Ambiguous Fullerene Patches

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

Boundary Code

(2,2,3,3,2,3,3,2,3,2,2,3,3,2,3,2,3,3,2,2,3,2,2,3)
Similar Patches

- Two patches are *similar* if they have the same boundary code.
A *convex patch* is a fullerene patch that satisfies the condition that there are no boundary segments of length 1.
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
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
  \[ \# \text{ of pents} = 6 - s_3 - 2s_4 - 3s_5 \leq 6 \]
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 $s_1 = s_3 = s_4 = s_5 = 0$
Thus, adding a layer of hexagons along the entire boundary yields a similar patch.

Two similar convex patches with 6 pentagons
Boundary Code (2,3,2,3,2,3,2,3,2,3,2,3,2,3,2,3,2,3,2,3,2,3,2,3,2,3,2,3,2,3,2,3,2,3,2,3,2,3,2,3,2,3,2,3,2,3,2,3)
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 - 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 $120^\circ$, 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
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 $\alpha$

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

![Diagram showing the transformation $\alpha$ applied to a convex patch $\Pi$ to find a similar patch $\alpha(\Pi)$]
The Transformation $\alpha$

- Applying $\alpha$ 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 $\Pi$.

$\Pi$ has a (3,2) pair of pentagons and 12 faces
$\alpha(\Pi)$ has 16 faces
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
Call this transformation $\beta$ and use it on any convex patch $\Pi$ to find a similar patch $\beta(\Pi)$. 

$\Pi$ $\beta(\Pi)$
Applying $\beta$ 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 $\Pi$.
Another transformation, $\gamma$ can be used when dealing with a specific configuration of 3 pentagons.
Applying $\gamma$ to a patch results in a patch with a larger number of faces.

$\gamma(\Pi)$ has 2 more faces than $\Pi$. 

$\Pi$ has 7 faces

$\gamma(\Pi)$ has 9 faces
Lemma: Let $\Pi = (V, E, F, B)$ be a convex patch with less than 6 pentagons. Then

$$|F| \leq \left(\frac{\ell(\Pi) + 1}{2}\right)$$

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

\[ |F| \leq \left( \frac{\ell(\Pi) + 1}{2} \right) \]

\[ |F| = 18 \quad \ell(\Pi) = 10 \]

\[ |F| = 19 \quad \ell(\Pi) = 11 \]
Proof of Lemma: \(|F| \leq \left( \frac{\ell(\Pi) + 1}{2} \right)\)

Case 1: \(\Pi\) is a linear patch.

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

Example: \(|F| = 6\) \(\ell(\Pi) = 10\)

Thus,

\[
\left( \frac{\ell(\Pi) + 1}{2} \right) = \left( \frac{2|F| - 1}{2} \right) \geq |F|
\]
Proof of Lemma: $|F| \leq \left( \frac{\ell(\Pi) + 1}{2} \right)$

Case 2: $\Pi$ is not linear.

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

\begin{align*}
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\end{align*}
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,
  
  $$|F| = |F'| + \text{length of deleted side} \leq \binom{\ell(\Pi)}{2} + \ell(\Pi) = \binom{\ell(\Pi) + 1}{2}$$
Performing $\alpha$, $\beta$, or $\gamma$ 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 $\alpha$, $\beta$, or $\gamma$ unless all the pentagons are next to each other.
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 $\alpha$, $\beta$, or $\gamma$ 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
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.
This is joint work with:
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Questions?