P. Consider two cases: (1) $q = 0$ and (2) $q > 0$.

Case 1. The area of the bounding rectangle is AB and $(d_i^2 + d_i)/2$ is the area within the bounding rectangle but not in P in diagonal section $i, i = 1, 2, 3, 4$. Therefore

$$n = |P| = AB - \frac{1}{2}\sum_{i=1}^{4}(d_i^2 + d_i).$$

In calculating $f(P)$, the contribution from boundary points on each diagonal section is $d_i + 3(d_i - 1)$, $i = 1, 2, 3, 4$. The contribution from boundary points on the bounding rectangle is $3(2A - \sum_{i=1}^{4} d_i + 2) + 3(2B - \sum_{i=1}^{4} d_i + 2)$. Thus the total is

$$f(P) = 6(A + B) - 2\sum_{i=1}^{4} d_i.$$

With n fixed, consider the problem of minimizing the function

$$F := F(A, B, d_1, d_2, d_3, d_4) = 6(A + B) - 2\sum_{i=1}^{4} d_i$$

subject to the constraint $n = AB - \frac{1}{2}\sum_{i=1}^{4}(d_i^2 + d_i)$. Regard this as an optimzation problem over the reals. Assume first that A, B, as well as n, are fixed. The problem is then to maximize $\sum_{i=1}^{4} d_i$ given the value of $\sum_{i=1}^{4}(d_i^2 + d_i)$. It follows from the Cauchy-Schwarz inequality that this maximum is achieved when $d := d_1 = d_2 = d_3 = d_4$, in which case

$$n = AB - 2(d^2 + d) \qquad\qquad F = 6(A + B) - 8d. \tag{11}$$

Letting $C := 2d + 1$ we have

$$n = AB - \frac{1}{2}C^2 + \frac{1}{2} \qquad F = 6(A + B) - 4C + 4 = 2(3A + 3B - 2C) + 4. \tag{12}$$

The problem is then to minimize $3A + 3B - 2C$ given that $AB - C^2/2 + 1/2 = n$. Using the Lagrange multiplier method yields

$$(3, 3, -2) = \lambda(2B, 2A, -2C) \qquad \text{and} \qquad 2n = 2AB - C^2 + 1,$$

giving a minimum when

$$A = B = \frac{3}{2}\sqrt{\frac{4n-2}{7}}, \quad C = \sqrt{\frac{4n-2}{7}},$$

which implies that

$$F \geqslant 14\sqrt{\frac{4n-2}{7}} + 4 = 2\sqrt{28n - 14} + 4.$$

Since the above bound holds over the reals, it must hold over the integers. Therefore,

$$f(P) \geqslant \lceil 2\sqrt{28n - 14}\, \rceil + 4.$$

Since $m_{\widehat{f}}(n)/2$ is an integer, we have

$$\frac{1}{2}m_{\widehat{f}}(n) \geqslant \lceil \sqrt{28n - 14}\, \rceil + 2.$$

By Theorem 11 this implies

$$M(n) \leqslant M_1(n) := 4n - \lceil \sqrt{28n - 14}\, \rceil. \tag{13}$$

Case 2. Proceed as in case 1 to minimize F over the reals. With n, A, B, q fixed we again deduce that $d := d_1 = d_2 = d_3 = d_4$. As in Equations (11) and (12) in case 1, we have

$$n = AB - 2(d^2 + d) + q \qquad\qquad F = 6(A + B) - 8d + 2.$$

The $+2$ in the formula for F above is from the addition of the incomplete outer layer, and notice that it does not depend on the number q of squares in incomplete outer layer. Again taking $C = 2d + 1$, we have

$$n - q = AB - \frac{1}{2}C^2 + \frac{1}{2} \qquad\qquad F = 6(A + B) - 4C + 6 = 2(3A + 3B - 2C) + 6.$$

With D as in Lemma 17, we have $q \leqslant D \leqslant d$. A similar use of the Lagrange mulitiplier method to that in case (1) yields

$$A = B = \frac{3}{2}\sqrt{\frac{4n-2-4q}{7}}, \quad C = \sqrt{\frac{4n-2-4q}{7}}.$$

Therefore

$$F = 6 + 2\sqrt{28n-14-28q}.$$

However,

$$q \leqslant d = \frac{1}{2}(C-1) = \frac{1}{14}\sqrt{28n-14-28q} - \frac{1}{2}.$$

Use the quadratic formula to obtain $q \leqslant (\sqrt{28n+1}-8)/14$, which implies that

$$f(P) \geqslant 6 + \left\lceil 2\sqrt{28n+2-2\sqrt{28n+1}}\, \right\rceil \quad \text{and} \quad \frac{1}{2}m_{\widehat{f}}(n) \geqslant 3 + \left\lceil \sqrt{28n+2-2\sqrt{28n+1}}\, \right\rceil.$$

By Theorem 11 this gives

$$M(n) \leqslant M_2(n) := 4n - 1 - \left\lceil \sqrt{28n+2-2\sqrt{28n+1}}\, \right\rceil.$$

Let $M_0(n) = 4n - \lceil \sqrt{28n-12}\, \rceil$. Referring to Equation (13) of Case (1), we have $M_1(n) = M_0(n)$ unless there is an integer m such that $\sqrt{28n-12} > m \geqslant \sqrt{28n-14}$, i.e., $28n-12 > m^2 \geqslant 28n-14$. Equivalently, $M_1(n) = M_0(n)$ unless either (a) $m^2 = 28n-14$ or (b) $m^2 = 28n-13$. In case (a), m must be even, hence m^2 is divisible by 4, hence 14 is divisible by 4, a contradiction. In case (b) m must be odd, i.e., $m = 2t+1$ for some integer t. Then $4t^2+4t+1 = 28n+4$ implies that 1 is divisible by 4, a contradiction. Therefore $M(n) \geqslant M_0(n) = M_1(n) \geqslant M(n)$ which implies $M(n) = M_0(n)$.

Referring to Equation (13), we leave to the reader the calculation showing that

$$4n - 1 - \sqrt{28n+2-2\sqrt{28n+1}} < 4n - \sqrt{28n-12},$$

hence $M_2(n) = 4n - 1 - \left\lceil \sqrt{28n+2-2\sqrt{28n+1}}\, \right\rceil \leqslant 4n - \lceil \sqrt{28n-12}\, \rceil = M_0(n)$. This implies $M(n) \geqslant M_0(n) \geqslant M_2(n) \geqslant M(n)$, which implies that $M(n) = M_0(n)$. Together with the lower bound in inequality (1), this gives $M(n) = M_0(n)$ in both case 1 and case 2. □

5 Open Problems

The analogs of a polyomino for unions of equilateral triangles and regular hexagons, rather than squares, are called polyiamonds and polyhexes, respectively; see Figure 11. The isoperimetric Question 6 can be posed for polyiamonds and polyhexes. For the polyiamond case the set of possible interior angles is $A = \{\pi/3, 2\pi/3, \pi, 4\pi/3, 5\pi/3\}$,

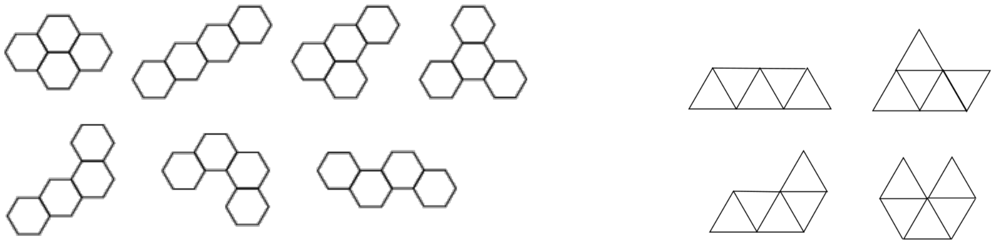

Figure 11: Polyhexes of order 4 and polyhiamonds of order 5.

and for the polyhex case $A = \{2\pi/3, 4\pi/3\}$. The polyhex case is easier as indicated by Theorem 19 below. The proof is essentially the same as for Theorem 10.

For a polyhex H, let n denote the number of hexagons in H, and let $\alpha(v)$ denote the internal angle of H at vertex $v \in \partial H$. Given an isoperimetric function $\widehat{f} : A \to \mathbb{R}$, define the $\widehat{f}$-*perimeter* of H by

$$f(H) = \sum_{v \in V(\partial H)} f\big(\alpha(v)\big).$$

Theorem 19. *If the isoperimetric function $\widehat{f} : A \to \mathbb{R}$ for polyhexes is*

$$\widehat{f}(2\pi/3) = a, \quad \textit{and} \quad \widehat{f}(4\pi/3) = b, \tag{14}$$

then

$$\min\{f(H) : H \textit{ is a polyhex with } |H| = n\} = (a+b)\left\lceil \sqrt{12n-3}\, \right\rceil + 3(a-b).$$

Theorem 19 provides a complete solution to the polyhex isoperimetric problem. Regarding the isoperimetric function (2) in Section 2 as a triple $(a, b, c) \in \mathbb{R}^3$, Corollary 10 provides a solution to the polyomino isomperimetric problem for all isoperimetric functions on a plane in $\mathbb{R}^3$.

Question 20. For which isoperimetric functions can the polyiamond isoperimetric problem be solved?

Question 21. Can the polyomino isoperimetric problem be solved for other isoperimetric functions, for example for values of (a, b, c) on planes in $\mathbb{R}^3$ in addition to the one in Corollary 10?

Questions 1 and 6 in Sections 1 and 2 can be generalized to higher dimensions. A higher dimensional question related to Theorem 7, for example, is the following, where a *polycube* is the 3-dimensional version of a polyomino.

Question 22. What is the minimum surface area, i.e., minimum number of squares on the surface, of a polycube consisting of n cubes?

The following continuous version of Question 6 generalizes the classical isoperimetric problem for the plane.

Question 23. Let $f : \mathbb{R} \to \mathbb{R}$ be a continuous function. Consider a smooth closed curve γ in the plane parametrized by arc length s and let $\kappa(s)$ be the curvature of γ. For a given area enclosed, what is the closed curve γ that minimizes the line integral $\int_\gamma f\big(\kappa(s)\big)\, ds$?

If $f(x) = 1$ for all x, then Question 23 is the classic isoperimetric problem, whose solution is a circle. It would be interesting to see how the minimal closed curve γ changes as f varies.

Acknowledgements

Thanks to Prof. Vince Vatter for bringing the landscape ecology question to my attention and to Prof. Kevin Keating for valuable conversations. The suggestions of the three referees resulted in a better paper.

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