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ORIGINAL PAPER

Counting symmetric and near-symmetric fullerene patches

Christina Graves · Stephen J. Graves

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Abstract We establish an exact method for drawing fullerene patches in the hexagonal tessellation of the plane. Using these embeddings, we then provide a closed form equation for the total number of symmetric and near-symmetric fullerene patches, up to isomorphism. The function depends only on parameters of the boundary code.

Keywords Fullerene · Fullerene patch · Boundary codes · Pseudoconvex patch · Nanocone

1 Introduction

A *fullerene* is a trivalent 2-connected plane graph with all faces hexagonal or pentagonal. A *fullerene patch* is a 2-connected plane graph with all faces hexagonal or pentagonal except one external face; all vertices not incident with the external face have degree three and those incident with the external face have degree two or three. The cycle bounding the external face is the *boundary* of the patch. Thus the *boundary code* is the sequence of degrees of vertices on the boundary in consecutive order, up to cyclic permutation or inversion. For instance, a pair of adjacent pentagons has boundary code 22232223, or equivalently $(2223)^2$.

Our interest is in a particularly nice type of fullerene patch. A patch is *pseudoconvex* if the boundary code does not contain consecutive 3's. Consecutive 3's on the boundary can be envisioned as a turn on the boundary "away from" the interior of the patch. An edge on the boundary incident with two 2-valent vertices is a *break edge*, and the

C. Graves (✉) · S. J. Graves
The University of Texas at Tyler, Tyler, TX 75799, USA
e-mail: cgraves@uttyler.edu

S. J. Graves
e-mail: sgraves@uttyler.edu

path on the boundary of a pseudoconvex patch between two break edges is a *side*. A pseudoconvex patch has boundary code $2(23)^{\ell_1}2(23)^{\ell_2}\cdots 2(23)^{\ell_k}$, and hence we say it has k sides with *lengths* $\ell_1, \ell_2, \ldots, \ell_k$. Following the notation of [5], a pseudoconvex patch with side lengths $\ell_1, \ell_2, \ldots, \ell_s$ has *side parameters* $[\ell_1, \ell_2, \ldots, \ell_s]$. A pseudoconvex patch with all sides of equal length is *symmetric*; a *near-symmetric patch* will have side parameters $[n, n+1, n+1, \ldots, n+1]$ for some nonnegative integer n. We will refer to a face incident with both an n-side and an $n+1$-side as an $(n, n+1)$-*corner*, and we similarly define an $(n+1, n+1)$-*corner*.

Boundary codes of fullerene patches have been extensively studied, and there have been many algorithms to determine if a specific boundary code is realizable as a patch (see [1,2,4]). In [5], it was shown that symmetric and near-symmetric patches exist for the following values of n and s:

- $s = 5$ and $n \geq 5$,
- $s = 4$ and $n \geq 2$,
- $s = 3$ and $n \geq 1$,
- $s = 2$ and $n \geq 1$ for symmetric patches,
- $s = 2$ and $n \geq 0$ for near-symmetric patches,
- $s = 1$ and $n \geq 0$, and
- $s = 0$ and $n \geq 0$ for symmetric patches.

These symmetric and near-symmetric patches are specifically of interest in the study of carbon nanocones, classified by Brinkmann and Van Cleemput [3]. In that article, the authors show that nanocones are in bijective correspondence with the set of symmetric and near-symmetric pseudoconvex fullerene patches, which they called *cone caps*. Further, Brinkmann and Van Cleemput provided an algorithm for generating all cone caps given the length of the shortest side. However, the algorithm is recursive in nature and no closed form for the number of patches as a function of minimum side length is provided via the algorithm.

This article is concerned with precisely that: to provide a constructive enumeration of pseudoconvex patches in order to give closed forms for the number of symmetric and near-symmetric patches. Unlike the algorithmic enumeration of [3], our construction is not recursive, and provides an exact value for the number of such patches as a function of the minimum side length n.

It suffices to determine the number of symmetric or near-symmetric patches with a pentagonal face on the boundary. If a patch does not have a pentagon on its boundary, it has some number of layers of hexagons before the first pentagonal face. Removing these layers of hexagons results in a symmetric or near-symmetric patch with shorter side lengths, as proven in [5]. We can then count all nonisomorphic patches on this "shorter" boundary inductively.

To this end, we provide a canonical method of embedding fullerene patches in the hexagonal tessellation of the plane, which we denote by Λ. Using this embedding and the geometry it provides, we determine an exact formula for the number of non-isomorphic symmetric and near-symmetric fullerene patches with two or three pentagonal faces, at least one of which is on the boundary.

Intuitively, we introduce a single pentagonal defect in the hexagonal tessellation Λ by identifying across a $60°$ sector with vertex at a face center. Carefully repeating

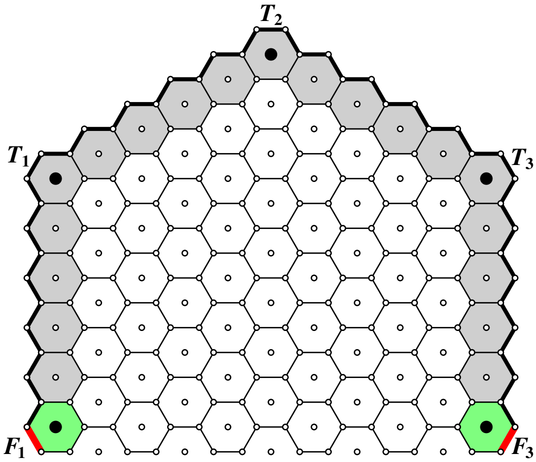


Fig. 1 The boundary of $[5, 5, 5, 5]$ in Λ

this process until twelve pentagonal faces are created produces a fullerene; we limit ourselves to patches with at most three pentagonal faces. We make the following definition for the purpose of easing notation.

Definition 1 We define ϕ_X to be a 60° counterclockwise rotation of the plane with center at X. Note that if X is a face center in Λ, then ϕ_X is an automorphism of Λ.

If X is a face center and Y is the center of an adjacent hexagon, we produce a defect at X by identifying vertices, faces, and edges across the sector between the rays XY and $\phi_X(XY)$. Hence the face with center X becomes a pentagon under the identification and all other resulting faces remain hexagonal.

2 Patches with 2 pentagonal faces

Drawing the patch in Λ

A patch Π with exactly two pentagonal faces will have side parameters $[n, n, n, n]$ if it is symmetric and $[n, n+1, n+1, n+1]$ if it is near-symmetric. Beginning with a break edge, we trace the boundary of Π in Λ. The boundary terminates with the same break edge. We label important faces on the boundary by their centers: F_1 is the initial face, T_1, T_2, and T_3 are the faces incident with the next three break edges in succession, and F_3 is the terminal face. See Fig. 1.

As we will identify F_1 and F_3 by the removal of two 60° sectors, we will (by the following lemma) demonstrate that the placement of the first pentagonal face uniquely determines the location of the second. Having determined the locations of P_1 and P_2, the removed sectors then are first between the ray P_1F_1 and P_1F_2, where $F_2 = \phi_{P_2}(F_1)$, and second between the rays P_2F_2 and P_2F_3.

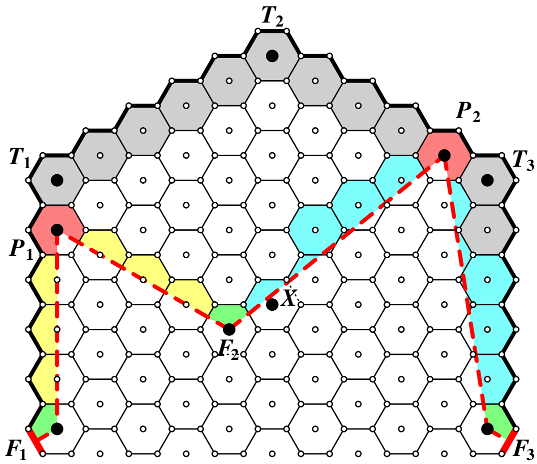


Fig. 2 A particular placement of P_1 and P_2

Lemma 1 *Given two distinct points F_1 and F_3 in a plane, let X be the unique point such that $\phi_X^2(F_1) = F_3$. Then for any point P_1, there is a unique point P_2 such that*

$$\phi_{P_2}\phi_{P_1}(F_1) = F_3.$$

Moreover, $\phi_X^{-2}(P_1) = P_2$.

Proof Suppose F_1, F_3, and P_1 are given. Let $F_2 = \phi_{P_1}(F_1)$, and let P_2 be the unique point such that $\phi_{P_2}(F_2) = F_3$. So then $\phi_{P_2}\phi_{P_1}(F_1) = F_3$, and $\phi_{P_2}\phi_{P_1}$ must be a counterclockwise rotation of 120° as a composition of rotations. Since $\phi_X^2(F_1) = F_3$ we have $\phi_X^2 = \phi_{P_2}\phi_{P_1}$, as both are rotations by the same angle carrying F_1 to F_3. Thus X is fixed by $\phi_{P_2}\phi_{P_1}$. Putting $X' = \phi_{P_1}(X)$, we observe that $\triangle P_1XX'$ is equilateral; similarly $\triangle P_2X'X$ is equilateral. Hence $\phi_X^2(P_2) = P_1$.

Let Π be a symmetric patch. Since there must be a pentagonal face on the boundary and all sides have the same length, we may assume without loss of generality that the first pentagon P_1 is centered on the line F_1T_1. Applying Lemma 1, the placement of P_1 uniquely determines the location of the second pentagonal face, P_2. The point X shown in Fig. 2 is the unique point such that $\phi_X^2(F_1) = F_3$. Moreover, $\phi_X^{-2}(F_1T_1) = T_2T_3$. Thus if P_1 is placed on the side of the boundary between F_1 and T_1, then P_2 will lie on the side between T_2 and T_3 (Fig. 3).

If Π is a near-symmetric patch with side-parameters $[n, n+1, n+1, n+1]$, there are three ways in which Π may be traced in Λ. We must consider whether the F_1T_1 side of the drawing is the n-side, an $(n+1)$-side adjacent to the n-side, or the other $(n+1)$-side, as we assume that P_1 will always be on F_1T_1. In the case where F_1T_1 is the n-side, we can quickly determine via Lemma 1 that placing P_1 on F_1T_1 requires that P_2 be outside the patch Π; this is shown in Fig. 4, where $F_1'T_1' = \phi_X^{-2}(F_1T_1)$.

Fig. 3 The patch from Fig. 2 with sectors removed

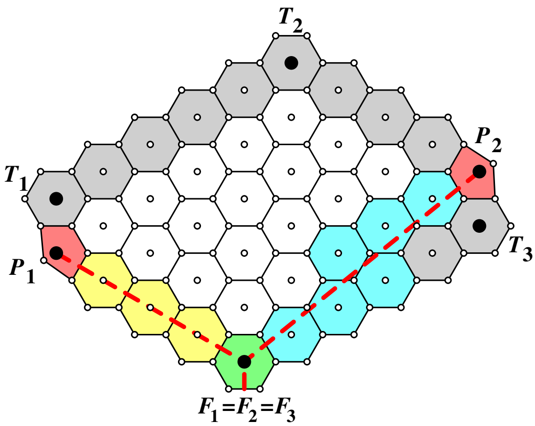
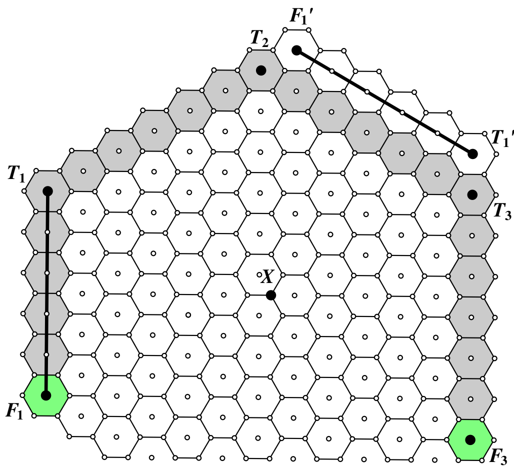


Fig. 4 A pentagon cannot lie on the n-side of a $[n, n+1, n+1, n+1]$-patch



Counting patches with exactly 2 pentagonal faces

To count the number of symmetric patches with side parameters $[n, n, n, n]$, we consider the embedding described in the previous section. There are $n+1$ hexagonal faces on F_1T_1 which are all valid locations for P_1. However, because all sides of this patch have length n, a pentagon on F_1T_1 at distance m from F_1 represents the same patch as one with a pentagon on F_1T_1 at distance m from T_1 via a reflection. Thus, we only count half of the positions for placement of P_1, and see that the total number of patches with side parameters $[n, n, n, n]$ is $\left\lceil \frac{n+1}{2} \right\rceil$.

The near-symmetric case is a little trickier. As seen in the previous section, there are no patches with side parameters $[n, n+1, n+1, n+1]$ with a pentagon on the side of length n. Now consider a patch Π with the same side parameters and a pentagon on an $(n+1)$-side adjacent to the n-side. We can draw Π in Λ by letting F_1T_1 be the side with the pentagon and T_1T_2 the side of length n. By Lemma 1, we see that if P_1 is distance m from F_1, then P_2 is distance $m+1$ from T_2. More importantly, P_2 is on the

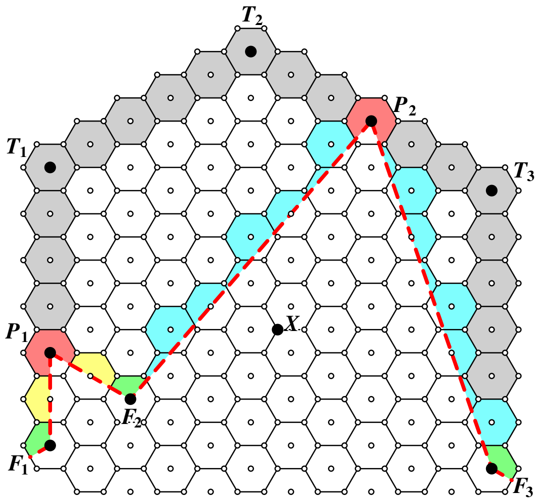


Fig. 5 A placement of P_1 on a $(n+1)$-side adjacent to an n-side

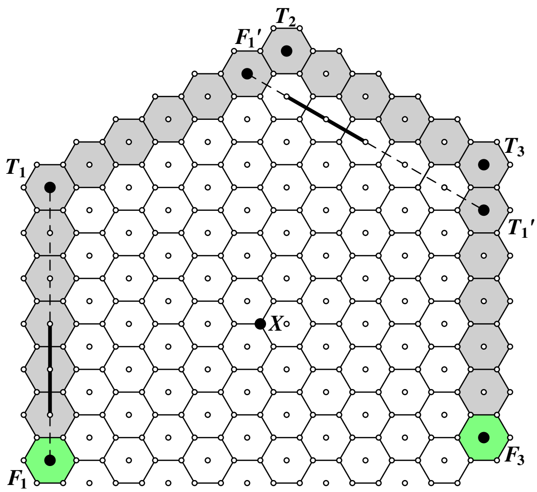


Fig. 6 P_1 may be placed at any hexagon center at distance $0 < m \leq \lceil \frac{n}{2} \rceil$ from F_1 on F_1T_1

boundary on the other $(n+1)$-side that is adjacent to the n-side. Because the side F_1T_1 can be mapped to T_2T_3 via a graph isomorphism, a patch with a pentagon distance m from F_1 is isomorphic to a patch with a pentagon distance m from T_3. Thus, we only count the patches where P_2 is distance at most $\lceil \frac{n-1}{2} \rceil$ from F_1; there are $\lceil \frac{n+1}{2} \rceil$ such patches; see Fig. 5.

Now consider a patch with the same side parameters $[n, n+1, n+1, n+1]$ but this time with a pentagon on the $(n+1)$-side that is not adjacent to the n-side. We again trace the boundary of the patch in Λ by letting F_1T_1 be the side with the pentagon and T_2T_3 the n-side. In this scenario, let $F_1'T_1' = \phi_X^{-2}(F_1T_1)$ as shown in Fig. 6. If P_1 is placed on F_1T_1, then P_2 will lie on $F_1'T_1'$. However, since F_1T_1 can be mapped to T_1F_1 via a graph isomorphism, we only consider placing P_1 distance at most $\lceil \frac{n}{2} \rceil$ from F_1. Finally, we note that if P_1 is placed on F_1, then the pentagon is on a corner and thus also on an $(n+1)$-side that is adjacent to the n-side; this patch was computed in the previous case. Thus, there are a total of $\lceil \frac{n}{2} \rceil$ more patches to count from this case that were not previously counted; see Fig. 6. Adding up the number of patches from both of these cases gives a total of $\lceil \frac{n+1}{2} \rceil + \lceil \frac{n}{2} \rceil = n + 1$ near-symmetric patches.

We summarize these results in the following proposition.

Proposition 1 *The number of non-isomorphic symmetric patches with side parameters $[n, n, n, n]$ and at least one pentagon on the boundary is $\left\lceil \frac{n+1}{2} \right\rceil$. The number of non-isomorphic near-symmetric patches with side parameters $[n, n+1, n+1, n+1]$ and at least one pentagon on the boundary is $n + 1$.*

3 Patches with 3 pentagonal faces

Drawing patches in Λ

Drawing a 2-pentagon symmetric or near-symmetric fullerene patch in Λ is straightforward compared to drawing a 3-pentagon patch; in the former, the placement of the second pentagonal face is wholly determined by the placement of the first. However, in the latter case there is an additional degree of freedom to the placement of the pentagonal faces. We begin similarly, by tracing the boundary of a patch Π in the hexagonal tessellation Λ. Beginning with a break edge, we trace the boundary back to the same break edge; the initial face is labelled F_1, the next two faces incident with break edges are T_1 and T_2, and the terminal face is F_4; refer to Fig. 7. We will again determine the locations of the pentagonal faces by assuming P_1 to lie on F_1T_1. Let the first pentagonal face P_1 be distance m from F_1 on the F_1T_1 side, and let $F_2 = \phi_{P_1}(F_1)$. We now can apply Lemma 1 to F_2 and F_4 to determine X such that $\phi_X^2(F_2) = F_4$. We must then be careful to place P_2 so that both P_2 and $P_3 = \phi_X^{-2}(P_2)$ are interior to Π. The following construction determines the possible locations for P_2, in both the symmetric and near-symmetric cases.

Let k be the line through T_2 and F_4, and let ℓ be the line through T_1 and T_2. Define $k' = \phi_X^2(k)$, $\ell' = \phi_X^2(\ell)$, and $Y = \phi_{F_2}(X)$; again refer to Fig. 7. Construct a circle $\mathcal{C}$ with center Y and radius XY. Finally, let R_1 be the intersection of ℓ and k', R_2 and R_3 respectively the intersections of $\mathcal{C}$ with ℓ and ℓ' both on the same side of k' as X, and R_4 the intersection of k' and ℓ'. We denote by $\mathcal{R}$ the region enclosed by line segment R_1R_2, arc R_2XR_3, and line segments R_3R_4 and R_4R_1, as shown in Fig. 7. While the location of P_2 is as yet unfixed, we consider $F_3 = \phi_{P_2}(F_3)$ and P_3 the unique point such that $\phi_{P_3}(F_3) = F_4$. The following two lemmas show that the face centers in $\mathcal{R}$, excluding X, are precisely the possible locations of P_2.

Lemma 2 *If P_2 is not on the same side of R_1R_2, R_3R_4, and R_4R_1 as X, then either P_2 or P_3 is outside the boundary of Π.*

Proof Since $k' = \phi_X^2(k)$, $\ell' = \phi_X^2(\ell)$, and $P_2 = \phi_X^2(P_3)$, the result is immediate.

Lemma 3 *The triangles $\triangle F_2P_2F_3$ and $\triangle F_3P_3F_4$ have nonintersecting interiors if and only if P_2 is inside $\mathcal{C}$.*

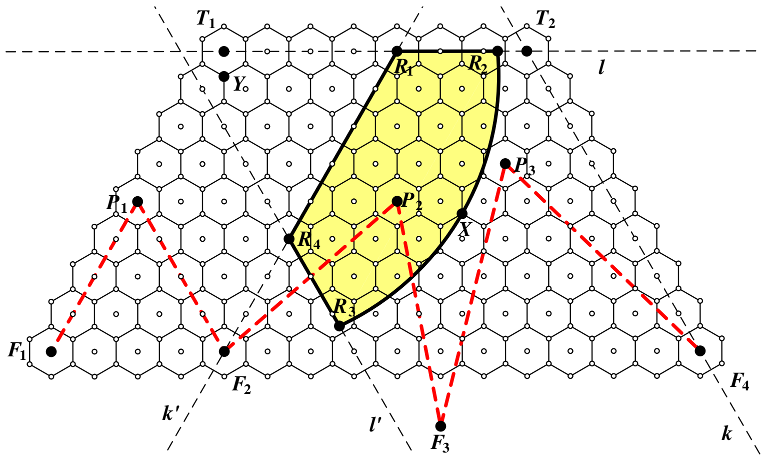


Fig. 7 Construction of the region $\mathcal{R}$ in a near-symmetric patch with $n = 7$, thus side parameters [8, 7, 8], and $m = 4$; P_2 is included as an arbitrarily-chosen face center in $\mathcal{R}$

Proof Consider a circle $\mathcal{C}'$ centered at X of radius XY; observe that $\phi_{F_2}(\mathcal{C}') = \mathcal{C}$. Since $F_3 = \phi_{F_2}^{-1}(P_2)$, F_3 is external to $\mathcal{C}'$ precisely when P_2 is external to $\mathcal{C}$. But whenever F_3 is external to $\mathcal{C}'$, $\angle F_4F_3F_2$ is less than $\angle F_2XF_4 = 120°$, since they subtend the same chord F_2F_4 of the circle $\mathcal{C}'$ centered at X. But then $\angle P_3F_3P_2$ is negative (since all angles are measured counterclockwise), and hence $\triangle F_2P_2F_3$, and $\triangle F_3P_3F_4$ have intersecting interiors.

If X falls upon a face center and P_2 is placed at X, then P_3 would also be at X. The deletion of the two sectors originating in P_2 and P_3 would result in a quadrilateral face, rather than two pentagonal faces; obviously this is not permitted. With this fact and the two preceding lemmas, P_2 can be located at any face center in $\mathcal{R}$ other than X.

However, while all these face centers are feasible, counting these face centers would double-count certain patches. Specifically, if both P_2 and P_3 lie in $\mathcal{R}$, then that patch would be counted twice. Hence we will construct a new region $\mathcal{R}'$ contained in $\mathcal{R}$ which avoids this problem without undercounting.

Let R_2' be the point on R_1R_2 such that XR_2' is perpendicular to R_1R_2; similarly define R_3' on R_3R_4 so that XR_3' is perpendicular to R_3R_4. Then $\angle R_2'XR_3' = 120°$. Thus if a face center in the pentagonal region $R_1R_2'XR_3'R_4$ has its rotation by ϕ_X^2 also in $R_1R_2'XR_3'R_4$, it must lie along XR_2'. Thus we define $\mathcal{R}'$ to be the pentagonal region $R_1R_2'XR_3'R_4$ less the boundary segment XR_2' where neither X nor R_2' is in $\mathcal{R}'$.

Counting symmetric patches with exactly 3 pentagonal faces

To count all $[n, n, n]$ patches, we begin by counting all $[n, n, n]$ patches with P_1 distance m from F_1. This is simply the number of faces centered in region $\mathcal{R}'$; for clarity, a face is in $\mathcal{R}'$ if its center is in $\mathcal{R}'$. We place P_1 at a distance of m from F_1 where $n/2 \le m \le n$. If P_1 is distance $m < n/2$ from F_1, then P_1 is distance $(n - m) > n/2$

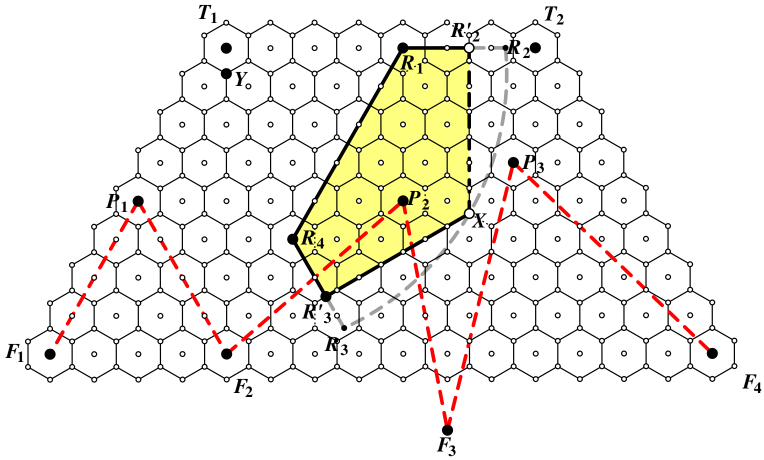


Fig. 8 The counting region $\mathcal{R}'$ in a near-symmetric patch with $n = 7$, thus side parameters [8, 7, 8] and $m = 4$

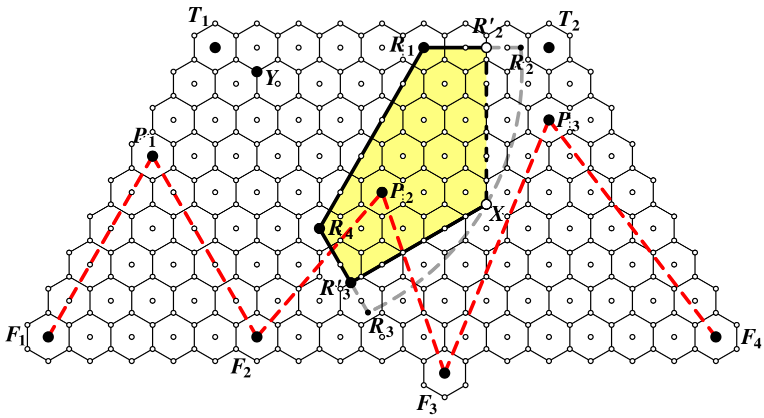


Fig. 9 The counting region $\mathcal{R}'$ in a symmetric patch with $n = 8$, thus side parameters [8, 8, 8], and $m = 5$

from T_1, and via a graph isomorphism is counted in the other configuration. The first of the following lemmas considers P_1 neither at the midpoint of F_1T_1 nor at T_1.

Lemma 4 *Let m and n be fixed positive integers with $n/2 < m < n$. Then the number of non-isomorphic patches that have side parameters $[n, n, n]$ and a pentagon distance m from a corner is*

$$h(n,m) = \begin{cases} \frac{1}{6}(n^2 + 2mn + 3n - 2m^2) & \textit{if } m + n \equiv 0 \pmod 3 \\ \frac{1}{6}(n^2 + 2mn + 3n - 2m^2 + 2) & \textit{else.} \end{cases}$$

Proof To prove this result, we need to count the number of faces in region $\mathcal{R}'$; for purpose of illustration, Fig. 9 may be consulted. First notice that the length of R_4R_1

is m and both R_4 and R_1 are in $\mathcal{R}'$, so the number of faces on R_4R_1 is $m+1$. Also, notice that the length of R_1R_2' (and thus of $R_3'R_4$) is $(n-m)/2$ with R_1 (respectively R_4) on the center of a face and R_2' (respectively R_3') on the center of face if and only if $(n-m)/2$ is an integer.

To proceed, we count the number of faces in each row starting at the row on R_4R_1. Each subsequent row has exactly one more face until the row just prior to or containing R_2' and R_3'. After this, the length of each row decreases by 3 until we reach the final row (prior to that row containing X) which has 0, 1, or 2 faces in it. If $(n-m)/2$ is an integer, the total number of faces in $\mathcal{R}'$ is

$$\sum_{k=1}^{(n-m)/2}(m+k)+\sum_{k=0}^{\lfloor (m+n)/6\rfloor}\left(m+\frac{n-m}{2}-3k\right).$$

The first sum counts all faces in the rows strictly before the row containing R_2', and the second sum counts all faces in the rows at R_2' or after it. The upper index of the second sum is $\lfloor (m+n)/6\rfloor$ because the summands are decreasing until $m+\frac{n-m}{2}-3k$ equals 0, 1, or 2. Solving for k gives the desired upper index.

If $(n-m)/2$ is not an integer, then the total number of faces in $\mathcal{R}'$ is

$$\sum_{k=1}^{(n-m+1)/2}(m+k)+\sum_{k=0}^{\lfloor (m+n-3)/6\rfloor}\left(m-2+\frac{n-m+1}{2}-3k\right).$$

The first sum again counts all faces in the rows strictly before the row containing R_2'. Notice the row directly preceding R_2' has two fewer faces than the row after it. Each subsequent row has three fewer faces which accounts for the the second sum.

These sums can be evaluated by considering the the parity of $n-m$ and the remainder of $n+m$ when dividing by 6. If n is even and $(n+m)/6$ is an integer, we see that the number of faces is

$$\sum_{k=1}^{(n-m)/2}(m+k)+\sum_{k=0}^{(m+n)/6}\left(m+\frac{n-m}{2}-3k\right)$$

which simplifies to

$$\frac{1}{6}(n^2+2mn+3n-2m^2).$$

The other cases can be evaluated similarly to get the closed form stated in the lemma.

We now consider a $[n,n,n]$ patch with P_1 distance exactly $m=n/2$ from a corner, where n is even. This configuration leads to additional double-counting when enumerating patches by placement of P_2 within $\mathcal{R}'$, as P_1 is the midpoint of the side of Π opposite T_2. Thus if P_2 and P_2' are possible positions for the second pentagonal face, with respective third pentagonal faces at P_3 and P_3', we must be careful that we do not count both configurations when P_3 and P_3' are symmetric in Λ with respect to the reflection through T_2X.

This can occur in exactly two ways; for the sake of explaining these cases, we let R_5 be the midpoint of R_4R_1 and note that XR_5 bisects $\mathcal{R}'$. The first case we must consider occurs when P_2 is in $\triangle XR_4R_5$. If P_2' is the reflection of P_2 through R_4X, $P_3 = \phi_X^{-2}(P_2)$, and $P_3' = \phi_X^{-2}(P_2')$, then it is trivial to see that P_3' is the reflection of P_3 through T_2X; we must not count both the positions of P_2 and P_2' as unique. On the other hand, suppose P_2 is in $\triangle XR_5R_1$ but not on XR_5. Then if $P_3 = \phi_X^{-2}(P_2)$ and P_3' is the reflection of P_3 through T_2X, then P_3' is in $\triangle XR_1R_2'$ inside $\mathcal{R}'$; we must not count both the positions of P_2 and P_3' as unique. So the face centers we must consider as all possible positions of P_2 with no double-counting are precisely those in the equilateral triangle $\triangle R_1XR_4$, not including X. There are $\frac{n}{2}+1$ faces on R_1R_4; each row of faces in $\triangle R_1XR_4$ distance k from R_1R_4 has $\frac{n}{2}+1-k$ faces with the farthest row being distance $\frac{n}{2}-1$ from R_1R_4 (since X isn't included). Thus, the total number of faces in $\triangle R_1XR_4$ is

$$\sum_{k=0}^{\frac{n}{2}-1} \frac{n}{2}+1-k = \frac{n(n+6)}{8}.$$

The following lemma summarizes this result.

Lemma 5 *Let n be a fixed even integer. Then the number of non-isomorphic patches that have side parameters $[n, n, n]$ and a pentagon distance $n/2$ from a corner is*

$$h(n, n/2) = \frac{n(n+6)}{8}.$$

So far, we have found the number of non-isomorphic symmetric patches having a fixed pentagon P_1 distance m from a corner with $n/2 \leq m < n$. We now explore the case where $m = n$. In this case, $R_1 = R_2'$ and $R_4 = R_3'$, so the region $\mathcal{R}'$ is simply the triangle XR_4R_1 (not including the line segment R_1X and its endpoints). This configuration will lead to double-counting when enumerating patches by placements of P_2 in $\mathcal{R}'$. Again, for notational purposes, we let R_5 be the midpoint of R_1R_4 and let $R_5' = \phi_X^{-2}(R_5)$, which is the midpoint of T_2F_4. Also, let P_2 and P_2' be possible positions for the second pentagonal face in $\mathcal{R}'$ and P_3 and P_3' their respective positions for the third pentagonal face. We must not count both positions P_2 and P_2' when P_3 and P_3' are symmetric about $R_5'X$. However, P_3 and P_3' being reflections about $R_5'X$ is the same as P_2 and P_2' being reflections about R_5X; thus, the region in $\mathcal{R}'$ that avoids double counting is the triangle $\triangle R_5XR_4$ not including X. The following lemma counts the number of faces in this region.

Lemma 6 *Let n be a fixed positive integer. Then the number of non-isomorphic patches that have side parameters $[n, n, n]$ and a pentagon on a corner is*

$$h(n,n) = \begin{cases} \frac{1}{12}(n^2+6n) & \text{if } n \equiv 0 \pmod 6 \\ \frac{1}{12}(n^2+6n+5) & \text{if } n \equiv 1, 5 \pmod 6 \\ \frac{1}{12}(n^2+6n+8) & \text{if } n \equiv 2, 4 \pmod 6 \\ \frac{1}{12}(n^2+6n-3) & \text{if } n \equiv 3 \pmod 6 \end{cases}$$

Proof If n is even, the number of faces on R_4R_5 is $n/2+1$. The subsequent rows distance d from R_4R_5 have

$$\frac{n}{2}+1-\left\lceil\frac{3d}{2}\right\rceil$$

faces with the farthest row distance $\lfloor(n+2)/3\rfloor$, since X is centered on a face only when n is a multiple of 3. Thus, if n is even, the total number of faces in $\triangle R_5XR_4$ not including X is

$$\sum_{d=0}^{\lfloor(n+2)/3\rfloor}\frac{n}{2}+1-\left\lceil\frac{3d}{2}\right\rceil.$$

If n is odd, the number of faces on R_4R_5 is $(n+1)/2$. The subsequent rows distance d from R_4R_5 have

$$\frac{n+1}{2}-\left\lfloor\frac{3d}{2}\right\rfloor$$

faces with the farthest row distance $\lfloor(n+2)/3\rfloor$. Thus, if n is odd, the total number of faces in $\triangle R_5XR_4$ not including X is

$$\sum_{d=0}^{\lfloor(n+2)/3\rfloor}\frac{n+1}{2}-\left\lfloor\frac{3d}{2}\right\rfloor.$$

The cases above show that the computations will differ based on the remainder of $n/6$. We examine the case where n is congruent to 1 mod 6 in detail, and note that the other cases are similar. In this case, we write $n=6q+1$ and see that the upper index on the sum is $2q$. The desired sum becomes

$$\sum_{d=0}^{2q}\left(3q+1-\left\lfloor\frac{3d}{2}\right\rfloor\right)=(3q+1)(2q+1)-\sum_{d=0}^{2q}\left\lfloor\frac{3d}{2}\right\rfloor.$$

The final sum can be evaluated by noting that

$$\sum_{d=0}^{2q}\left\lfloor\frac{3d}{2}\right\rfloor=\sum_{k=1}^{3q}k-\sum_{k=1}^{q}(3k-1).$$

Thus the total number of faces in $\triangle R_5XR_4$ not including X is

$$(3q+1)(2q+1)-\frac{3q(3q+1)}{2}+\frac{3q(q+1)}{2}-q=3q^2+4q+1.$$

By rewriting q in terms of n, we get the desired result.

We now have a formula for the number of symmetric patches with a pentagon at fixed distance m from a corner. However, summing over all m overcounts the number of nonisomorphic patches because more than one pentagon may lie on the boundary. For instance, if m is fixed and the second pentagon P_2 is placed on the line R_1R_4, P_3 is forced to be on the boundary F_4T_2, and then P_3 is some distance m' from a corner. Hence its patch would be counted when P_1 is distance m' from F_1.

The next lemmas consider the case where either P_2 or P_3 is also on the boundary of Π and nearer to a corner than P_1 is to T_1. We will exclude such cases in the overall count.

Lemma 7 *Let n and m be fixed positive integers with $n/2 < m < n$. Then there are $2n - 2m - 1$ patches having side parameters $[n, n, n]$, a pentagon distance m from a corner, and another pentagon on the boundary distance less than $n - m$ to a corner.*

Proof Let P_1 be distance m from F_1. Then R_1 is distance m from T_1, making R_1R_2' nearer to the corner T_2 than to T_1. If P_2 is on the boundary of Π, it must be on R_1R_2'; if also the distance from P_2 to T_2 is less than $n - m$, then P_2 cannot be R_1.

On the other hand, if P_3 is on the boundary of Π, then either P_3 is on $R_2'T_2$ or on T_2F_4. If P_3 is on $R_2'T_2$, then this distance from P_3 to T_2 is less than $n-m$; this occurs only when P_2 is on $R_3'R_4$. If instead P_3 is on T_2F_4 and distance less than $n - m$ from T_2, then P_2 must be on R_4R_1 and distance less than $n - m$ from R_4. So we can count exactly those positions of P_2 along the boundary of $\mathcal{R}'$ which we have just described. The line segments $R_3'R_4$ and R_1R_2' excluding R_1 and R_2' give $(n - m)$ positions for P_2, and the portion of the segment R_4R_1 distance less than $n - m$ to R_4 but not at R_4 gives $(n - m - 1)$ positions. Summing these, the result holds.

Lemma 8 *Let n be a fixed even integer. Then there are $n/2$ patches having side parameters $[n, n, n]$, a pentagon distance $n/2$ from a corner, and another pentagon on the boundary distance less than $n/2$ to a corner.*

Proof The pentagon distance $n/2$ from a corner will be P_1. Then as before, for another pentagon to be on the boundary, P_2 must be on $R_3'R_4$ (including endpoints), R_1R_2' (not including endpoints), or on the closest $n - m - 1$ faces to R_4 on R_4R_1 not including R_1. Accounting for our previous isomorphisms, P_2 must be on R_4R_1 not including R_1. There are $n/2$ such faces.

Combining these lemmas yields the following theorem.

Theorem 1 *The number of non-isomorphic patches with side parameters $[n, n, n]$ and a pentagon on the boundary is*

$$\begin{cases} \frac{1}{18}(2n^3 + 24n - 18) & \textit{if } n \equiv 0 \pmod 6 \\ \frac{1}{18}(2n^3 + 15n + 1) & \textit{if } n \equiv 1 \pmod 6 \\ \frac{1}{18}(2n^3 + 24n - 10) & \textit{if } n \equiv 2 \pmod 6 \\ \frac{1}{18}(2n^3 + 15n - 9) & \textit{if } n \equiv 3 \pmod 6 \\ \frac{1}{18}(2n^3 + 24n - 8) & \textit{if } n \equiv 4 \pmod 6 \\ \frac{1}{18}(2n^3 + 15n - 1) & \textit{if } n \equiv 5 \pmod 6 \end{cases}$$

Proof We first count the number of non-isomorphic patches with a pentagon on the corner; then we count the number of non-isomorphic patches with a pentagon distance m from a corner with $n/2 < m < n$ and subtract the number of patches that are counted twice. Finally, if n is even, we count the number of patches with a pentagon distance $n/2$ from a corner and subtract the number of patches that are counted twice. Thus, if n is even, we evaluate the sum

$$h(n,n) + \left(\sum_{m=n/2+1}^{n-1} (h(n,m) - (2n - 2m - 1)) \right) + h(n, n/2) - n/2,$$

and the total number if n is odd is

$$h(n,n) + \sum_{m=(n+1)/2}^{n-1} (h(n,m) - (2n - 2m - 1)) .$$

The simplification of these sums requires knowing the remainder of n when dividing by 6. We examine the case where $n = 6q + 2$ in detail and note that the other cases are similar. Notice the sum

$$\sum_{m=n/2+1}^{n-1} (h(n,m) - (2n - 2m - 1))$$

has $3q$ terms. Of these terms, q of them come from an index m which is congruent to 1 mod 3 (thus ensuring $n + m$ is congruent to 0 mod 3). Using the formula in Lemma 4, the sum can be rewritten as

$$\sum_{m=n/2+1}^{n-1} \left(\frac{1}{6}(n^2 + 2nm + 3n - 2m^2 + 2) - (2n - 2m - 1) \right) - \frac{1}{3}q$$

or more simply

$$\frac{1}{72} \left(8n^3 - 15n^2 + 42n - 88 \right).$$

Thus, using Lemmas 5 and 6, the total number of patches is given by

$$\frac{1}{12}(n^2 + 6n + 8) + \frac{1}{72} \left(8n^3 - 15n^2 + 42n - 88 \right) + \frac{n(n+6)}{8} - \frac{n}{2}$$

which can be simplified to the desired result.

These results agree with the numbers found by Brinkmann and Van Cleemput in their recursive algorithm in [3].

Counting near-symmetric patches with exactly 3 pentagonal faces

The construction of the region $\mathcal{R}'$ in the near-symmetric case is exactly the same as in the symmetric case; in fact, Fig. 7 depicted a near-symmetric patch, and Fig. 8 depicted its counting region $\mathcal{R}'$. However, determining whether F_1T_1 or T_1T_2 is on the shorter side or a longer side has an effect on the enumeration of positions for P_2. We first consider all near-symmetric patches that have a pentagon on a longer side. For near-symmetric patches with side parameters $[n, n+1, n+1]$ and a pentagon on a side of length $n+1$, we draw the patch such that T_1T_2 has length n. We again fix P_1 at distance m from F_1, and as long as $m \neq 0$, the counting process is the same.

Lemma 9 *Let n and m be fixed positive integers with $1 \leq m \leq n+1$. Then the number of non-isomorphic patches that have side parameters $[n, n+1, n+1]$ with a pentagon on a side of length $n+1$ distance m from the $(n+1, n+1)$-corner is*

$$f(n,m) = \begin{cases} \frac{1}{6}(n^2 + 2mn + 7n - 2m^2 - 2m + 4) & \textit{if } n + m - 1 \equiv 0 \pmod 3 \\ \frac{1}{6}(n^2 + 2mn + 7n - 2m^2 - 2m + 6) & \textit{else.} \end{cases}$$

Proof After fixing P_1, we need to count the number of possible positions for P_2 which is equivalent to the number of faces in region $\mathcal{R}'$. Notice that the length of R_4R_1 is $m+1$ and both R_4 and R_1 are in $\mathcal{R}'$, so the number of faces on R_4R_1 is $m+2$. Also, notice the length of R_1R_2' is $(n-m)/2$ with R_1 on the center of a face if and only if $(n-m)/2$ is an integer. This proof is almost identical to the proof of Lemma 4, so we omit some of the details here. If $(n-m)/2$ is an integer, the total number of faces in $\mathcal{R}'$ is

$$\sum_{k=1}^{(n-m)/2} (m+1+k) + \sum_{k=0}^{\lfloor (m+n+2)/6 \rfloor} \left(m + 1 + \frac{n-m}{2} - 3k\right),$$

and if $(n-m)$ is odd, the total number of faces in $\mathcal{R}'$ is

$$\sum_{k=1}^{(n-m+1)/2} (m+1+k) + \sum_{k=0}^{\lfloor (m+n+3)/6 \rfloor} \left(m - 1 + \frac{n-m+1}{2} - 3k\right).$$

When $m = 0$, which occurs when $P_1 = F_1$, it is not the case that placing P_2 at each face center in $\mathcal{R}'$ results in a non-isomorphic patch. Since the patch Π has three sides and three corners, we can think of P_1 as the opposite corner to the side T_1T_2. If P_2 and P_2' are possible positions for the second pentagonal face, with respective third pentagonal faces P_3 and P_3', we must ensure that we do not count both configurations when P_3 and P_2' are symmetric with respect to reflection through $R_2'X$.

Again we denote by R_5 the midpoint of R_1R_4. Suppose P_2 is in the quadrilateral $R_3'R_4R_5X$, excluding X and $P_3 = \phi_X^{-2}(P_2)$. Then the reflection of P_3 through XR_2' is in the quadrilateral $R_1R_2'XR_5$. Hence we count only those face centers in one of those quadrilaterals as possible locations for P_2.

Lemma 10 *Let n be a fixed positive integer. Then the number of non-isomorphic patches that have side parameters* $[n, n+1, n+1]$ *and a pentagon on the* $(n+1, n+1)$*-corner is*

$$f(n,0) = \begin{cases} \frac{1}{12}(n^2+10n+12) & \text{if } n \equiv 0,2 \pmod 6 \\ \frac{1}{12}(n^2+10n+1) & \text{if } n \equiv 1 \pmod 6 \\ \frac{1}{12}(n^2+10n+9) & \text{if } n \equiv 3,5 \pmod 6 \\ \frac{1}{12}(n^2+10n+4) & \text{if } n \equiv 4 \pmod 6 \end{cases}$$

Proof This proof is very similar to the proof of Lemma 6.

We count the number of faces centered in the quadrilateral $R_1R_2'XR_5$, excluding X. The length of R_1R_2' is $n/2$. Thus there are $n/2+1$ faces on the row if n is even and $(n+1)/2$ faces if n is odd.

If n is even, each subsequent row at distance d from R_1R_2' has

$$\frac{n}{2} + 2 - \left\lceil \frac{3d}{2} \right\rceil$$

faces with the farthest row at distance $\lfloor (n+1)/3 \rfloor$. The reason for this is that X is centered on a face only when $n+2$ is divisible by 3. Thus, if n is even, the total number of faces in quadrilateral $R_1R_2'XR_5$ (excluding X) is

$$\frac{n}{2} + 1 + \sum_{d=1}^{\lfloor (n+1)/3 \rfloor} \left(\frac{n}{2} + 2 - \left\lceil \frac{3d}{2} \right\rceil \right).$$

If n is odd, we have a similar scenario and see that the number of faces in $R_1R_2'XR_5$ (excluding X) is

$$\frac{n+1}{2} + \sum_{d=1}^{\lfloor (n+1)/3 \rfloor} \left(\frac{n+1}{2} + 1 - \left\lfloor \frac{3d}{2} \right\rfloor \right).$$

These expressions can be algebraically simplified to the closed form above.

For near-symmetric patches with side parameters $[n, n+1, n+1]$ and a pentagon on the side of length n, we draw the patch with F_1T_1 of length n and both T_1T_2 and T_2F_4 of length $n+1$. For such patches, we only need to consider the pentagon P_1 being distance m from F_1 where $n/2 \le m \le n$. If P_1 is distance less than $n/2$ from F_1, then it is at least $n/2$ distance from T_1; such a patch would be counted in the other configuration. As the cases for $m = \frac{n}{2}$ and $m = n$ require extra care, we begin by excluding them.

Lemma 11 *Let n and m be positive integers with* $n/2 < m < n$*. Then the number of non-isomorphic patches that have side parameters* $[n, n+1, n+1]$ *and a pentagon on the side of length n at distance m from a corner is*

$$g(n,m) = h(n,m) = \begin{cases} \frac{1}{6}(n^2 + 2mn + 3n - 2m^2) & \textit{if } n+m \equiv 0 \pmod 3 \\ \frac{1}{6}(n^2 + 2mn + 3n - 2m^2 + 2) & \textit{else.} \end{cases}$$

Proof Note that R_1R_4 has length m and R_1R_2' has length $(n-m)/2$. Thus, to count the face centers in $\mathcal{R}'$ we use the same technique as Lemma 4.

When there is a pentagon on the side of length n and distance exactly $n/2$ from a corner, we use similar arguments as the symmetric case and get the following lemma extending the definition of g.

Lemma 12 *Let n be a fixed even integer. Then the number of non-isomorphic patches that have side parameters $[n, n+1, n+1]$ and a pentagon on the side of length n at distance $n/2$ from a corner is*

$$g(n, n/2) = h(n, n/2) = \frac{n(n+6)}{8}.$$

Each of these lemmas allows us to count the number of non-isomorphic near-symmetric patches when a pentagon is in a fixed position on a particular side. However, some of these cases overlap; for instance, those cases with pentagons on two sides could be counted twice. Therefore, we need to consider all ways we could possibly be double-counting before finding the total. The next result counts those patches with one pentagon on each long side of the boundary, F_1 in the $(n+1, n+1)$-corner, and the distance from P_2 to F_4 greater than P_1 to F_1.

Lemma 13 *Let n and m_1 be fixed positive integers with $0 \le m_1 \le n+1$. The number of non-isomorphic patches having side parameters $[n, n+1, n+1]$, a pentagon on a long side at distance m_1 from the $(n+1, n+1)$-corner, and another pentagon on the other long side at distance $m_2 > m_1$ from the $(n+1, n+1)$-corner is*

$$\begin{cases} 1 & \textit{if } m_1 = 0, \\ m_1 + 2 & \textit{if } 0 < m_1 < n/2, \textit{ and} \\ n - m_1 + 1 & \textit{if } m_1 \ge n/2. \end{cases}$$

Proof We draw the patch as usual with P_1 distance m_1 from F_1. The other long side of the patch is T_2F_4 and P_2 cannot be on that side. If P_3 is on the long side and is distance $m_2 > m_1$ from F_4, the P_3 is less than $n+1-m_1$ from T_2. Since T_2 maps to R_4 in our 120 degree rotation about X, we see that P_2 must be on R_4R_1 and be distance less than $n+1-m_1$ from R_4. There are exactly m_1+2 faces on R_1R_4.

If $m = 0$, our acceptable region is the quadrilateral $R_5R_1R_2'X$, and there is only 1 place for P_2 on the line R_5R_1. If $m_1 < n/2$ and P_2 is anywhere on R_4R_1, P_3 will be on the other long side at distance more than m_1 from the $(n+1, n+1)$-corner. There are m_1+2 possible positions for P_2. On the other hand, if $m_1 \ge n/2$, then P_2 can only be in the first $n - m_1 + 1$ positions along R_4R_1.

Now we consider double-counting patches with a pentagon on both a long side and short side.

Lemma 14 *Let n be a fixed positive integer. The number of non-isomorphic patches having side parameters* $[n, n+1, n+1]$*, a pentagon on a long side, and a pentagon on a short side not including the short side's corners is* $\lfloor n^2/2 \rfloor$.

Proof Consider fixing P_1 at distance m from F_1. If $m = 0$ and P_2 is on T_1T_2 (the short side), then P_2 is on R_1R_2' including R_2' (which is in the allowable region in this case) but not including R_1 which is on the corner T_1. Thus there are $\lfloor n/2 \rfloor$ positions for P_2.

If $0 < m < n+1$, then P_2 could be on all of R_1R_2' not including R_2' (which is not in $\mathcal{R}'$). There are $\lfloor (n-m)/2 \rfloor + 1$ valid positions. However, P_3 could also be on the short side T_1T_2, which occurs when P_2 is on $R_3'R_4$. In this case, P_2 cannot be on R_4 because then P_3 would be on the corner T_2. Thus, there are $\lceil (n-m)/2 \rceil - 1$ positions for P_2 here for a total of $n - m$ places.

If $m = n+1$, neither P_2 nor P_3 can be on T_1T_2, so there are no patches to count in this case. Summing over all m yields a total of

$$\left\lfloor \frac{n}{2} \right\rfloor + \sum_{m=1}^{n} (n-m) = \left\lfloor \frac{n^2}{2} \right\rfloor$$

patches satisfying the given criteria.

The final theorem gives a formula for the total number of near-symmetric patches with at least one pentagon on the boundary. These results agree with the values found by the recursive algorithm in [3].

Theorem 2 *The number of non-isomorphic patches with side parameters* $[n, n+1, n+1]$ *and at least one pentagon on the boundary is*

$$\begin{cases} \frac{1}{6}(2n^3 + 4n^2 + 8n) & \text{if } n \equiv 0, 2 \pmod 6 \\ \frac{1}{6}(2n^3 + 4n^2 + 5n + 1) & \text{if } n \equiv 1 \pmod 6 \\ \frac{1}{6}(2n^3 + 4n^2 + 5n + 3) & \text{if } n \equiv 3, 5 \pmod 6 \\ \frac{1}{6}(2n^3 + 4n^2 + 8n - 2) & \text{if } n \equiv 4 \pmod 6 \end{cases}$$

Proof We start by counting all such patches with a pentagon on the $(n+1, n+1)$-corner. There are $f(n, 0)$ of these. We then count the patches with a pentagon on a side of length $n+1$ at distance m from the $(n+1, n+1)$ corner where $1 \le m \le n+1$; however, we must subtract the number of patches that have two pentagons on long sides that will be counted twice. We then add in all patches with a pentagon on the short side and subtract those that were previously counted if they also had a pentagon on the long side. Finally, we notice that some patches have a pentagon on all three sides, and we need to add those back in. This occurs exactly when there is a pentagon on the long side at distance m from the $(n+1, n+1)$-corner with $1 \le m < n/2$ and P_2 is at R_1, equalling $\left\lfloor \frac{n}{2} \right\rfloor - 1$ cases. Thus, the total number is

$$f(n,0)+\sum_{m=1}^{n+1} f(n,m)-\left(1+\sum_{m=1}^{\lfloor n/2\rfloor -1}(m+2)+\sum_{m=\lfloor n/2\rfloor}^{n+1}(n-m+1)\right)$$
$$+\sum_{\lfloor n/2\rfloor +1}^{n-1} g(n,m)+(n-1 \mod 2)g(n,n/2)-\left\lfloor \frac{n^2}{2}\right\rfloor+\left\lceil \frac{n}{2}\right\rceil -1$$

Again, these sums require some care to simplify. Using similar techniques to those used previously, the stated result holds.

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