Ambiguous Fullerene Patches

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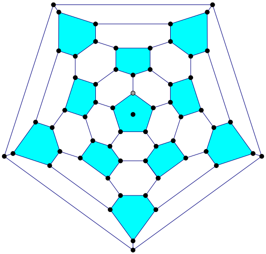
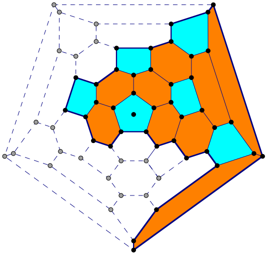
Definitions

- A *fullerene* is a trivalent plane graph with only hexagonal and (12) pentagonal faces.
- A *fullerene patch* is the graph obtained by taking a simple closed curve in a fullerene and deleting all vertices on one side.



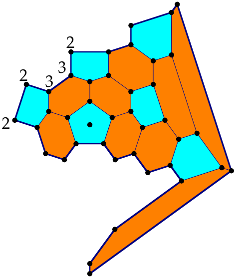
Fullerene



Fullerene Patch

Boundary Code

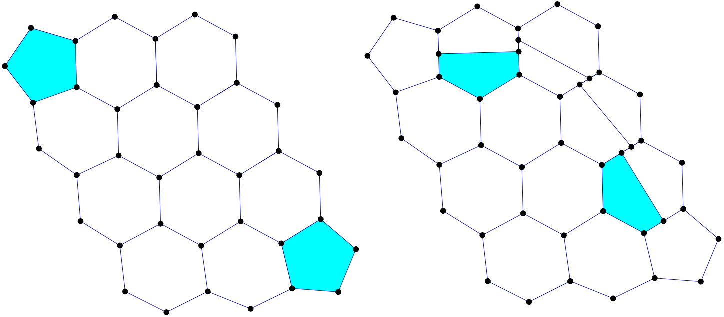
- The *boundary code* of a patch is the sequence of valences of boundary vertices.



Boundary Code
(2,2,3,3,2,3,3,2,3,2,3,2,2,2,3,3,2,3,2,3,3,2,2,3)

Similar Patches

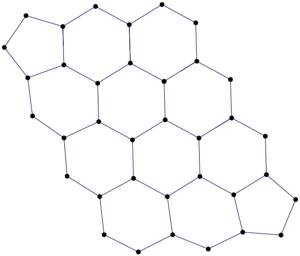
- Two patches are *similar* if they have the same boundary code.



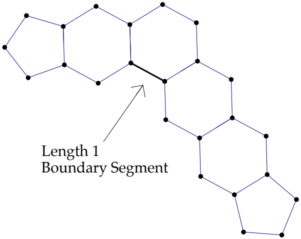
Two Similar Patches

Convex Patch

A *convex patch* is a fullerene patch that satisfies the condition that there are no boundary segments of length 1.



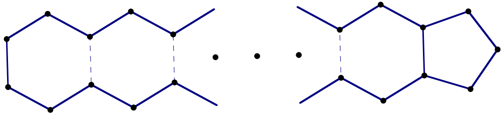
Convex Patch



Non-Convex Patch

Convex Patch

FACT - A convex patch is either linear or there are no boundary segments of length 5.



Linear Patch with a
Boundary Segment of Length 5

Convex Patch

FACT - A convex patch has at most 6 pentagonal faces.

- A previous result for fullerene patches gives

$$\# \text{ of pents} = 6 + s_1 - s_3 - 2s_4 - 3s_5$$

  where s_i is the number of boundary segments of size i.

- For convex patches this becomes

$$\# \text{ of pents} = 6 - s_3 - 2s_4 - 3s_5 \leq 6$$

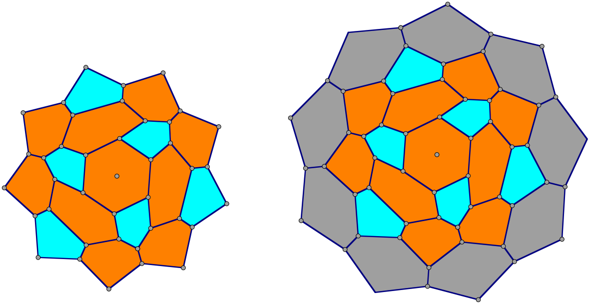
Convex Patch

FACT - A convex patch with 6 pentagons only has boundary segments of length 2 and is similar to an infinite number of patches.

- $\#$ of pents $= 6 - s_3 - 2s_4 - 3s_5$
- Thus $s_1 = s_3 = s_4 = s_5 = 0$

Convex Patch

Thus, adding a layer of hexagons along the entire boundary yields a similar patch.



Two similar convex patches with 6 pentagons
Boundary Code (2,3,2,3,2,3,2,3,2,3,2,3,2,3,2,3,2,3)

Convex Patch

Summary: A convex patch satisfies the following conditions:

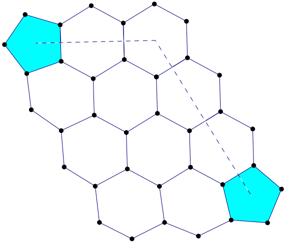
- There are no boundary segments of length 1.
- It is either linear or there are no boundary segments of length 5.
- There are at most 6 pentagonal faces.

Goal

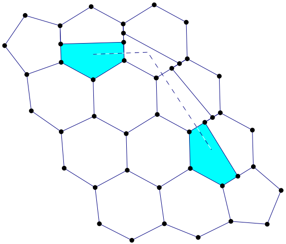
Goal - Given a convex patch, describe all other patches similar to it.

Coxeter Coordinates

- Given two (close together) pentagons in a patch, we can find the *Coxeter Coordinates* between them.
- Start at one pentagon, take a straight ahead path of length n, turn left 120°, and take a straight ahead path of length k to get to the next pentagon.
- The Coxeter coordinates of these two pentagons is (n, k).



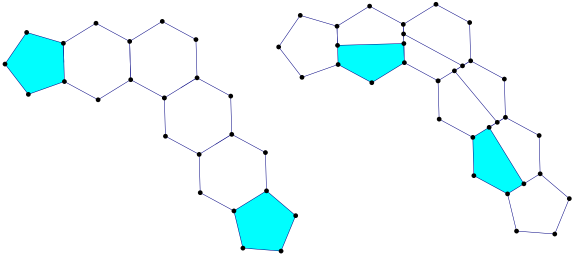
A (3,2)-pair of pentagons



A (2,1)-pair of pentagons

The Transformation α

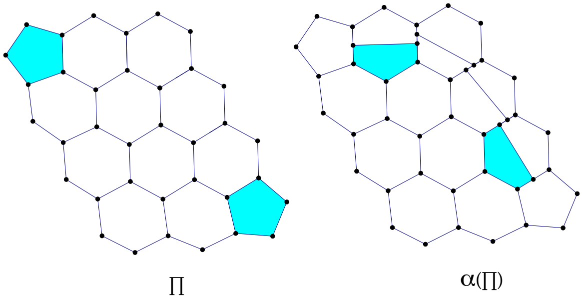
An extension of the Endo-Kroto transformation shows a way to find two similar patches by sending an (n, k) pair of pentagons to an $(n-1, k-1)$ pair of pentagons.



Endo-Kroto Transformation
A (3,2)-patch and a similar (2,1)-patch

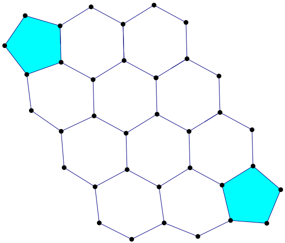
The Transformation α

Call this transformation α and use it on any convex patch Π (with "nearby" pentagons) to find a similar patch $\alpha(\Pi)$.

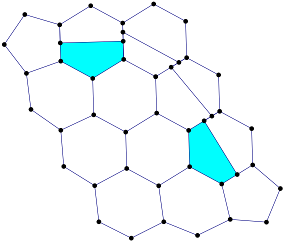


The Transformation α

- Applying α to a patch results in a patch with a larger number of faces.
- For every hexagon in the path between the pentagons, we are adding an extra face.
- Thus, $\alpha(\Pi)$ has $n + k - 1$ more faces than Π



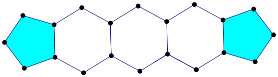
$\prod$ has a (3,2) pair of pentagons and 12 faces



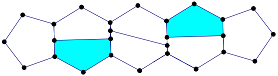
$\alpha(\prod)$ has 16 faces

The Transformation β

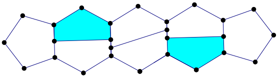
Another extension of the Endo-Kroto transformation shows a way to find two similar patches by sending a (n) pair of pentagons to an $(n-2, 1)$ or $(1, n-2)$ pair of pentagons.



A (4)-pair of pentagons



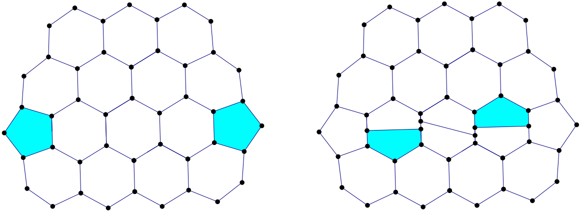
A similar (2,1)-pair of pentagons



A similar (1,2)-pair of pentagons

The Transformation β

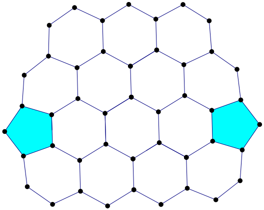
Call this transformation β and use it on any convex patch Π to find a similar patch $\beta(\Pi)$.



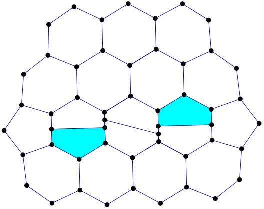
Π $\qquad$ $\beta(\Pi)$

The Transformation β

- Applying β to a patch results in a patch with a larger number of faces.
- For every hexagon in the path between the pentagons, we are adding an extra face.
- Thus, $\beta(\Pi)$ has $n-1$ more faces than Π



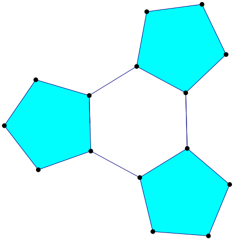
$\prod$ has a (4) pair of pentagons and 16 faces



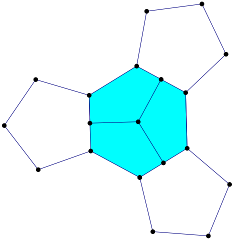
$\beta(\prod)$ has 19 faces

The Transformation γ

Another transformation, γ can be used when dealing with a specific configuration of 3 pentagons.



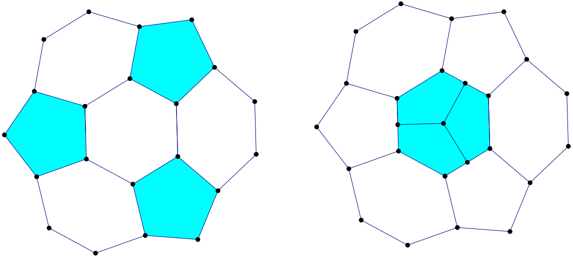
$\prod$



$\gamma(\prod)$

The Transformation γ

- Applying γ to a patch results in a patch with a larger number of faces.
- $\gamma(\Pi)$ has 2 more faces than Π.



$\prod$ has 7 faces

$\gamma(\prod)$ has 9 faces

Technical Lemma

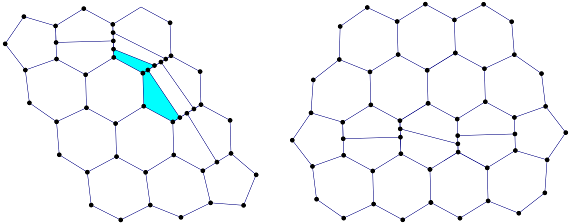
Lemma: Let $\Pi = (V, E, F, B)$ be a convex patch with less than 6 pentagons. Then

$$|F| \leq \binom{\ell(\Pi)+1}{2}$$

where $\ell(\Pi)$ is the length of the perimeter in terms of boundary segments.

Example of Technical Lemma

$$|F| \leq \binom{\ell(\Pi)+1}{2}$$



$|F| = 18$

$\ell(\prod) = 10$

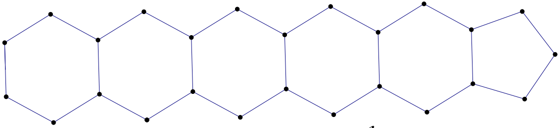
$|F| = 19$

$\ell(\prod) = 11$

Proof of Lemma: $|F| \leq \binom{\ell(\Pi)+1}{2}$

Case 1: Π is a linear patch.

- A linear patch implies that $\ell(\Pi) = 2|F| - 2$.



Example: $|F| = 6$ $\quad \ell(\prod) = 10$

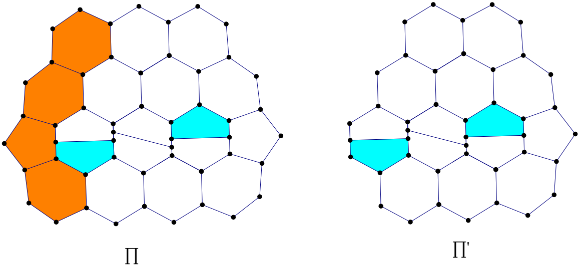
- Thus,

$$\binom{\ell(\Pi)+1}{2} = \binom{2|F|-1}{2} \geq |F|$$

Proof of Lemma: $|F| \leq \binom{\ell(\Pi)+1}{2}$

Case 2: Π is **not** linear.

- Use induction on $\ell(\Pi)$. Delete all faces on one "side" of Π leaving Π'.



Proof of Lemma: $|F| \leq \binom{\ell(\Pi)+1}{2}$

- Now $\ell(\Pi') \leq \ell(\Pi) - 1$
- Using induction, we have

$$|F'| \leq \binom{\ell(\Pi')+1}{2} \leq \binom{\ell(\Pi)}{2}$$

- Thus,

$$|F| = |F'| + \text{length of deleted side} \leq \binom{\ell(\Pi)}{2} + \ell(\Pi) = \binom{\ell(\Pi)+1}{2}$$

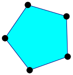
Main Idea

- Performing α, β, or γ keeps the boundary fixed ($\ell(\Pi)$), but the number of faces increase. Thus, we can only perform so many transformations before the number of faces is maxed out.
- In a convex patch, we can always perform an α, β, or γ unless all the pentagons are next to each other.

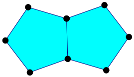
Main Idea

- We're working on showing that there are exactly eight minimal configurations with all of the pentagons together.
- The idea is that if you are not in one of the minimal configurations, you could perform an α, β, or γ on the patch and be similar to one.

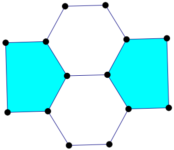
Eight Minimal Configurations



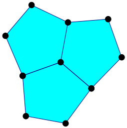
Case 1
1 pentagon



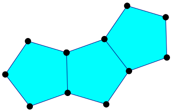
Case 2
2 pentagons



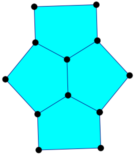
Case 3
2 pentagons



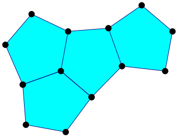
Case 4
3 pentagons



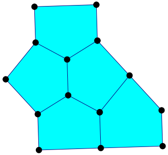
Case 5
3 pentagons



Case 6
4 pentagons



Case 7
4 pentagons



Case 8
5 pentagons

Finishing Touches

- Bound the number of similar patches to a given convex patch.
- Characterize all patches that can be extended to a convex patch by adding hexagonal faces.
- Extend result to all of these patches.

Acknowledgements

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References

G. Brinkmann, G. Caporossi and P. Hansen, *A survey and new results on computer enumeration of polyhex and fusene hydrocarbons,* Journal of Chemical Information and Computer Sciences **43**, 2003, 842–851.

M. Endo and H. W. Kroto, *Formation of carbon nanofibers*, J. Phys. Chem. **96**, 6941-6944 (1992).

J. E. Graver, *The (m,k)-patch boundary code problem*, MATCH **48** (2003) 189-196.

J. E. Graver and C. Graves, *Fullerene Patches I*, Ars Mathematica Contemporanea, **3** (2010) 104–120.

X. Guo, P. Hansen and M. Zheng, *Boundary Uniqueness of Fusenes*, Tech. Report G-99-37, GERAD (1999).

A. J. Stone and D. J. Wales, *Theoretical studies of icosahedral C_{60} and some related species*, Chem. Phys. Lett., (1986), 501–503.

Questions

Questions?