Polycycles and their boundaries

Mathieu Dutour

ENS/CNRS, Paris and Hebrew University, Jerusalem

Michel Deza

ENS/CNRS, Paris and ISM, Tokyo

and Mikhail Shtogrin

Steklov Institute, Moscow

I. $(p, 3)$-polycycles

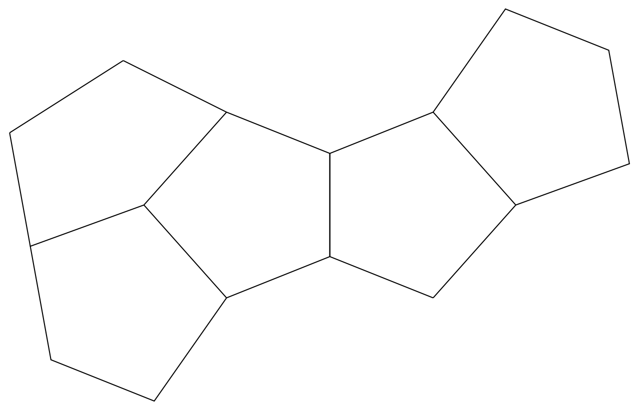
Polycycles

A finite $(p, 3)$-polycycle is a plane 2-connected finite graph, such that :

(i) all interior faces are (combinatorial) p-gons,

(ii) all interior vertices are of degree 3,

(iii) all boundary vertices are of degree 2 or 3.

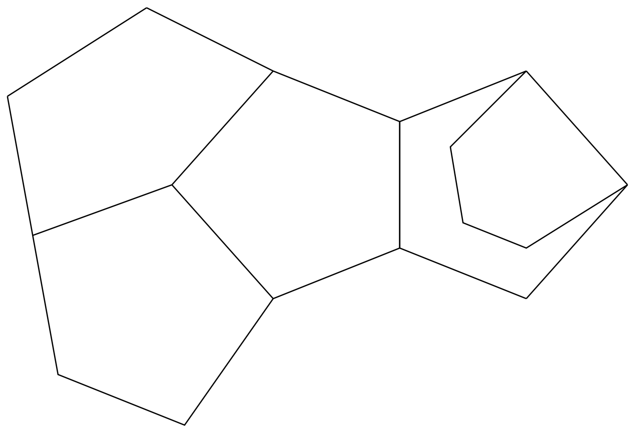


Theorem

The skeleton of a plane graph is the graph formed by its vertices and edges.

Theorem

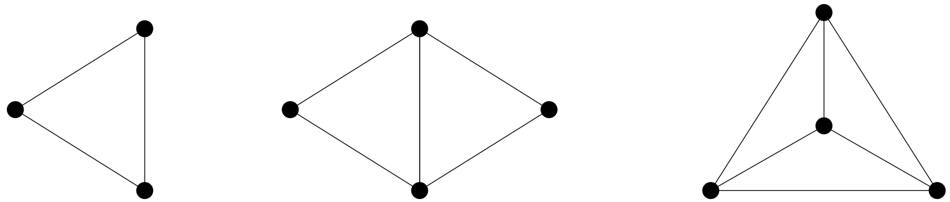
A $(p, 3)$-polycycle is determined by its skeleton with the exception of the Platonic solids, for which any of their faces can play role of exterior one



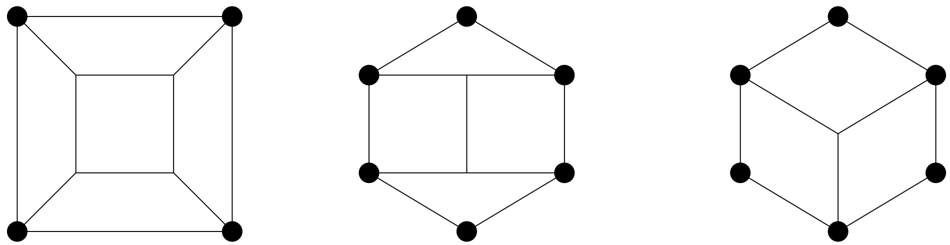
an unauthorized plane embedding

$(3,3)$ and $(4,3)$-polycycles

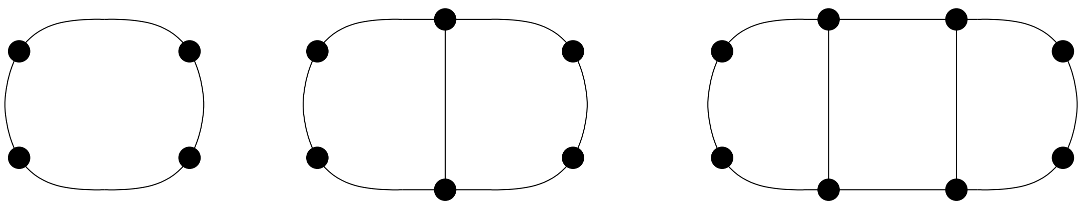
(i) Any $(3,3)$-polycycle is one of the following 3 cases:



(ii) Any $(4,3)$-polycycle belongs to the following 3 cases:



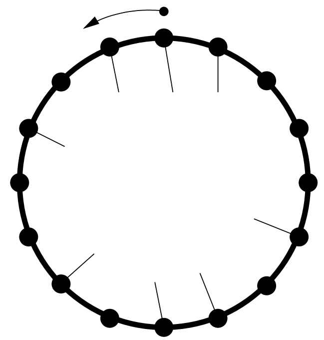
or belong to the following infinite family of $(4,3)$-polycycles:



So, those two cases are trivial.

Boundary sequences

The boundary sequence is the sequence of degrees (2 or 3) of the vertices of the boundary.

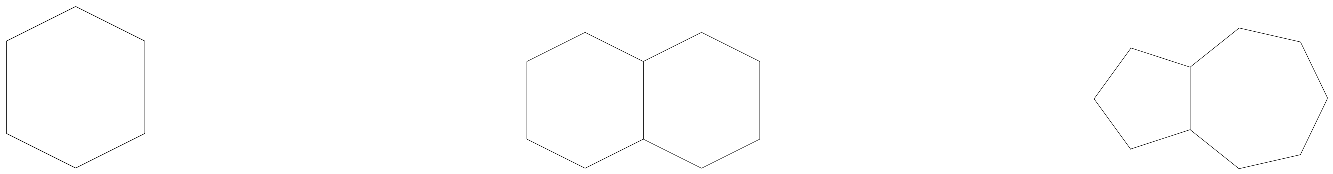


Associated sequence is 3323223233232223

- The boundary sequence is defined only up to action of D_n, i.e. the dihedral group of order $2n$ generated by cyclic shift and reflexion.
- The invariant given by the boundary sequence is the smallest (by the lexicographic order) representative of the all possible boundary sequences.

Enumeration of $(p, 3)$-polycycles

There exist a large litterature on enumeration of $(6, 3)$-polycycles; they are called benzenoids.

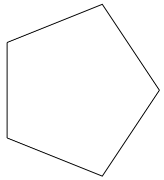


benzene C_6H_6 naphtalene $C_{10}H_8$ azulene $C_{10}H_8$

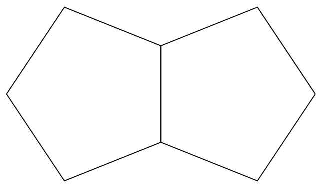
Algorithm for enumerating $(p, 3)$-polycycles with n p-gons:

1. Compute the list of all p-gonal patches with $n-1$ p-gons
2. Add a p-gon to it in all possible ways
3. Compute invariants like their smallest (by the lexicographic order) boundary sequence
4. Keep a list of nonisomorph representatives (we use here the program **nauty** by Brendan Mc Kay)

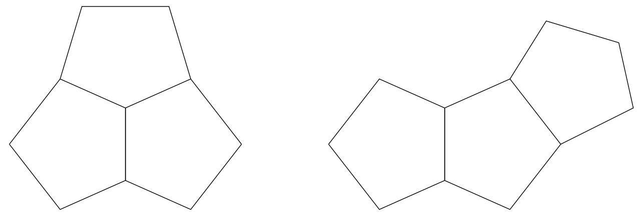
Enumeration of small $(5,3)$-polycycles



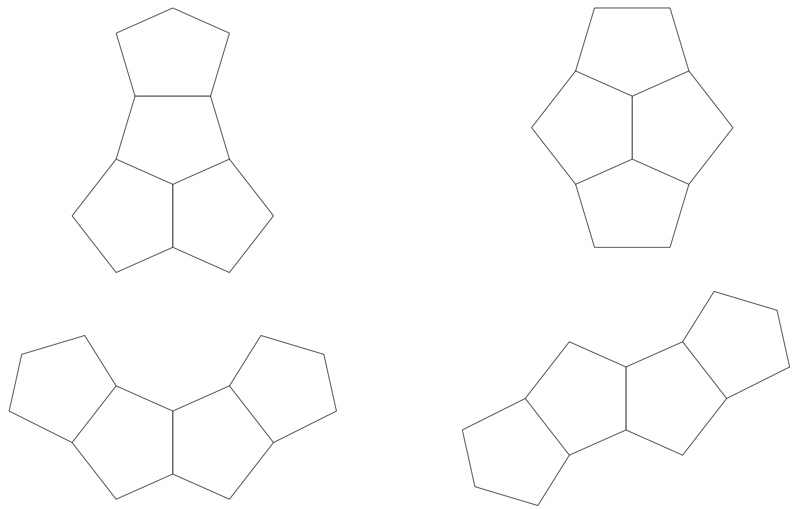
$n = 1$



$n = 2$



$n = 3$

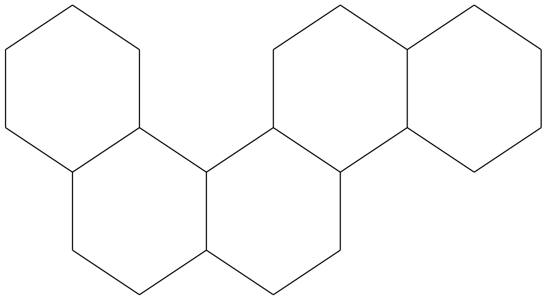


$n = 4$

1	1	6	18	11	1337
2	1	7	35	12	3524
3	2	8	87	13	9262
4	4	9	206	14	24772
5	7	10	527	15	66402

Benzenoids of lattice type

We say that a $(6,3)$-polycyle has lattice type if its skeleton is a partial subgraph of the skeleton of the partition of the plane into hexagons.



Such $(6,3)$-polycycles are uniquely defined by their boundary sequence.

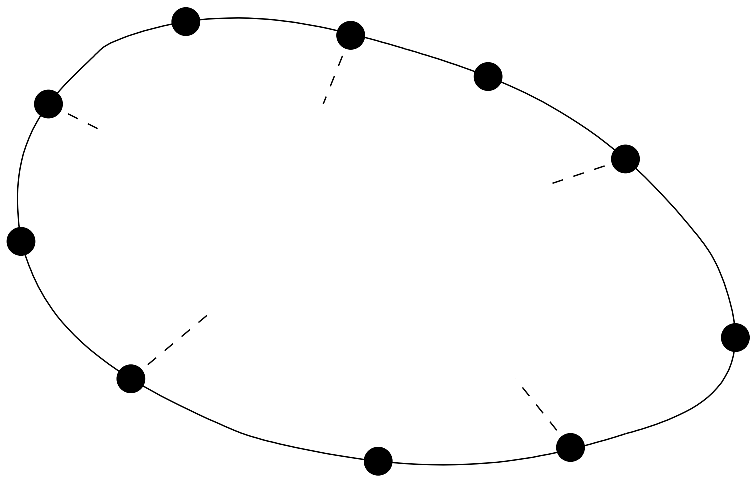
M. Deza, P.W. Fowler, V.P. Grishukhin, *Allowed boundary sequences for fused polycyclic patches, and related algorithmic problems*, Journal of Chemical Information and Computer science **41-2** (2001) 300–308.

II. $(p, 3)$-polycycles with given boundary

The filling problem

- Does there exist $(p, 3)$-polycycles with given boundary sequence?
- If yes, is this $(p, 3)$-polycycle unique?
- Find an algorithm for solving those problems computationally.

Remind, that the cases $p = 3$ or 4 are trivial.
Let $p = 5$; consider, for example, the sequence 2323232323



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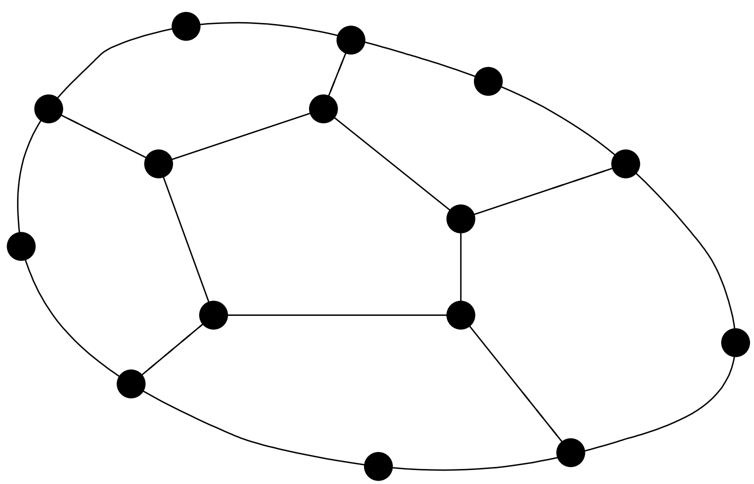
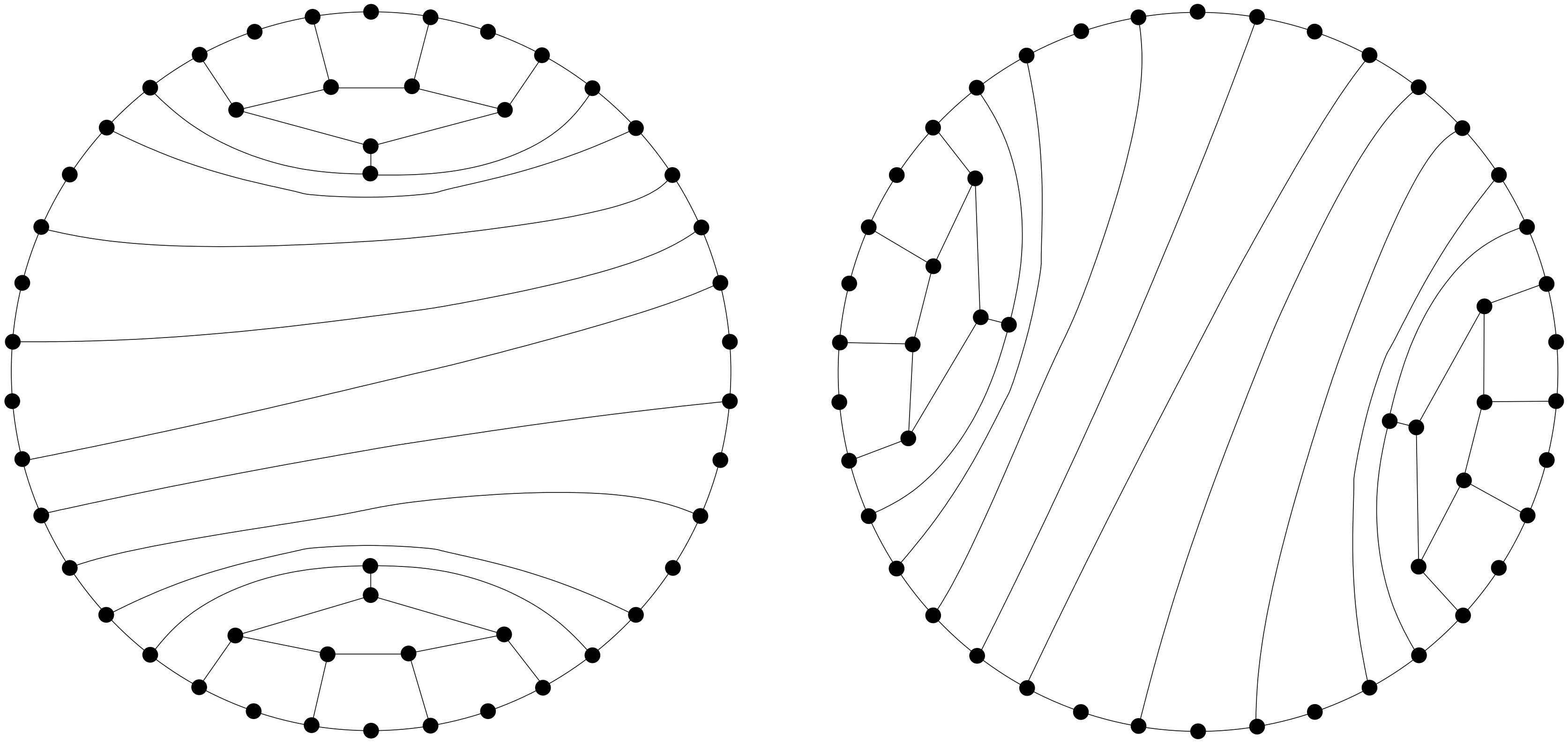


The case of $(5,3)$-polycycles

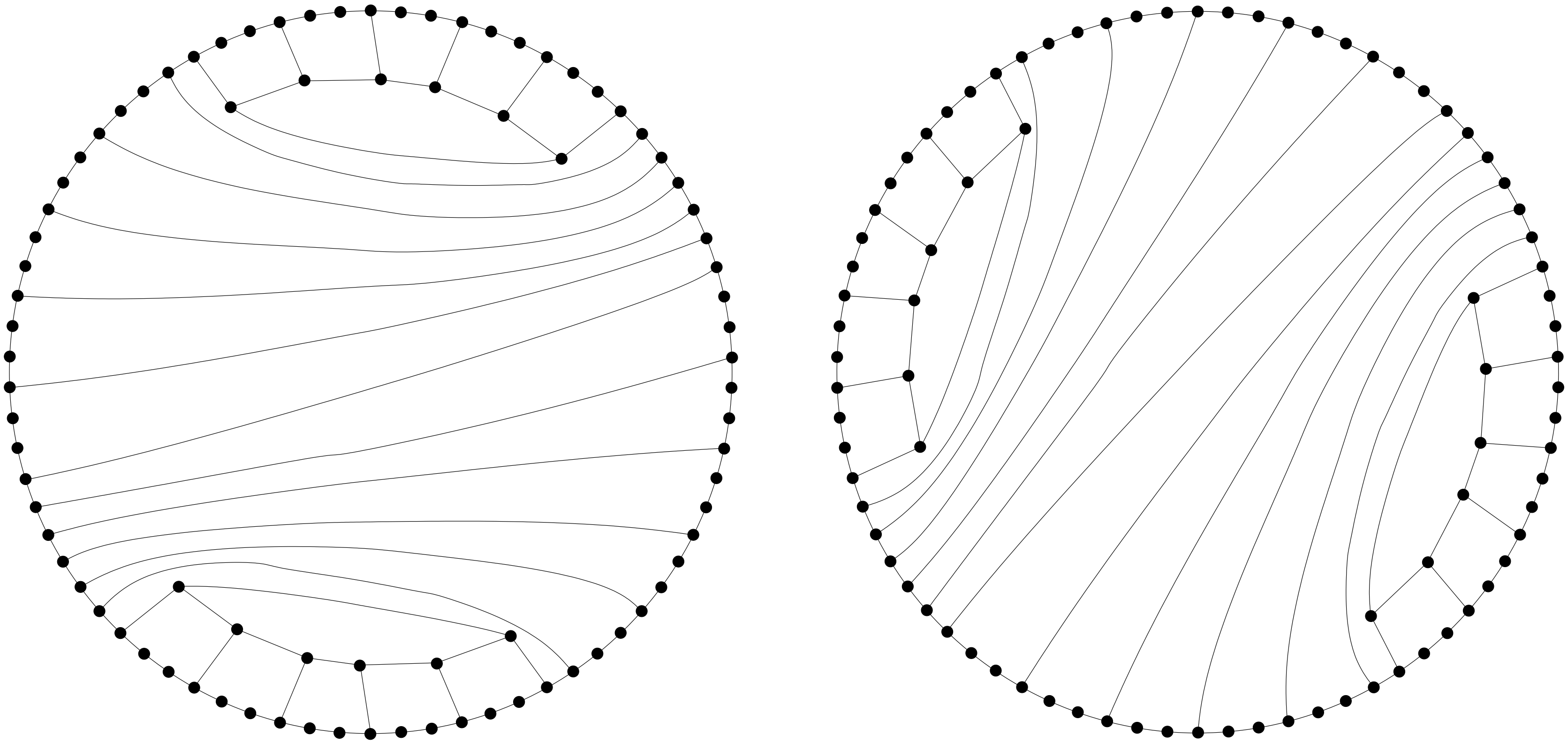
Two $(5,3)$-polycycles with the same boundary.



Boundary sequence: 12, 26 vertices of degree 2, 3, resp.
Symmetry groups: of boundary: C_{2v}, of polycycles: C_2.
Fillings: 20 pentagons, 12 interior points.

The case of $(6,3)$-polycycles

Two $(6,3)$-polycycles with the same boundary.

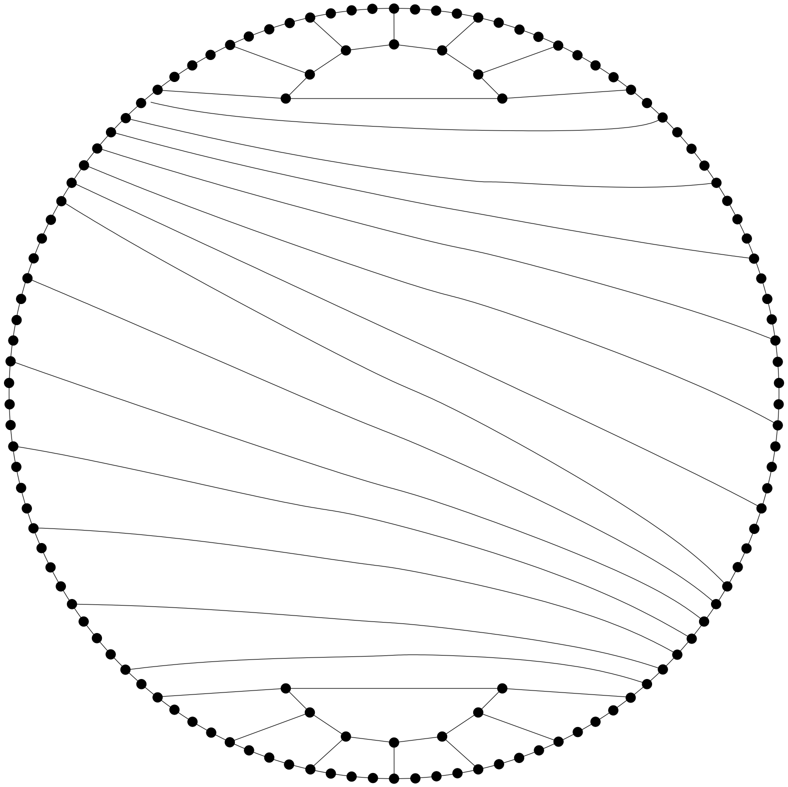


Boundary sequence: 40, 34 vertices of degree 2, 3, resp.

Symmetry groups: of boundary: C_{2v}, of polycycles: C_2.

Fillings: 24 hexagons, 12 interior points.

Non-uniqueness for any $p \geq 6$



Boundary sequence is:
$b = u2^{p-1}u3^{p-6}u2^{p-1}u3^{p-6}$
$u = (23^{p-4})^{p-1}2$;
$6p-2$ vertices of degree 3 and $4p^2-18p+4$ of degree 2.

Symmetry groups are:
of boundary: C_{2v},
of polycycles: C_2.

This domain is filled in two ways (by $4p$ p-gons; $2p$ interior 3-valent vertices).
Thm.: The boundary does not determine $(p, 3)$-polycycle if $p \geq 5$. Conj.: but it determines it if the filling is by less than $4p$ p-gons.

Euler formula for $(p, 3)$-polycycles

Let P be a $(p, 3)$-polycycle. Let v_2, v_3 be the number of vertices of degree 2 or 3 on the boundary. Let f_p the number of p-gonal faces and x the number of interior vertices

Theorem

(i) one has the relations

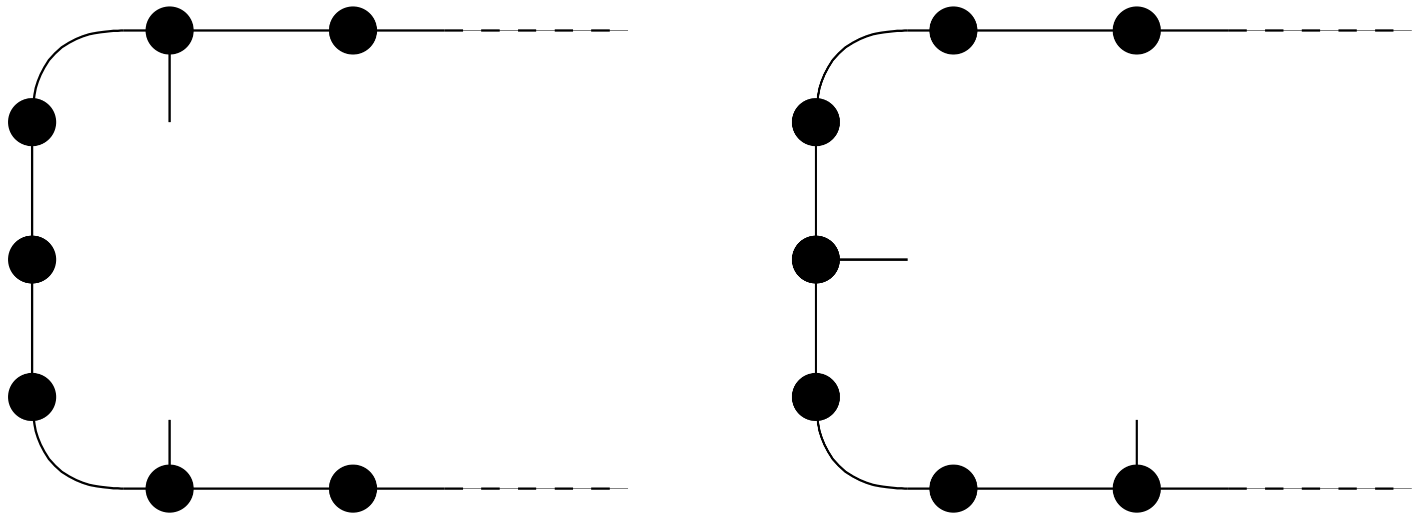
$$\begin{cases} f_p - \frac{x}{2} & = & 1 + \frac{v_3}{2} \\ pf_p - 3x & = & v_2 + 2v_3 \end{cases}$$

(ii) If $p \neq 6$, then f_p and x are determined by the boundary sequence.

(iii) If $p = 6$, then $v_2 = 6 + v_3$.

Possible filling

Let us illustrate the algorithm for the simplest case $p = 5$. In some cases we can complete the patch directly.



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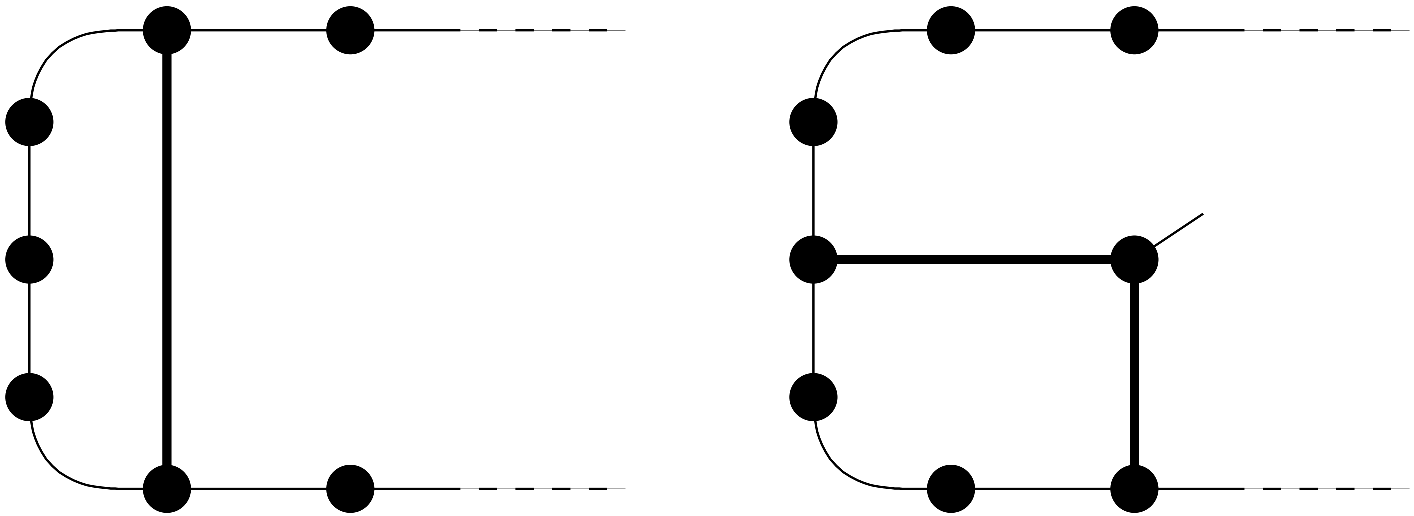

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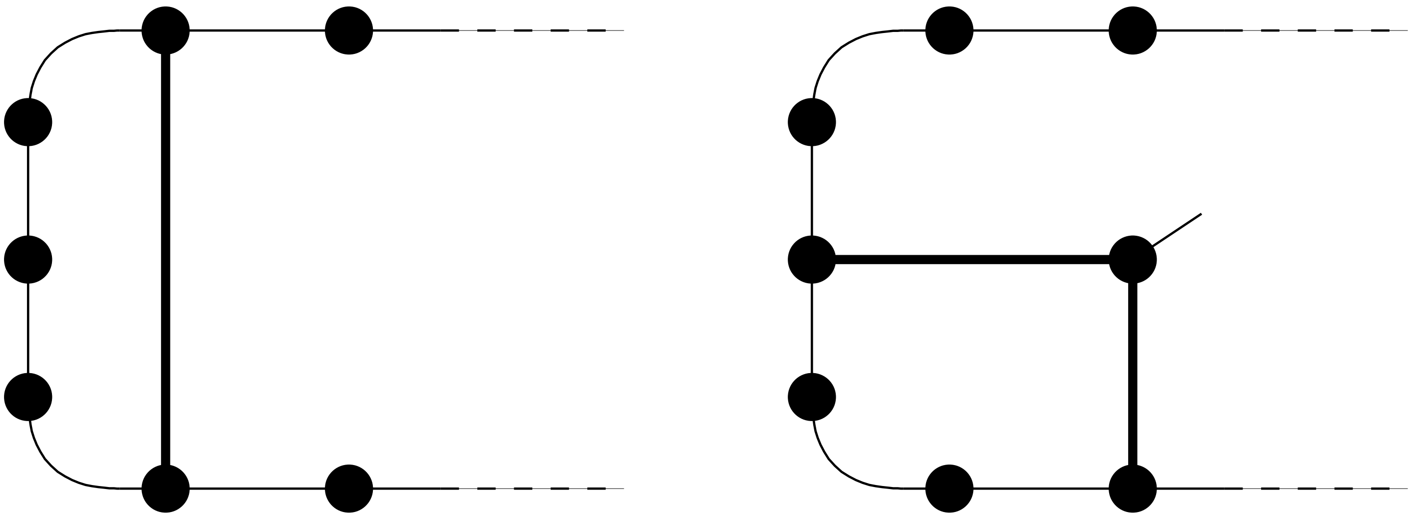
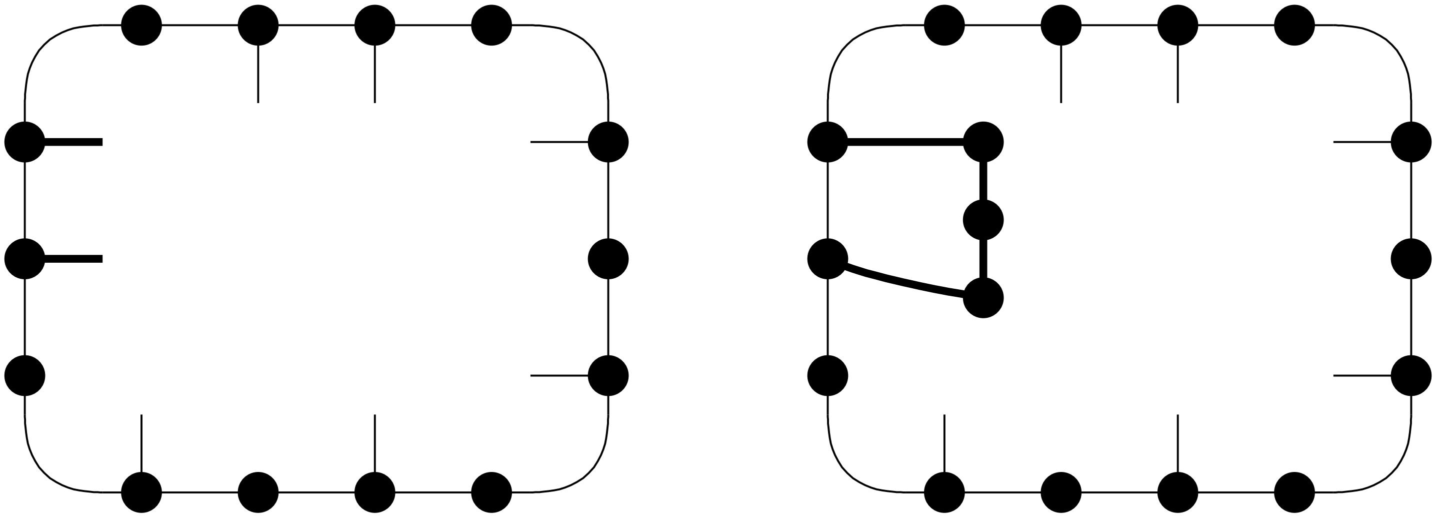
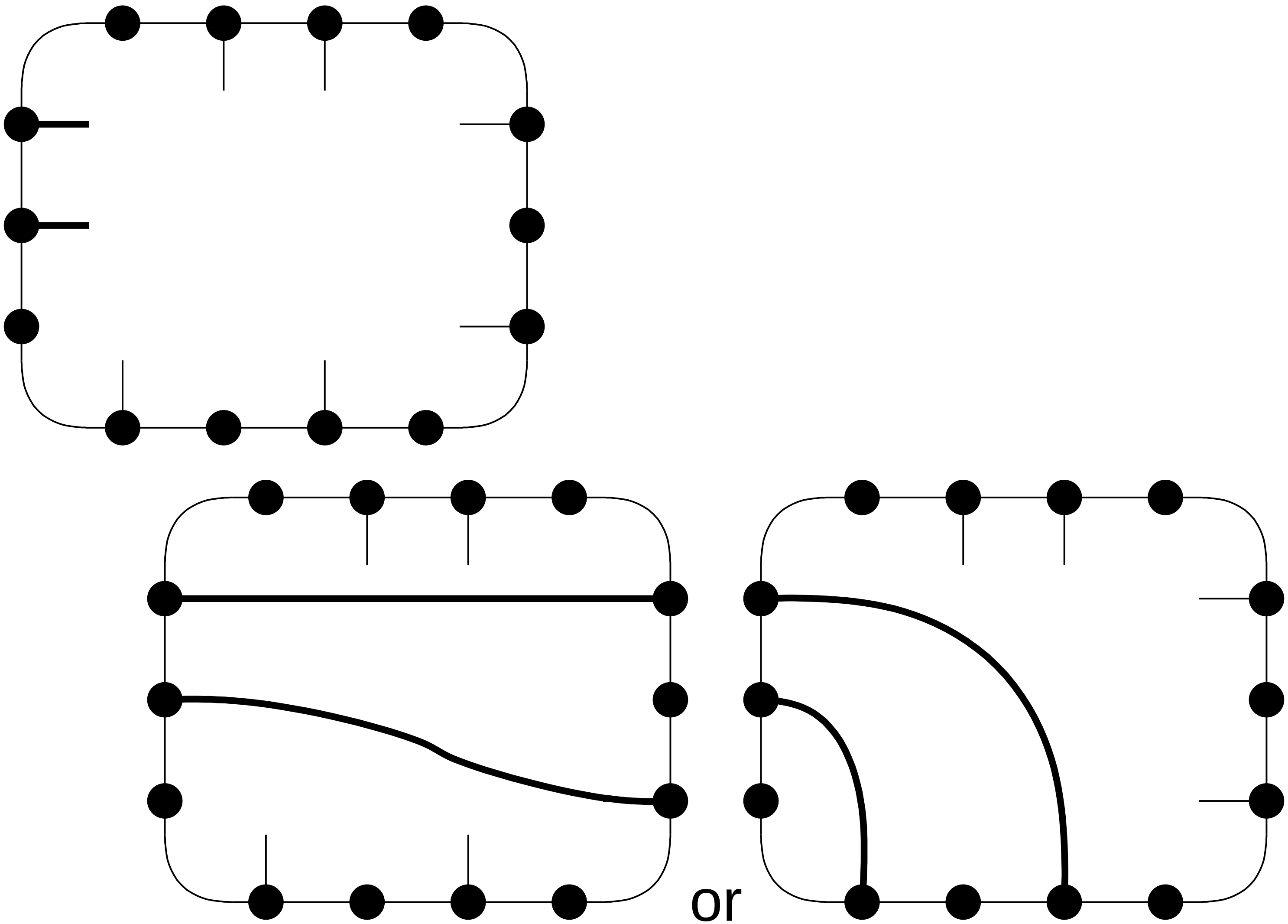


But in some cases more is needed:

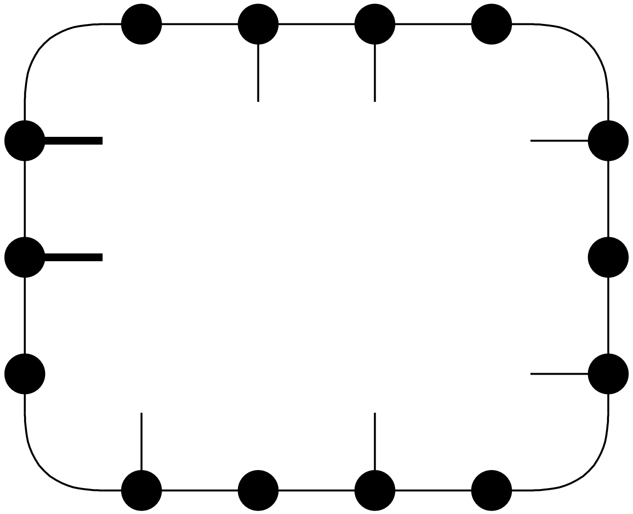
Different possible options

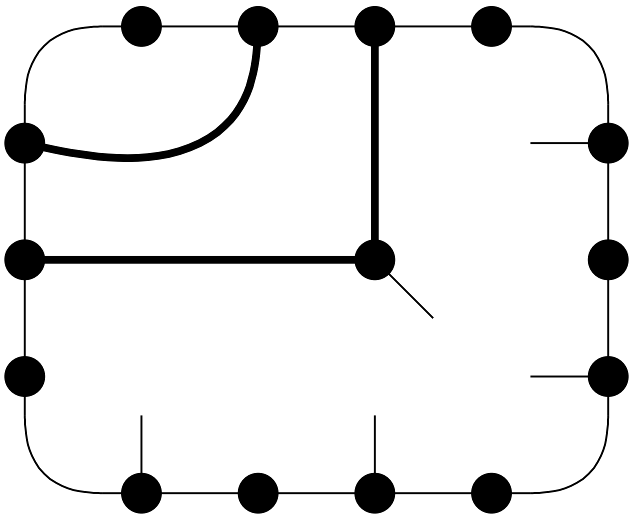


Different possible options

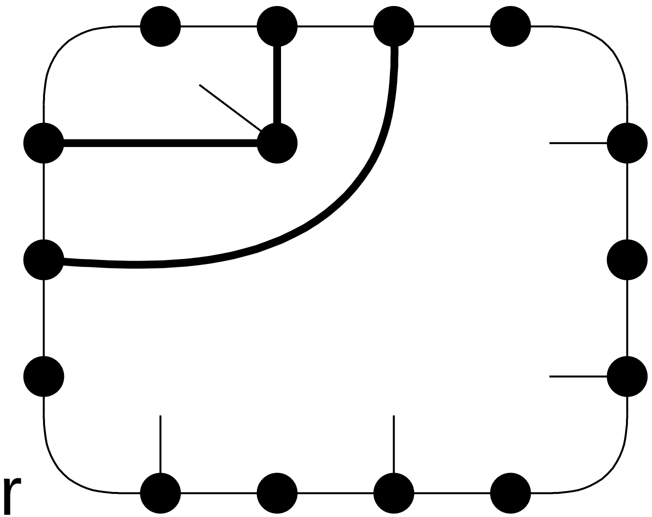


Different possible options





or



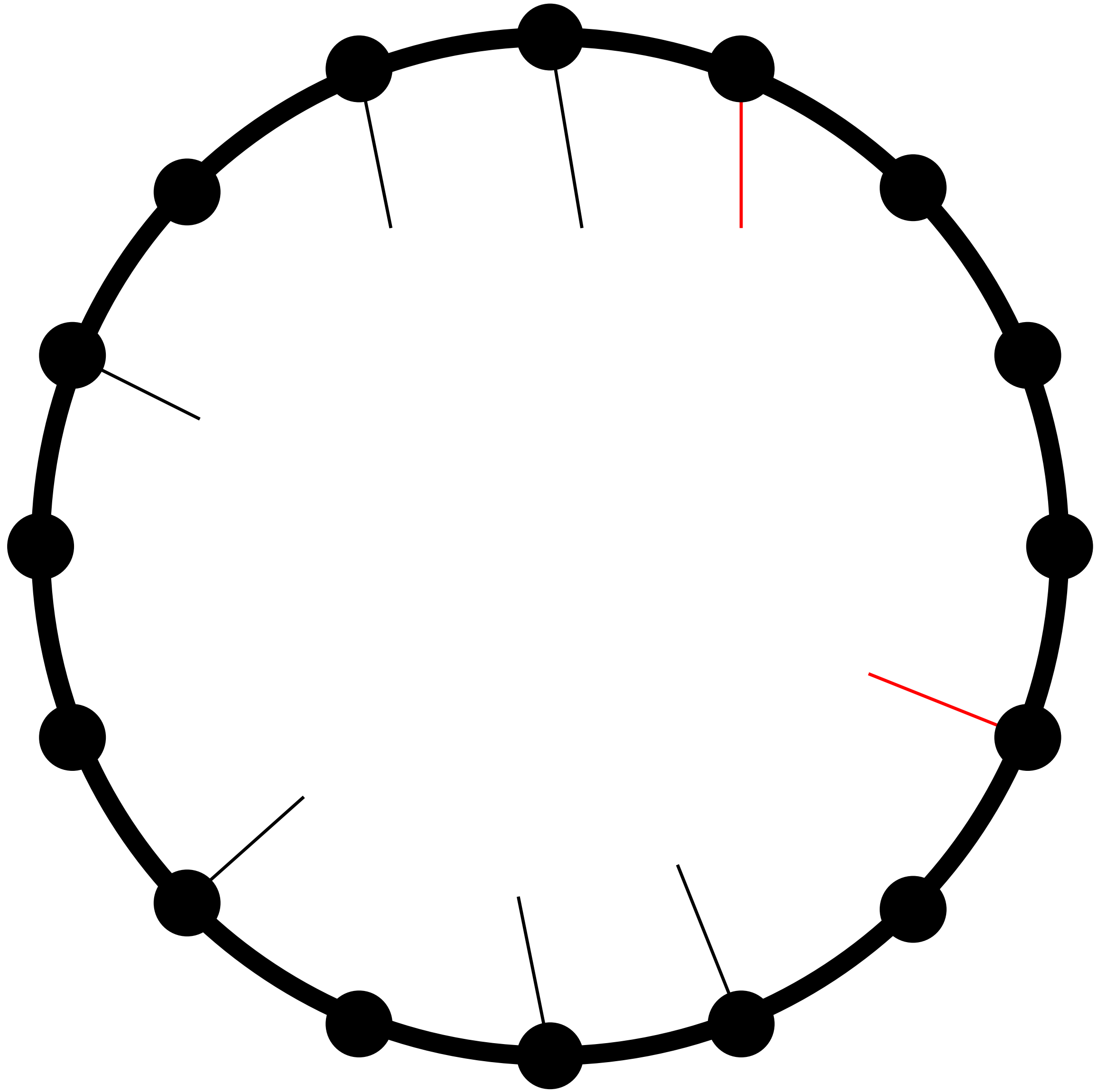
Algorithm

A patch of p-gonal faces is a group of faces with one or more boundaries.
Take a boundary of a patch of faces. Then:

1. Take a pair of vertices of degree 3 on the boundary and consider all possible completions to form a p-gon.
2. Every possible case define another patch of faces. Depending on the choice, the patch will have one or more boundaries.
3. For any of those boundaries, reapply the algorithm.

This algorithm is a tree search, since we consider all possible cases.

An example of a search



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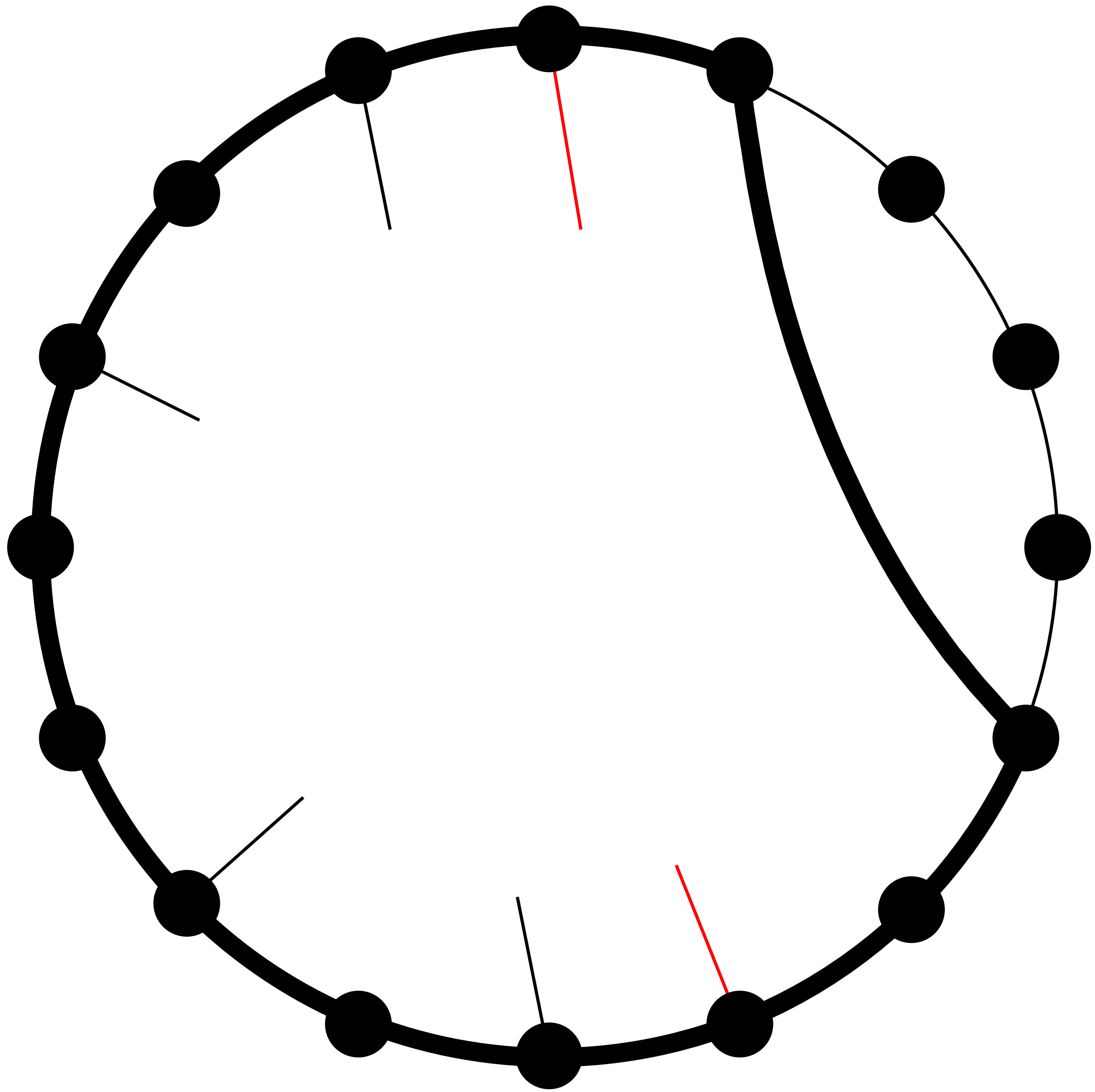

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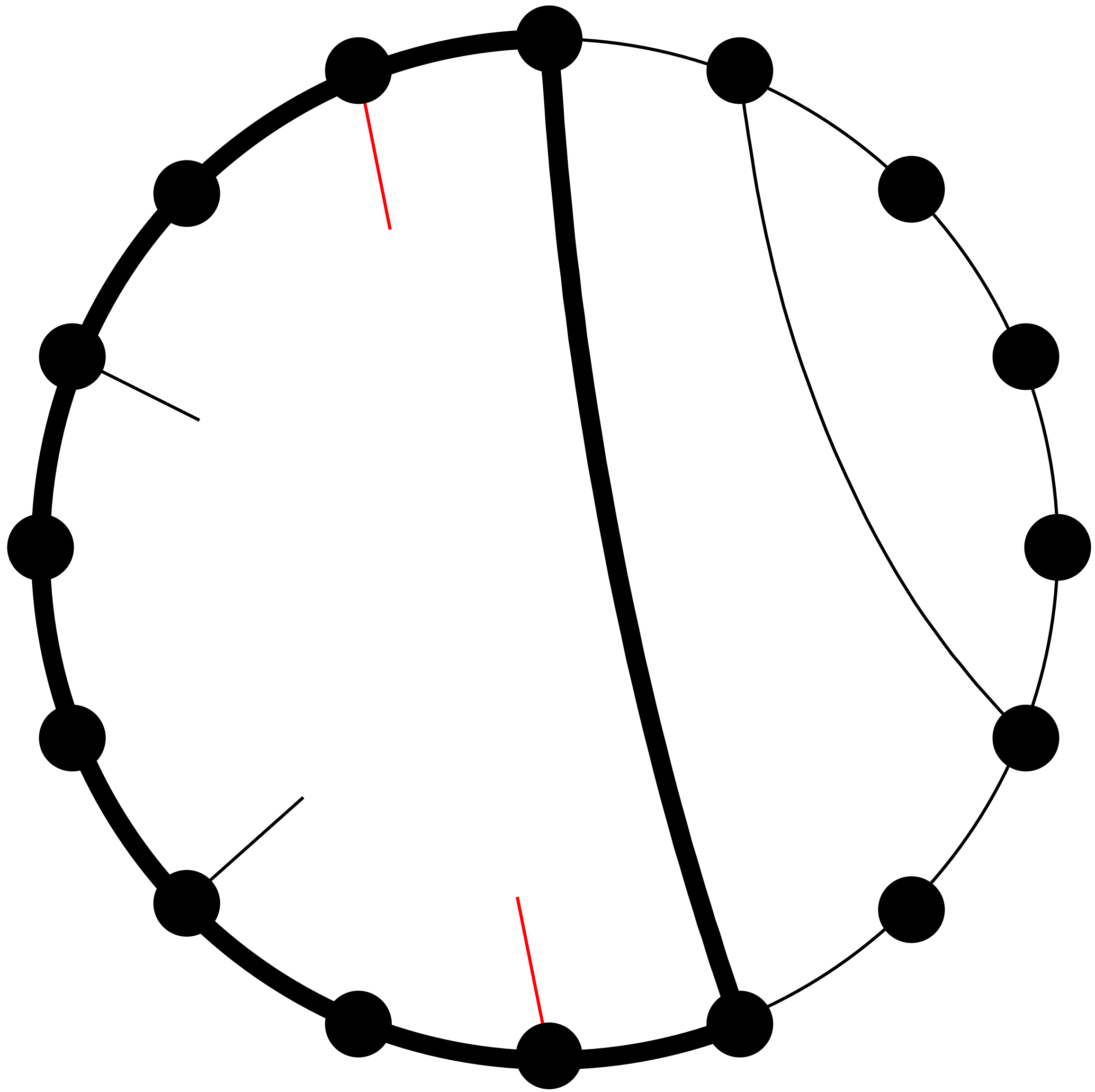

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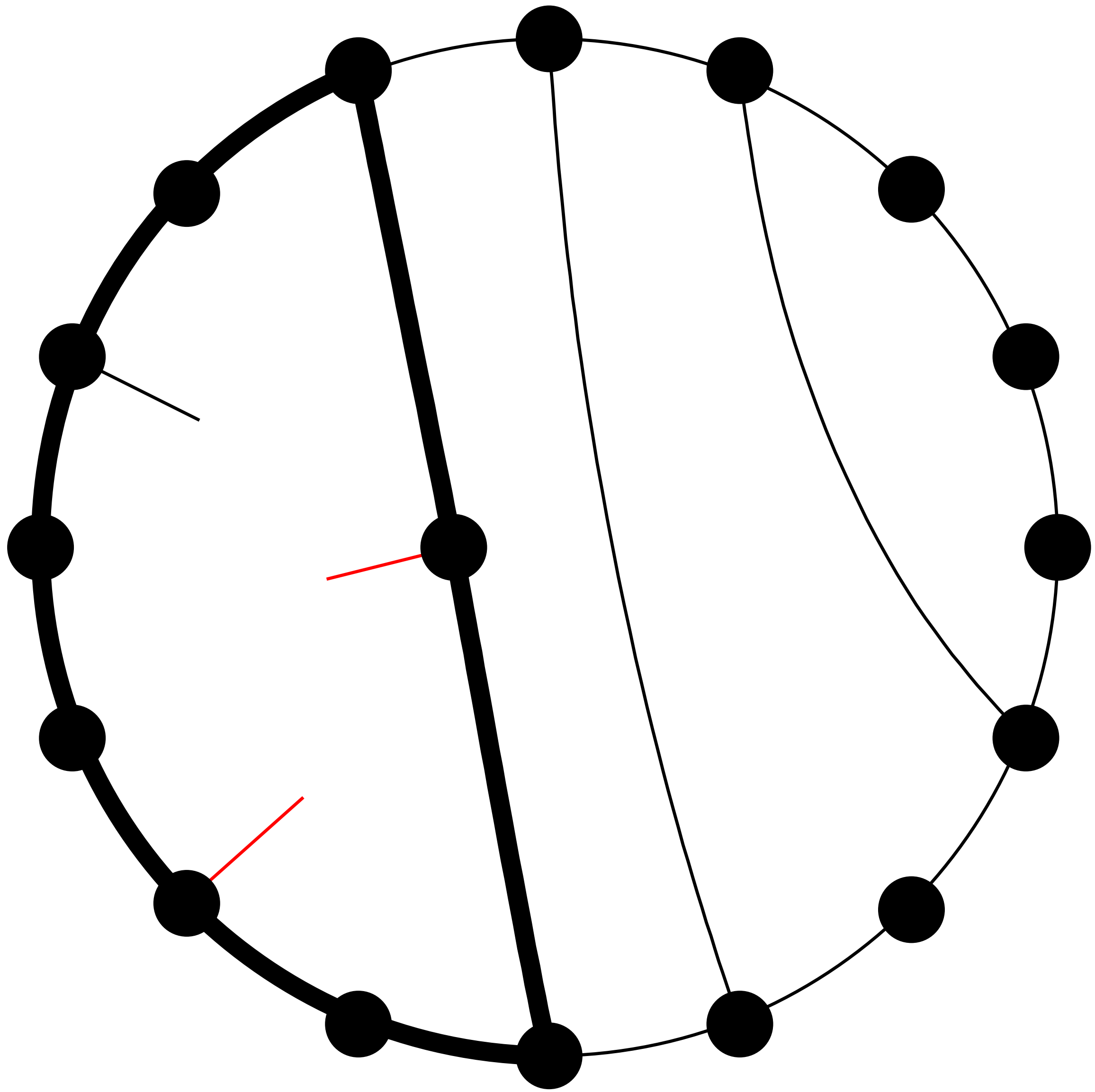

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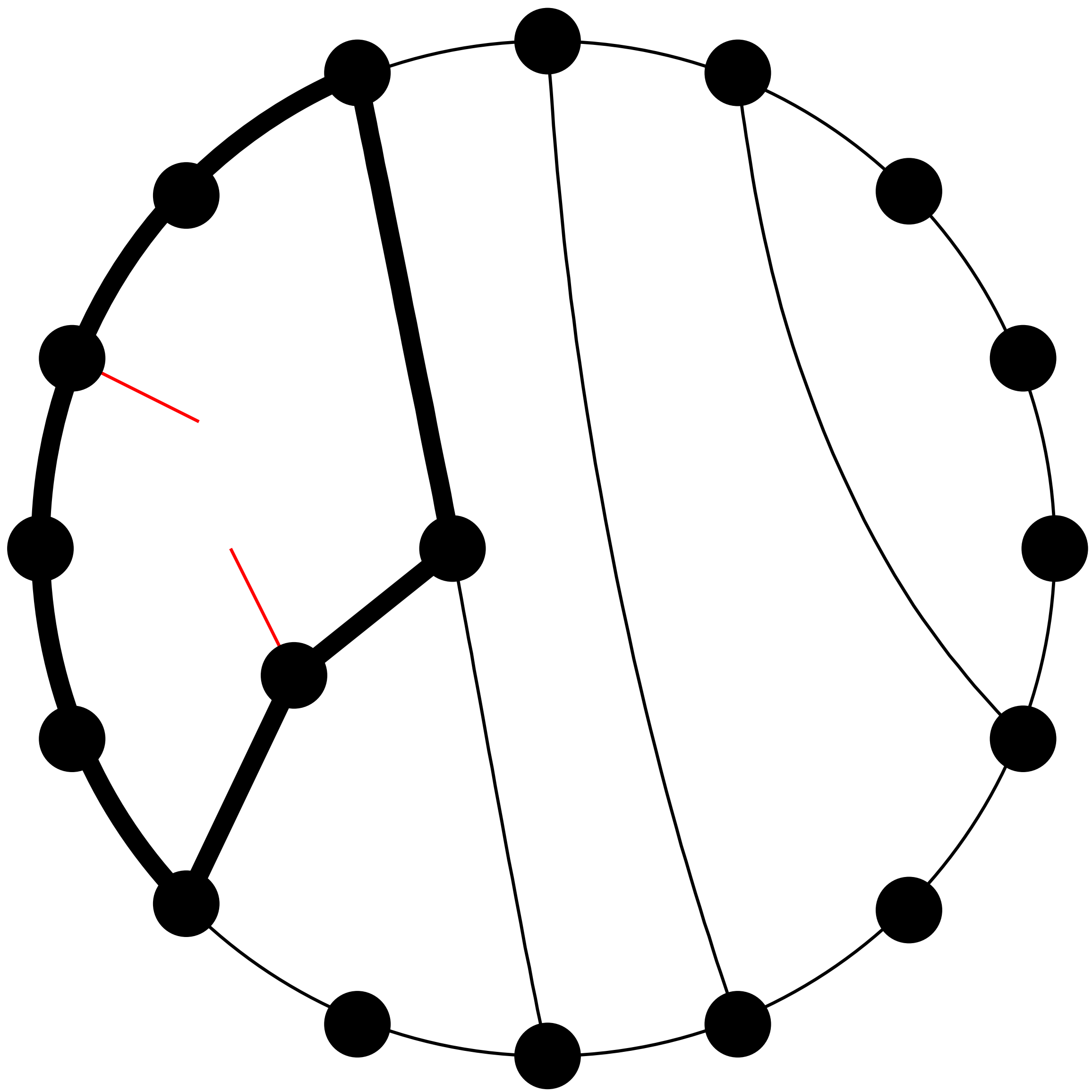

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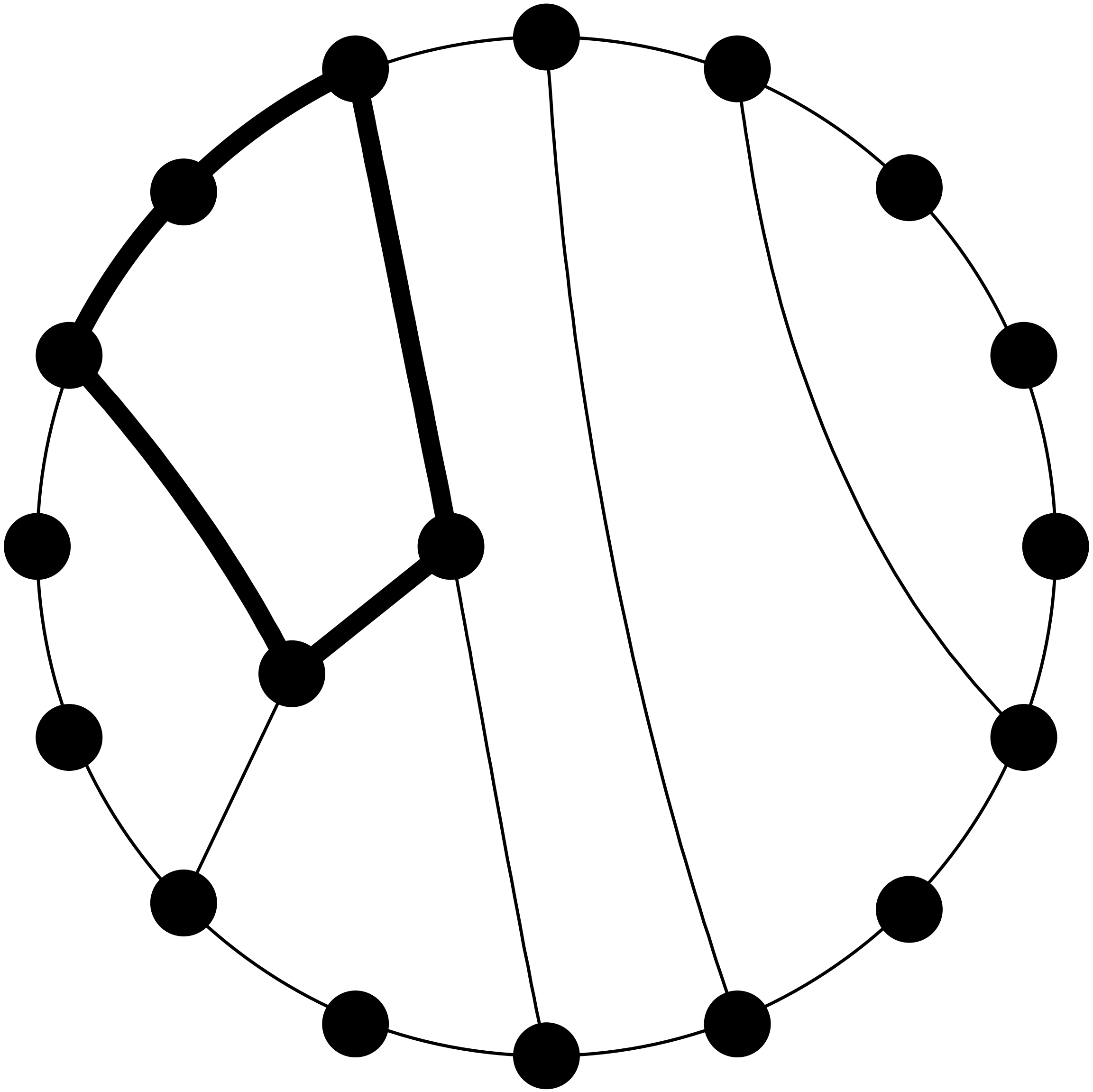

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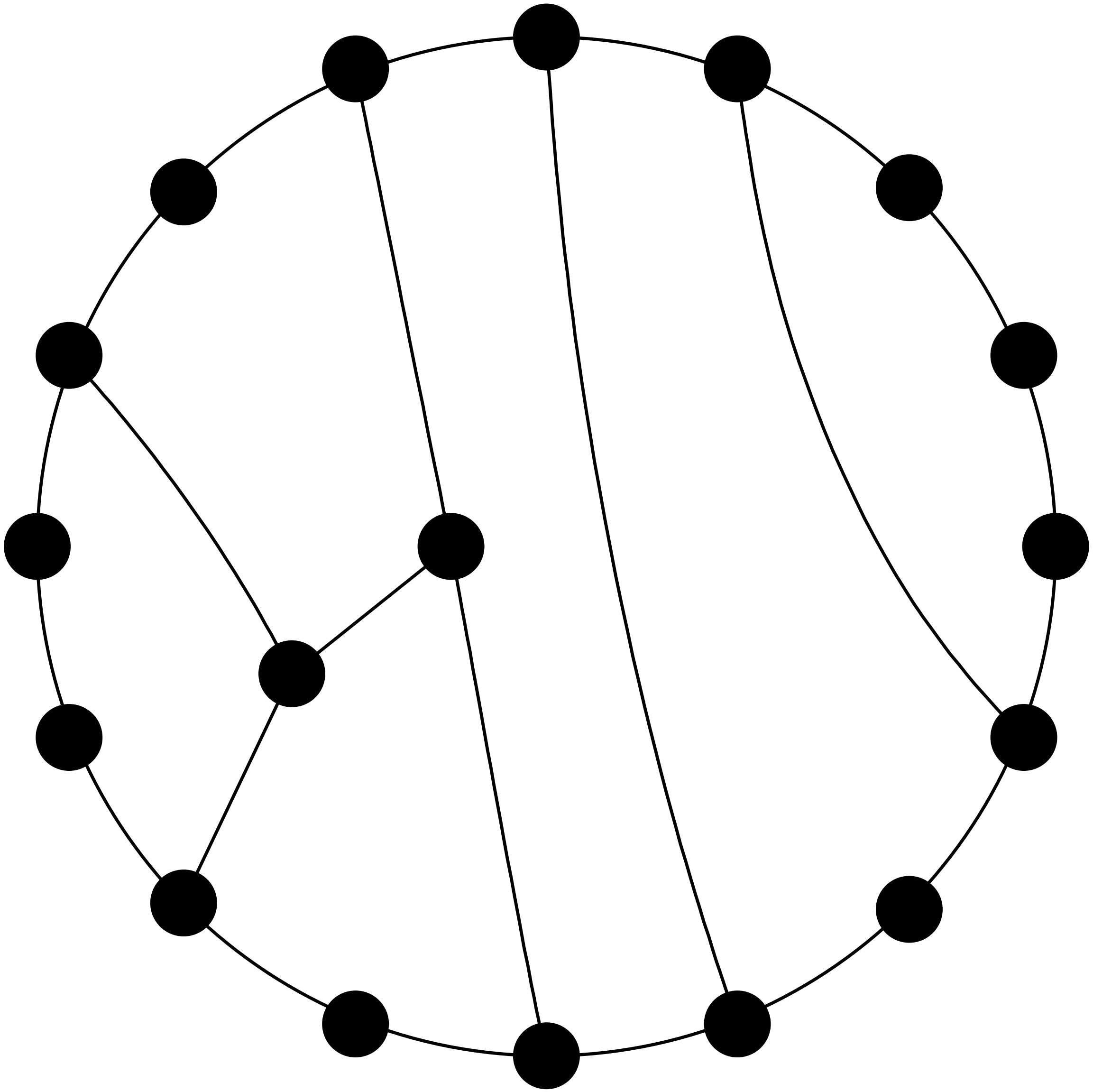
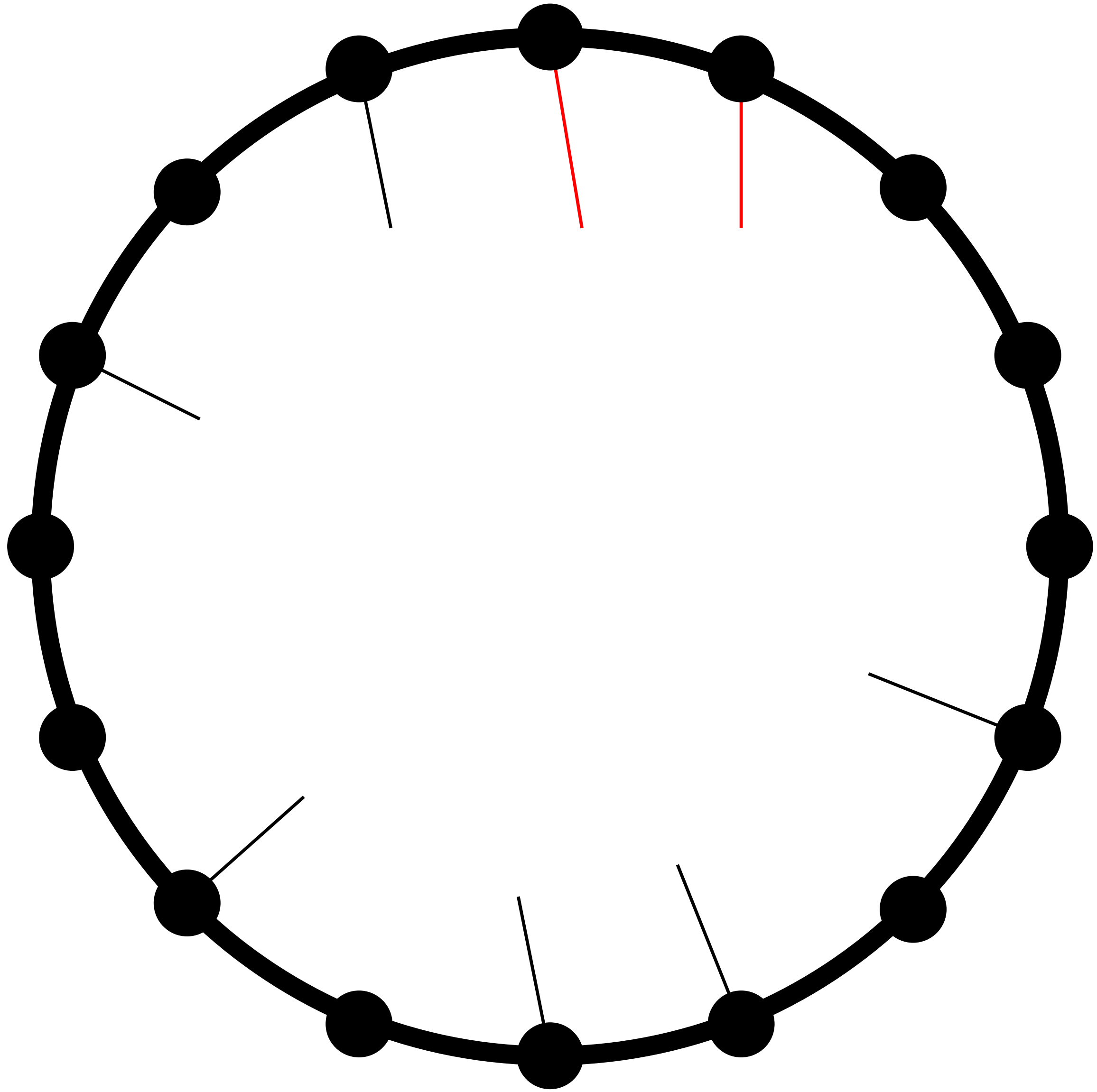
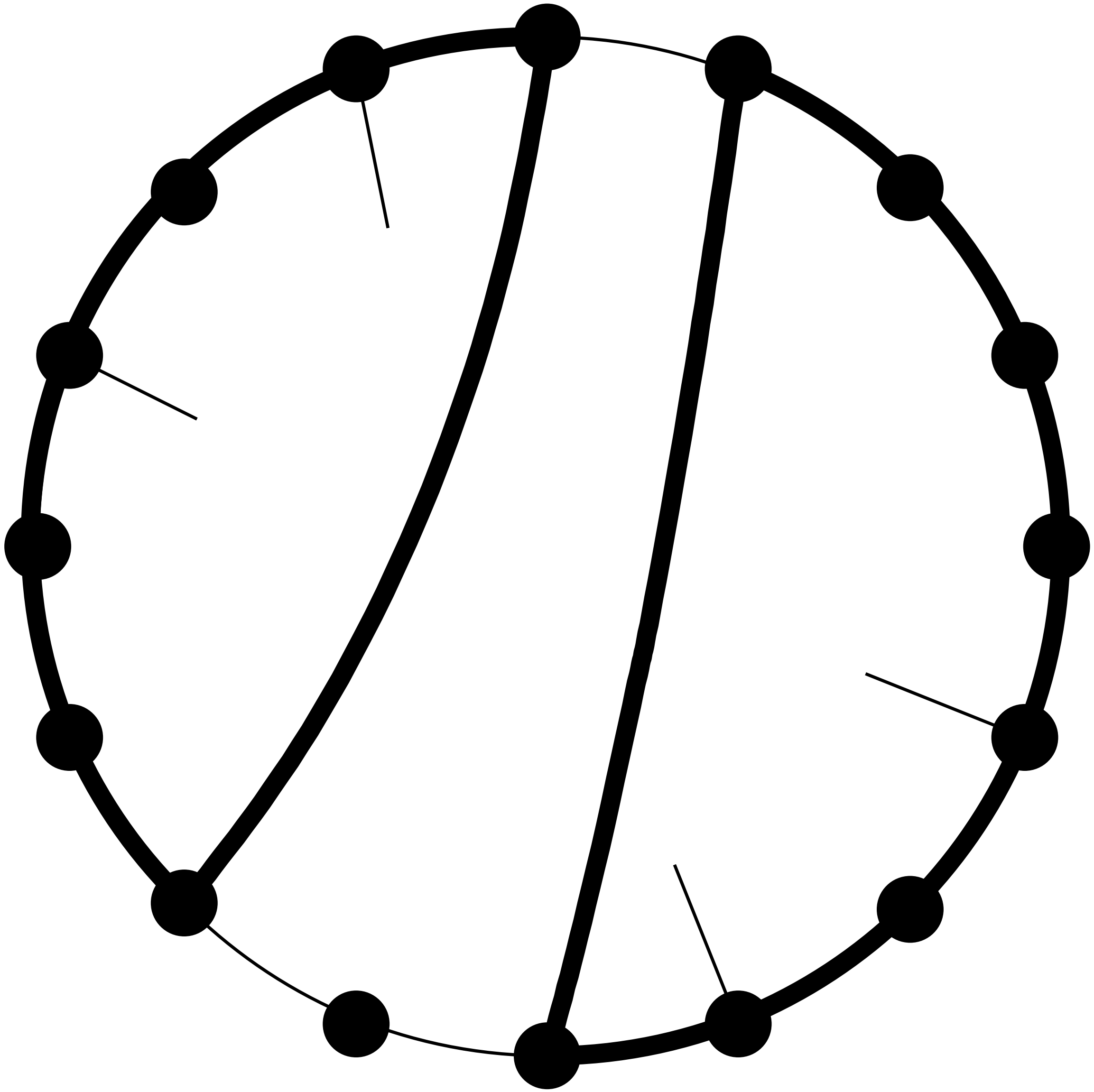


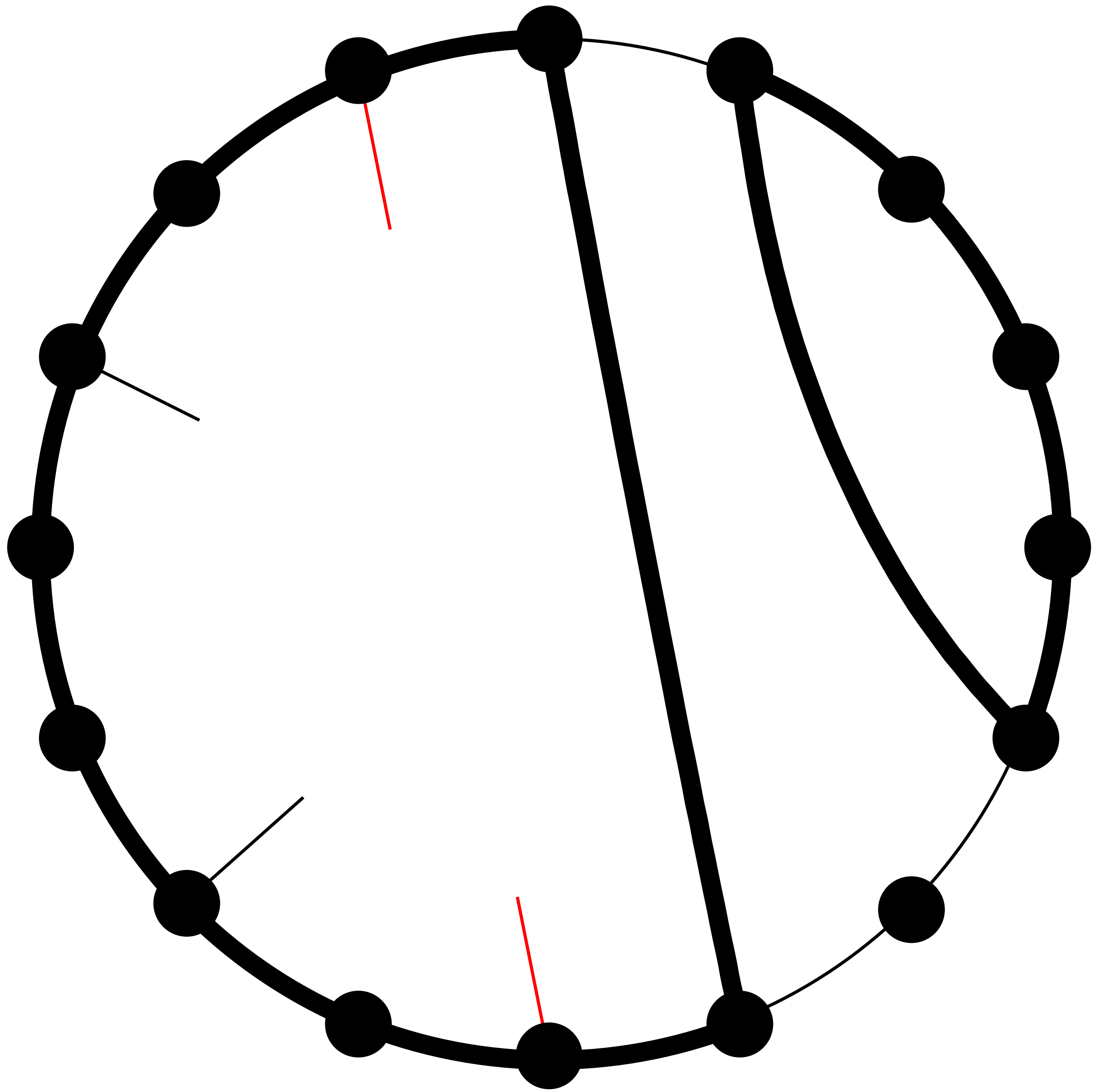
Another possible search



Another possible search



Another possible search



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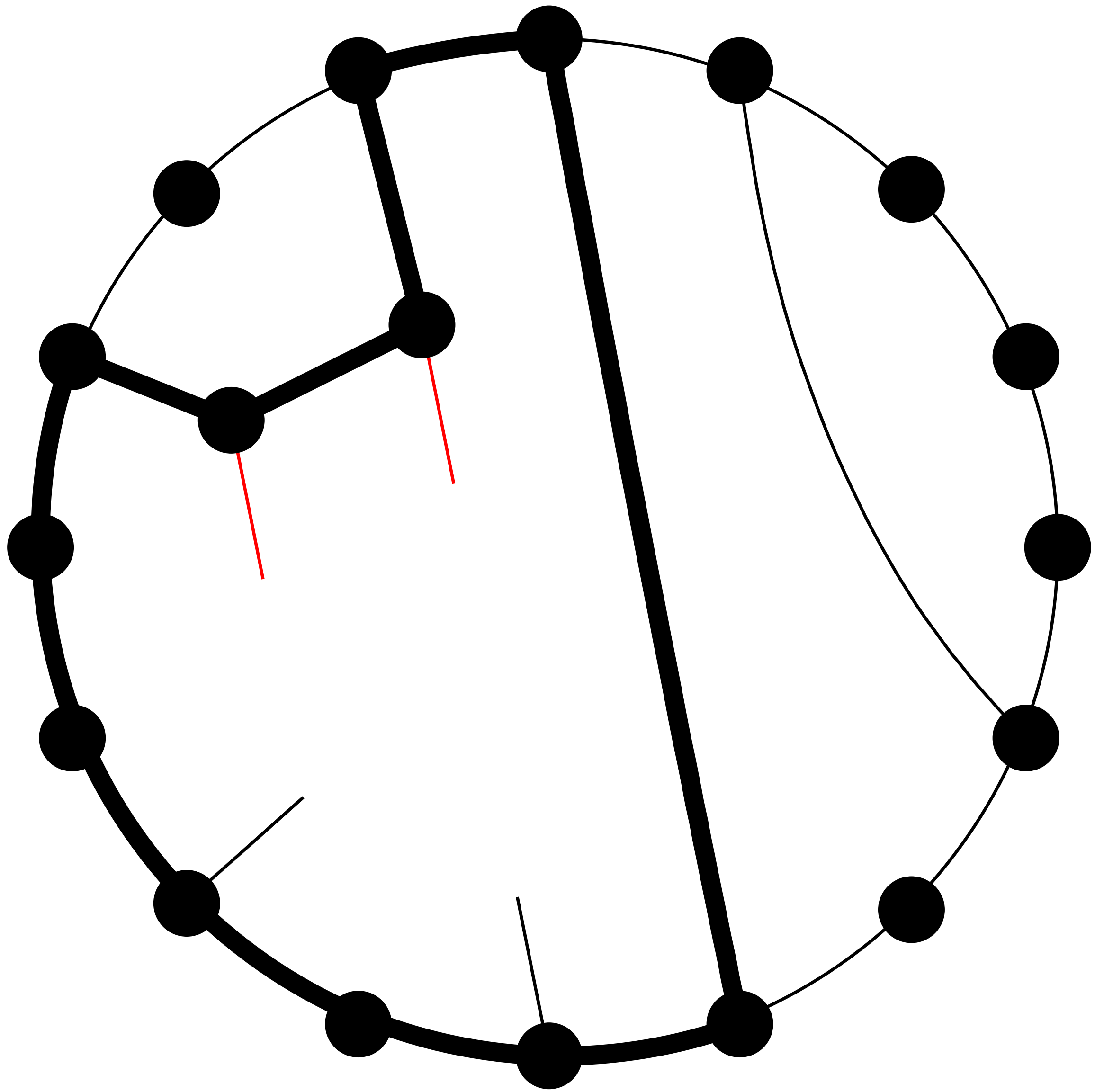
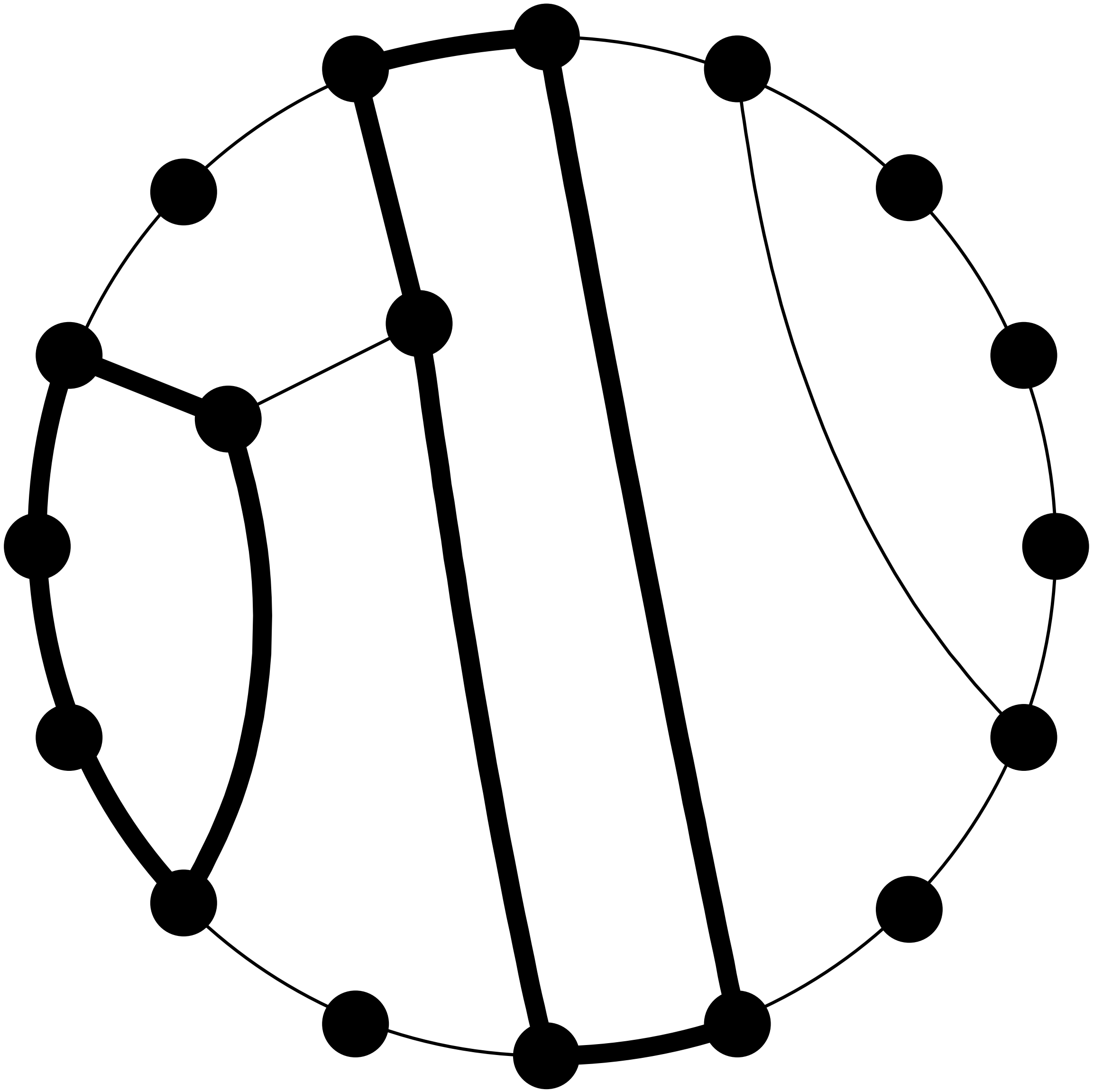
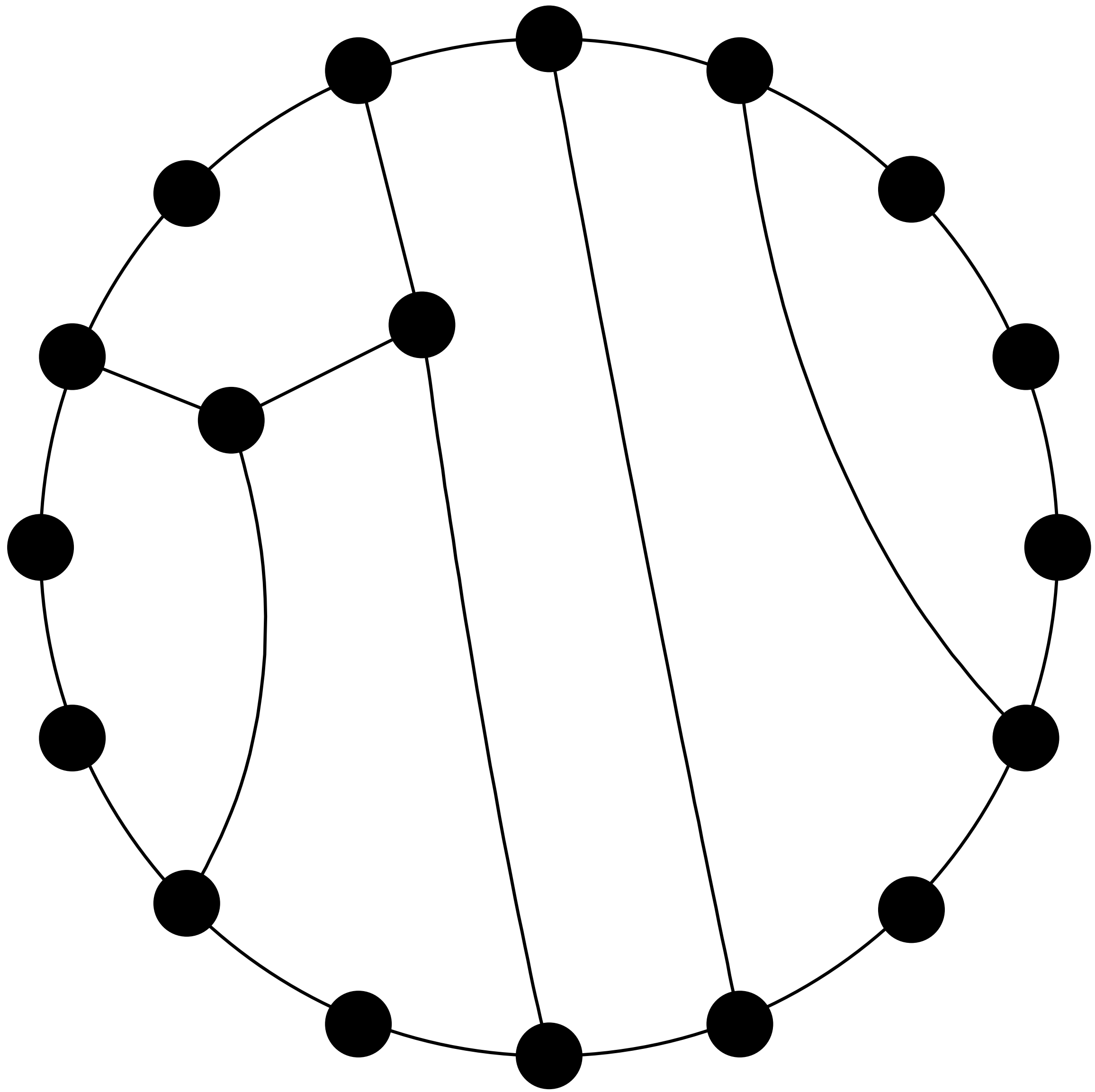


Another possible search



Another possible search



Possible speedups

- Limitation of tree size:
  - Do all “automatic fillings” when there are some.
  - Then, we can select the pair of consecutive vertices of degree 3 with maximal distance between them.
- Kill some branches if :
  - f_p or x are not non-negative integers (they are computed from the boundary sequence by Euler formula).
  - two consecutive vertices of degree 3 do not admit any extension by a p-gon.

The combination of those tricks is insufficient in many cases. For the enumeration of the maps $M_n(p, q)$ below, this is the critical bottleneck.

III. maps of p-gons with a ring of q-gons

The problem

A $M_n(p,q)$ denotes a 3-valent plane graph having only p-gonal and q-gonal faces, such that the q-gonal faces form a ring, i.e. a simple cycle, of length n.

Theorem: *One has the equation*

$$((4-p)(q-4)+4)n+(6-p)(x+x')=4p$$

with x and x' being the number of interior vertices in two $(p,3)$-polycycles defines by the ring of n q-gons.

M. Deza and V.P. Grishukhin, *Maps of p-gons with a ring of q-gons*, Bull. of Institute of Combinatorics and its Applications **34** (2002) 99–110.

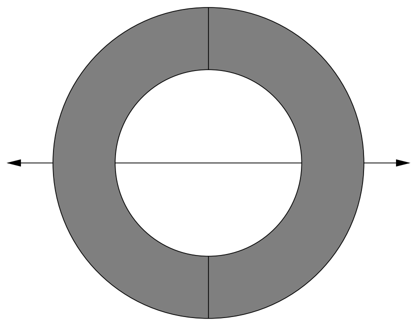
Classification theorem

Main Theorem

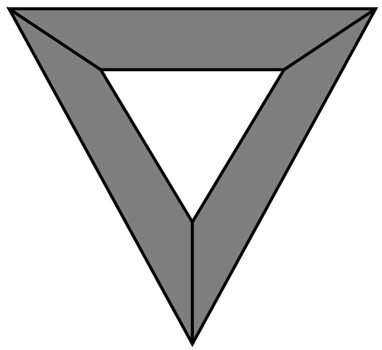
Besides the cases (p,q)=$(7,5)$ *and* $(5,q)$ *with* $q \geq 8$, *all such maps are known;*

If $q=4$, then the map is $Prism_{p=n}$; from now, let $q \geq 5$.

If $p=3$, two possibilities:



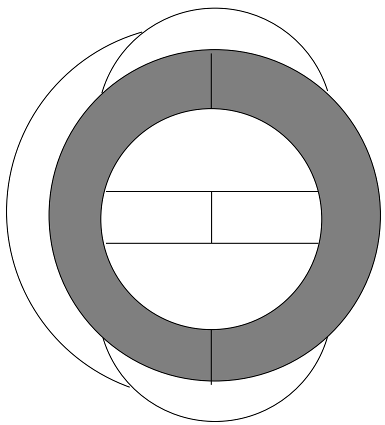
$M_2(3,6)(D_{2h})$



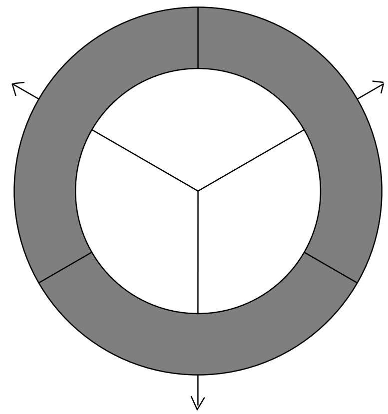
$M_3(3,4)(D_{3h})$

Case $p = 4$

If $p = 4$, two possibilities:

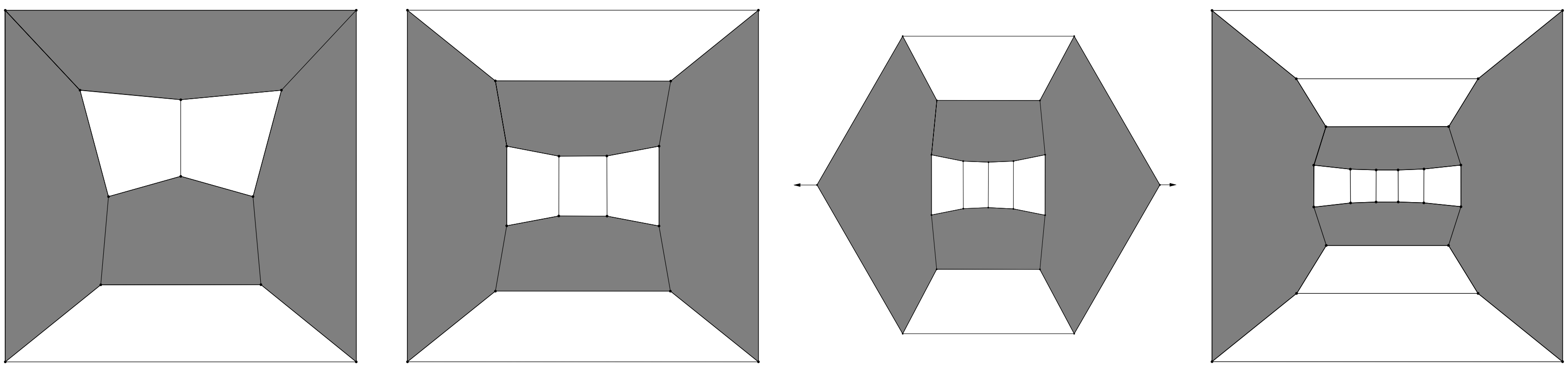


$M_2(4, 8)(D_{2h})$



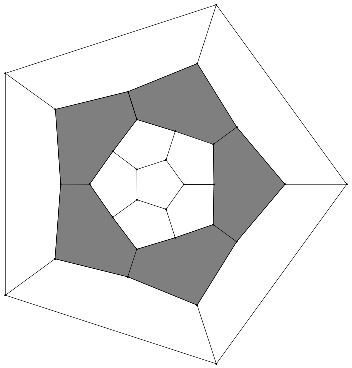
$M_3(4, 6)(D_{3h})$

and an infinite serie

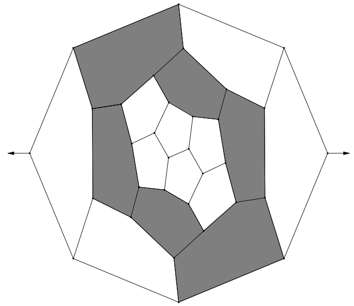


Case $p = 5$

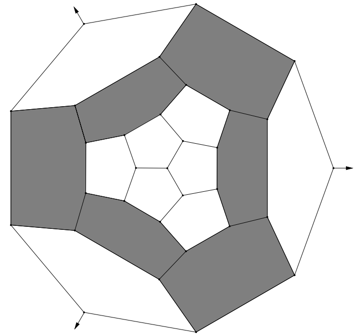
- If $q = 5$, then this is Dodecahedron
- If $q = 6$, then five possibilities:



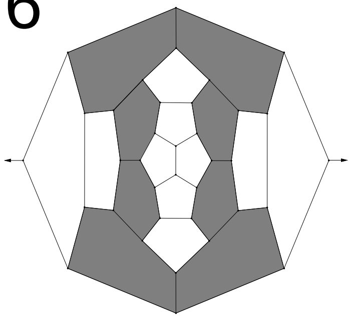
5, D_{5h};6,6



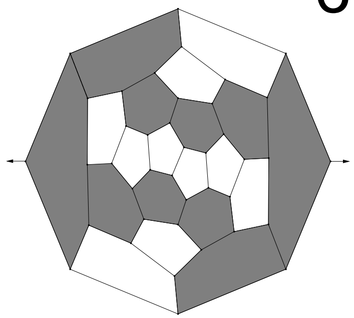
6, D_2;6,6



6, D_{3d};6,6



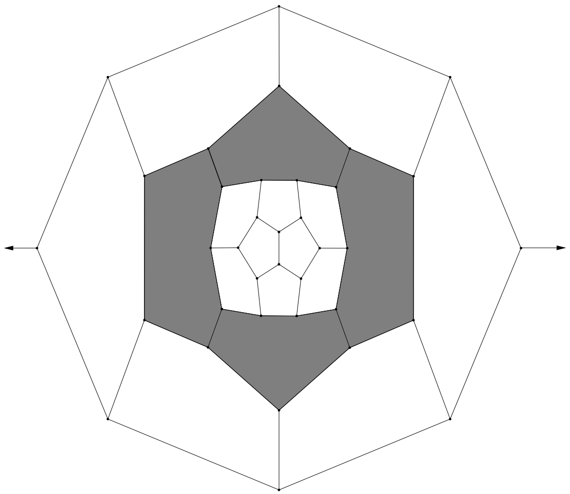
8, D_{2d};6,6



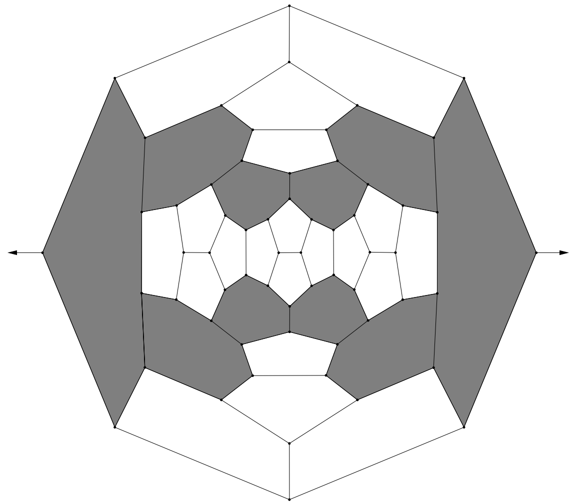
10, D_2;6,6

- If $q = 7$, then ten possibilities
- If $q \geq 8$, we expect infinity of possibilities

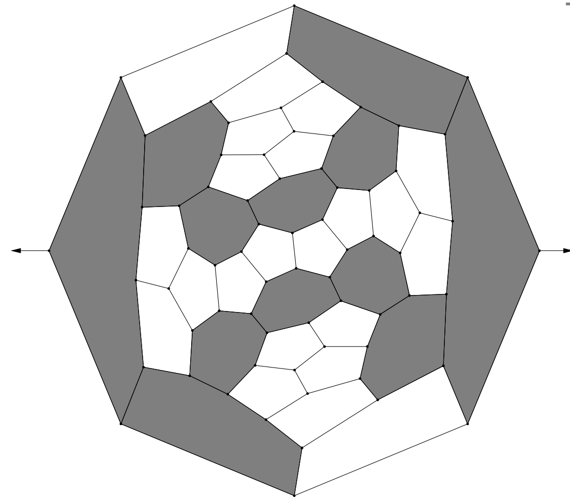
All $M_n(5,7)$



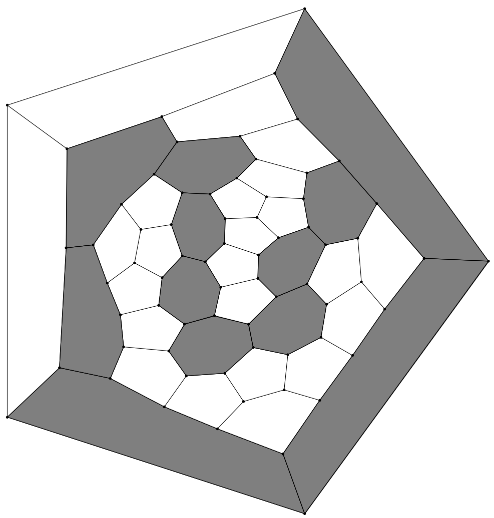
4, D_{2d};8,8



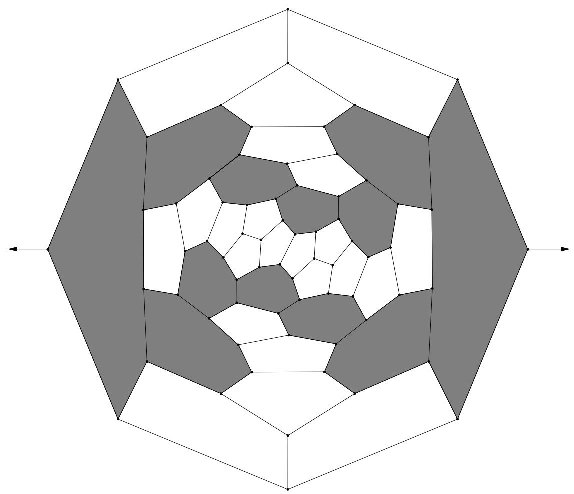
10, C_{2v};12,10



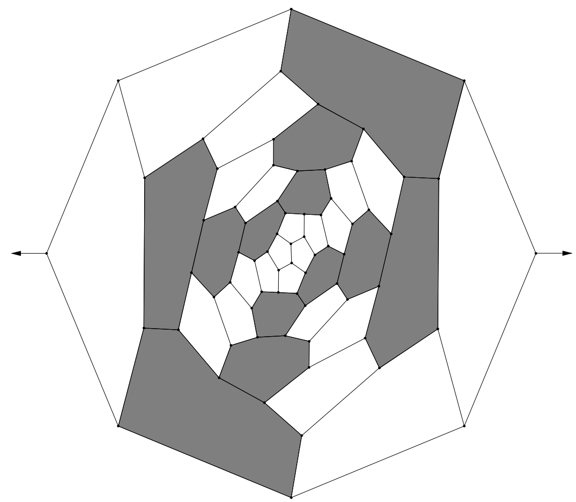
12, C_2;10,14



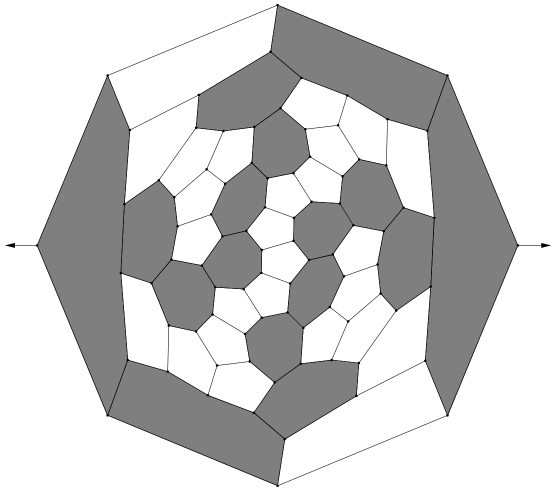
12, C_1;13,11



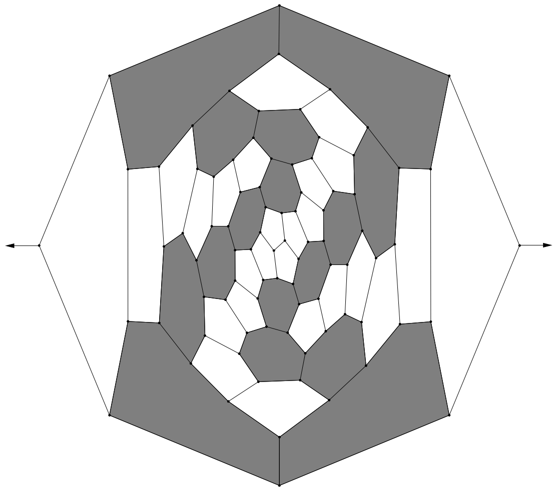
12, D_2;12,12



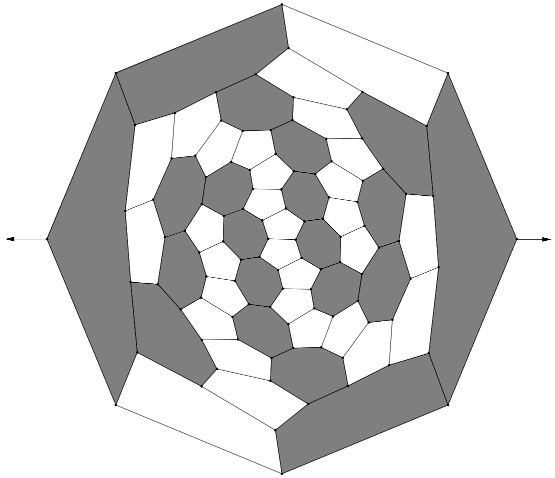
12, S_4;12,12



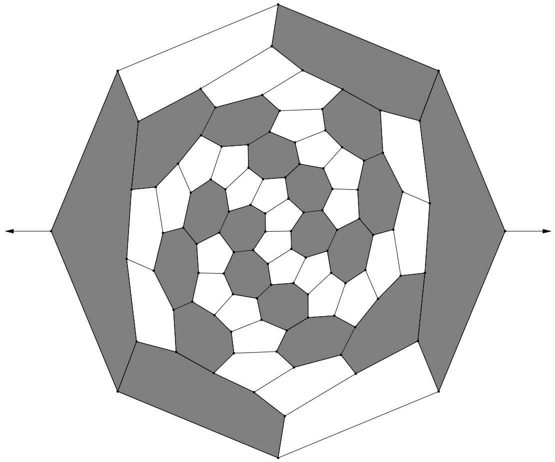
16, D_2;14,14



16, D_2;14,14



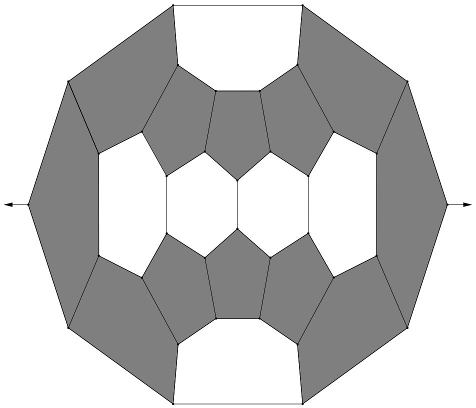
20, D_2;16,16



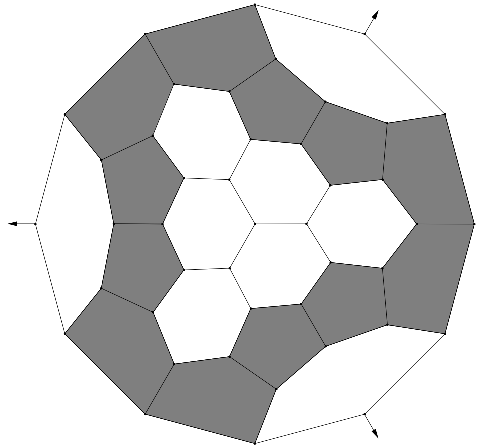
20, C_2;16,16

Case $p = 6$

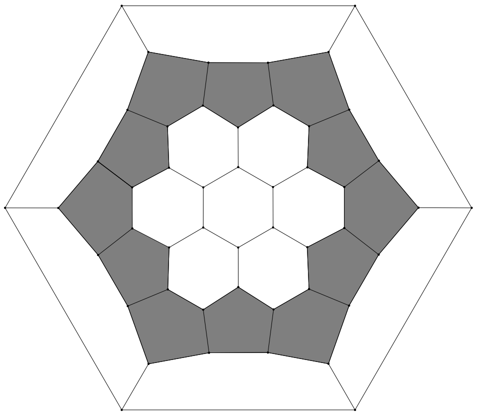
If $p = 6$, then $q = 5$. There are four possibilities:



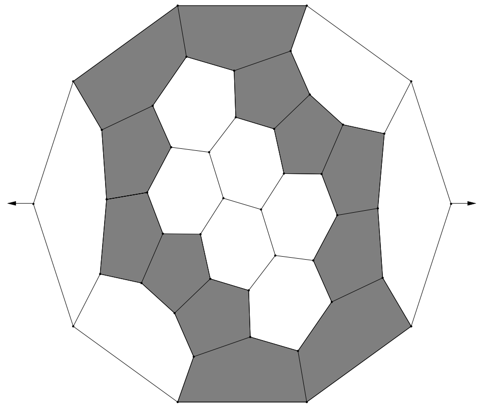
12, D_{2d};4,4



12, D_{3d};6,6



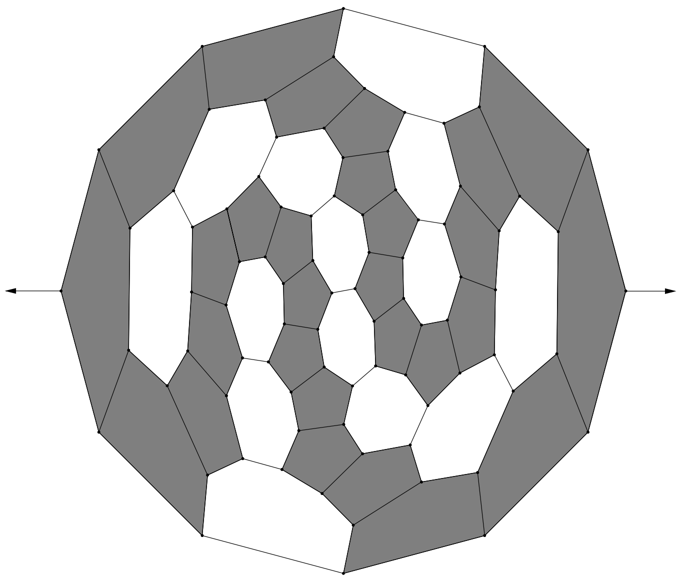
12, D_{6d};7,7



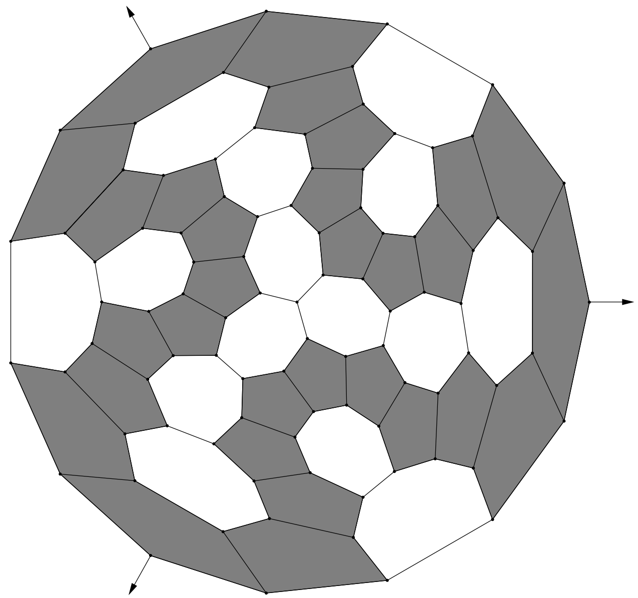
12, D_2;6,6

Two remaining undecided cases

If $p = 7$, then $q = 5$ and $n - (x + x') = 28$. Two examples:



28, D_2;8,8



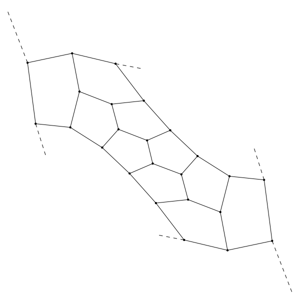
30, D_3;9,9

The remaining undecided case is $M_n(5, q)$ with $q \geq 8$.

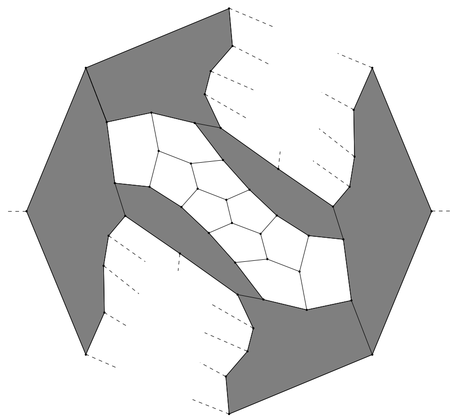
- Hadjuk and Soták found an infinity of maps $M_n(7, 5)$,
- Madaras and Soták found infinity of maps $M_n(5, q)$ for $q = 10$ and $q \equiv 2, 3 \pmod 5$, $q \geq 8$.

Enumeration techniques

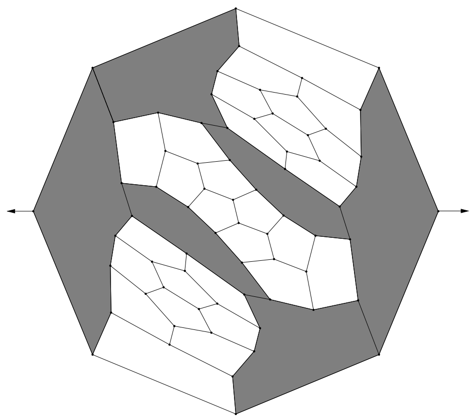
- Harmuth enumerated all 3-valent plane graphs with at most 84 vertices, faces of gonality 5 or 7 and such that every faces of gonality 7 is adjacent to two faces of gonality 7 (i.e. 7-gons are organised into disjoint simple cycles). It gives all $M_n(5, 7)$ with $n \leq 16$.
- Remaining case $17 \leq n \leq 20$ is treated by following algorithm:



Generating patches

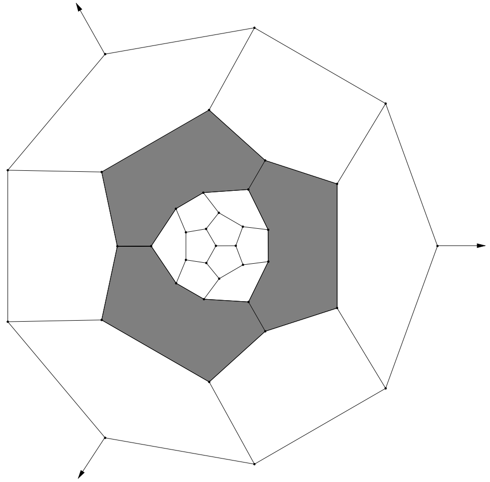


Adding ring of q gons

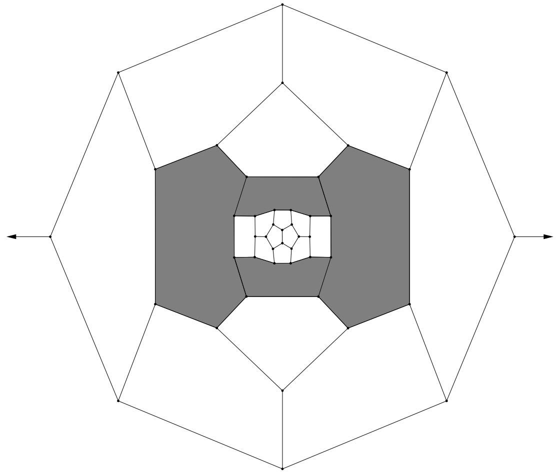


completing (if possible).

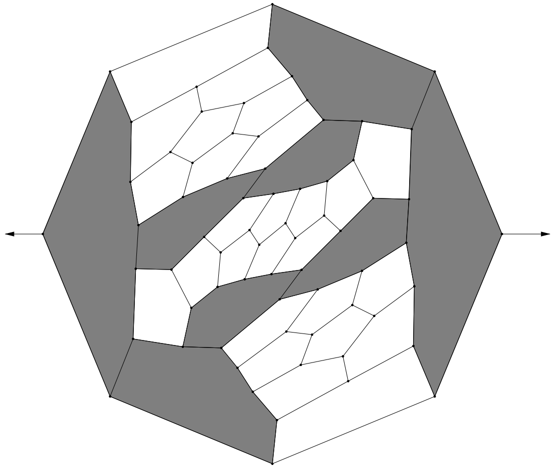
Known $M_n(5,8)$



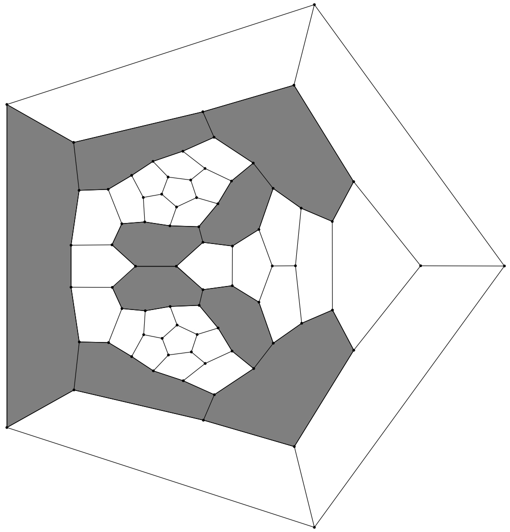
3, D_{3h};9,9



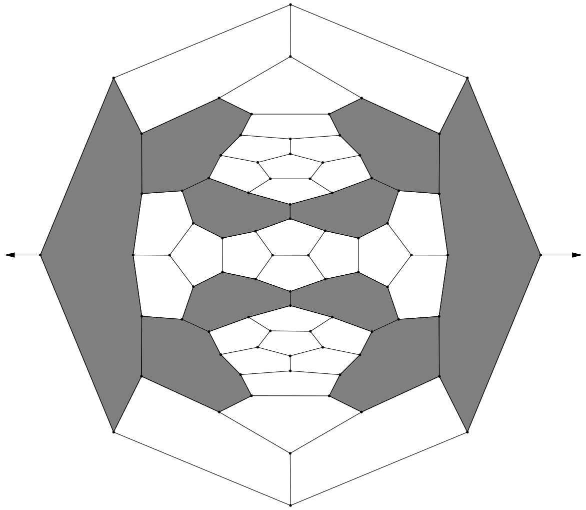
4, D_{2d};10,10



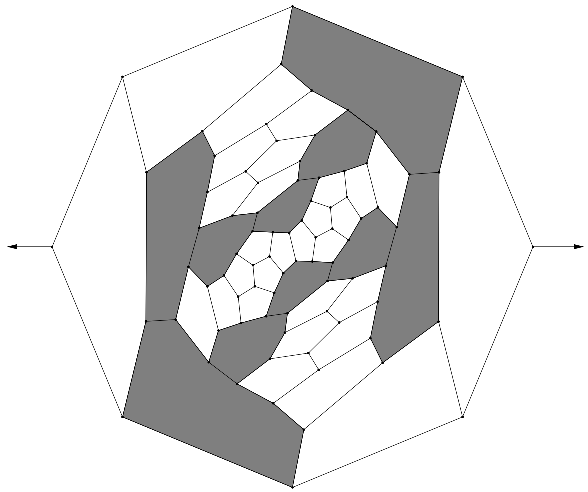
8, C_2;10,18



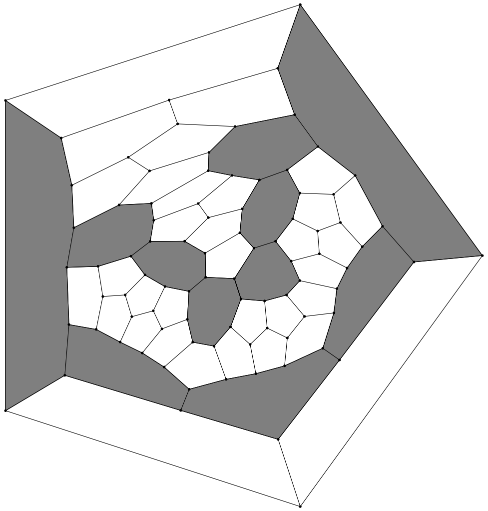
9, C_s;19,11



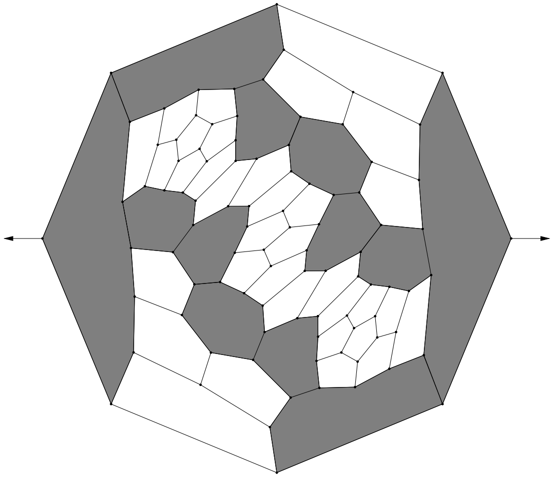
10, C_{2v};10,22



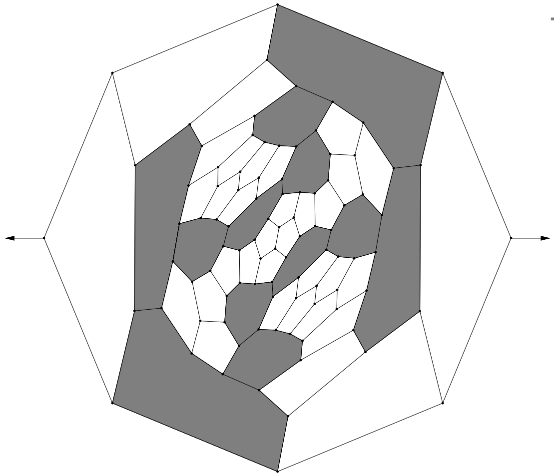
10, C_2;14,18



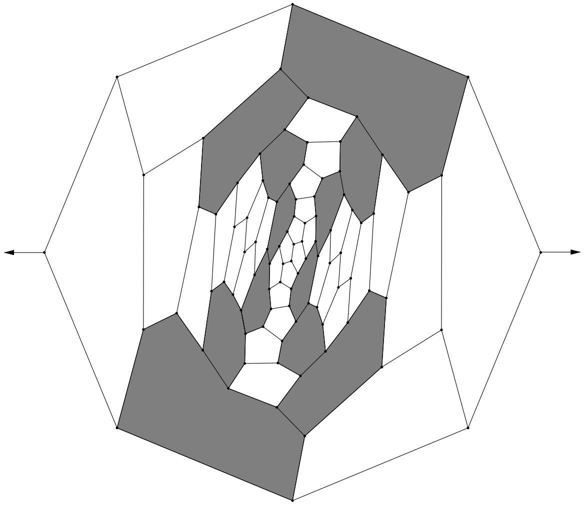
11, C_1;20,14



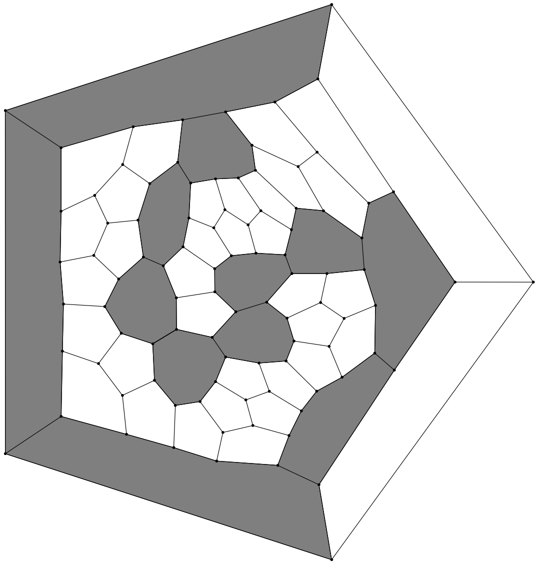
12, C_2;26,10



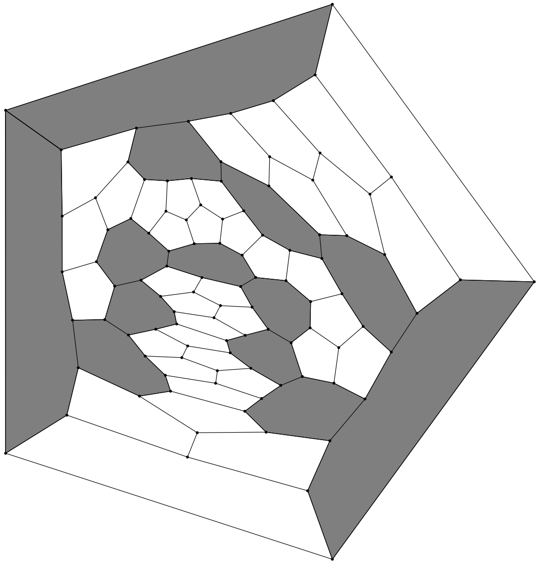
12, C_2;14,22



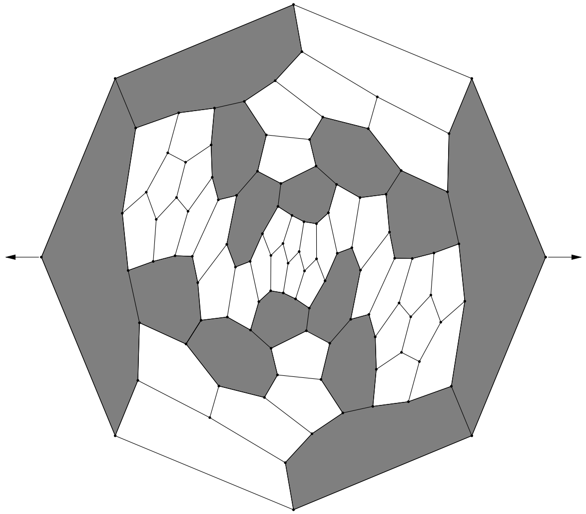
12, C_2;14,22



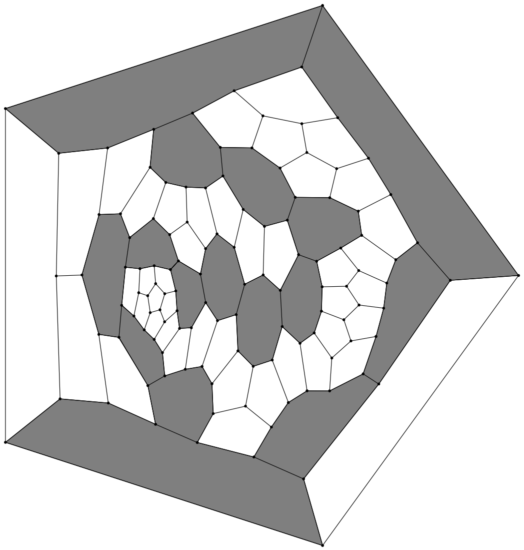
12, C_1;21,15



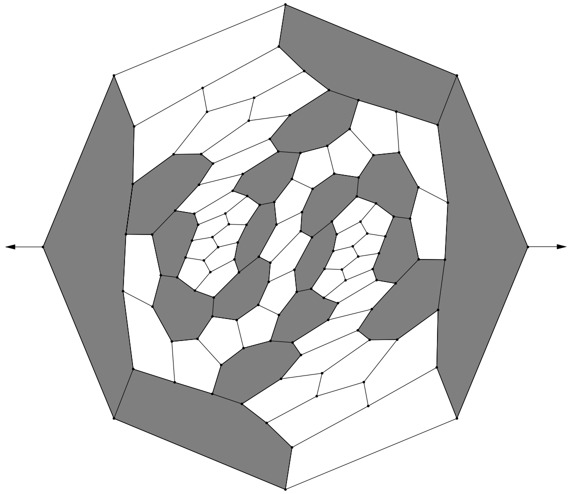
13, C_1;15,23



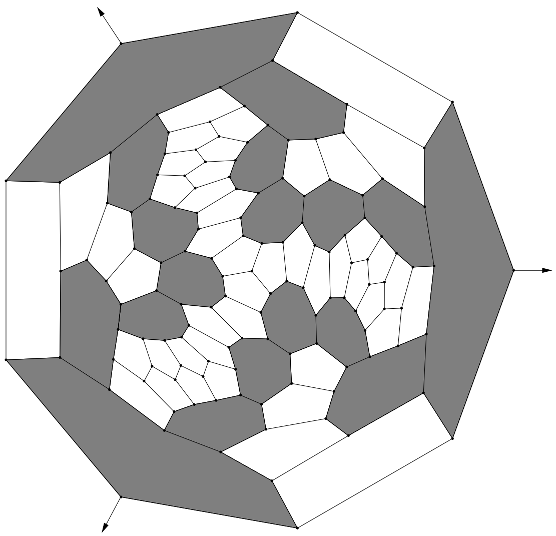
14, C_2;28,12



16, C_1;30,14

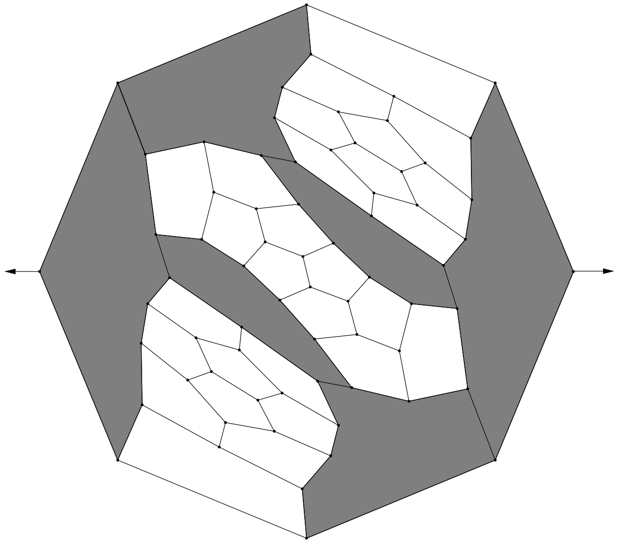


18, C_2;14,34

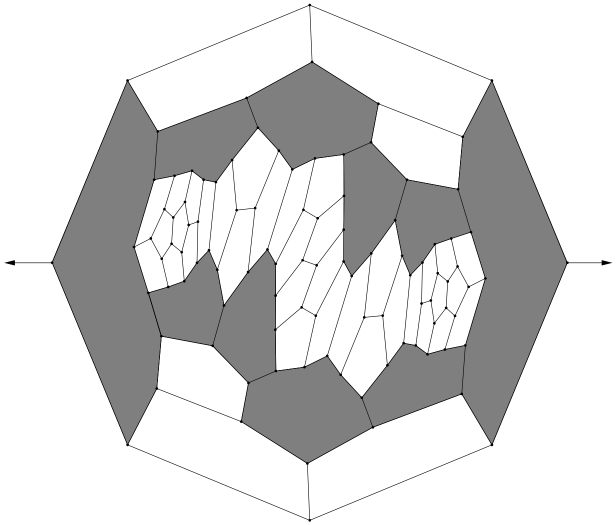


18, C_3;33,15

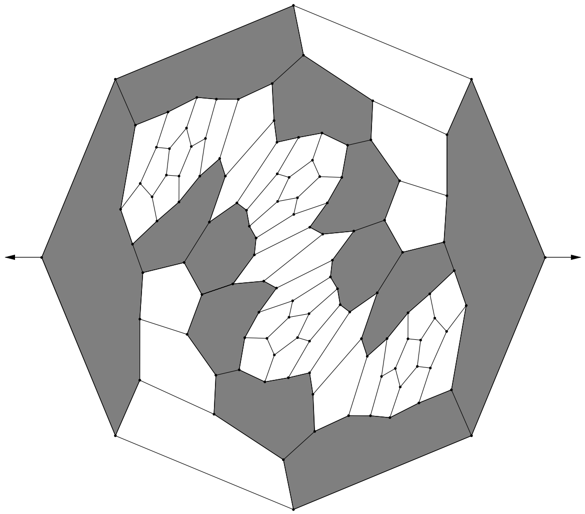
Known $M_n(5,9)$



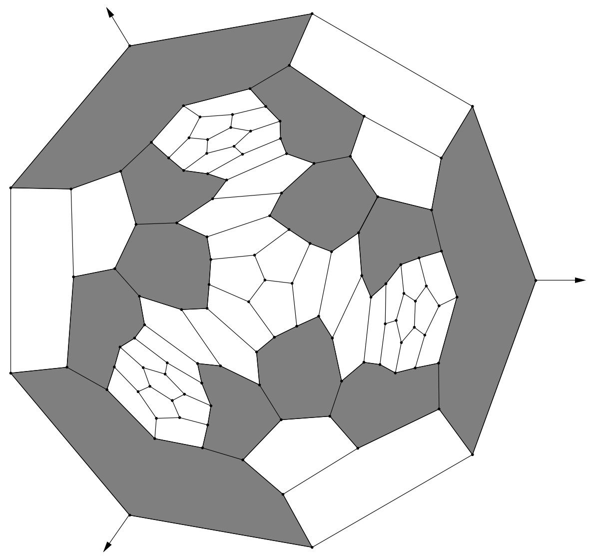
6, C_2;10,20



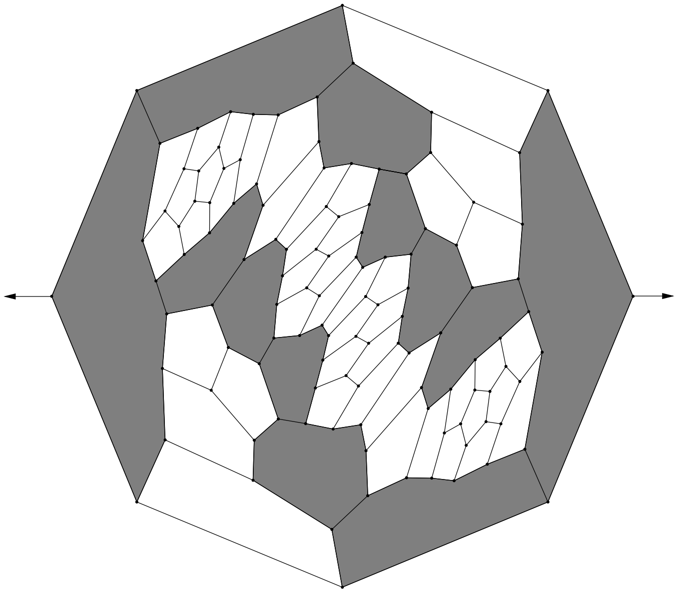
10, C_2;34,8



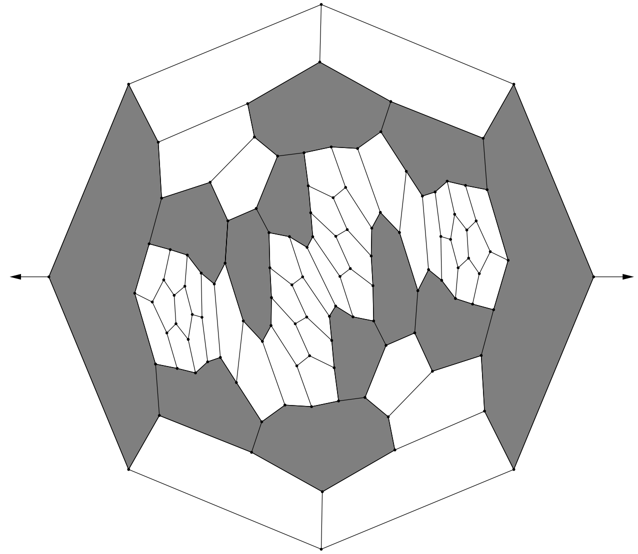
12, C_2;40,8



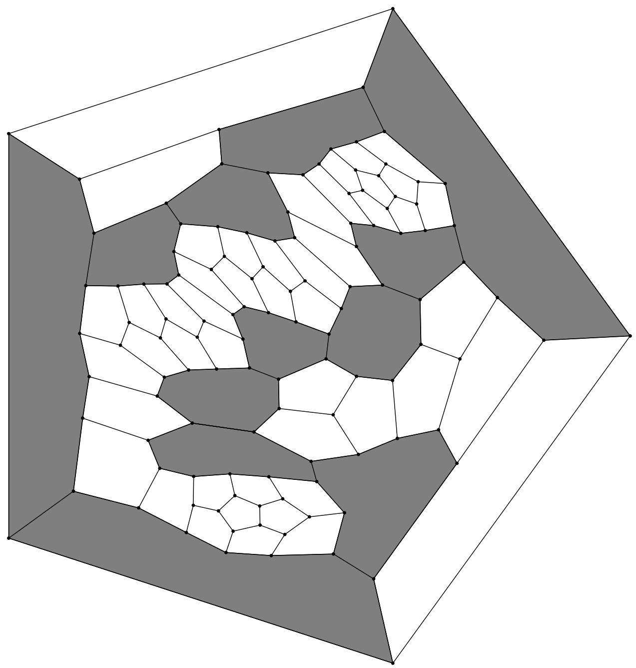
12, C_3;39,9



12, C_2;38,10

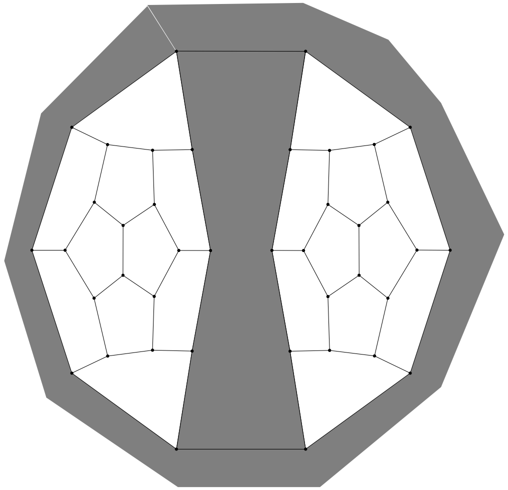


12, C_2;38,10

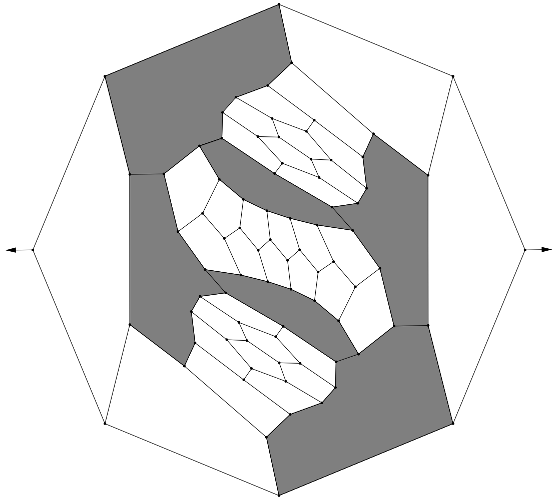


12, C_1;38,10

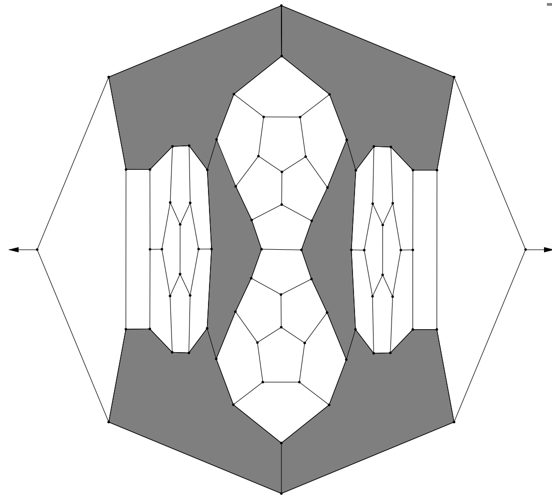
Known $M_n(5,10)$



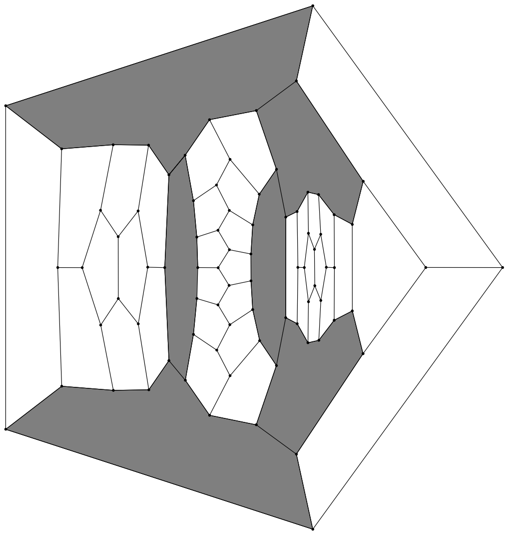
2, D_{2h};10,10



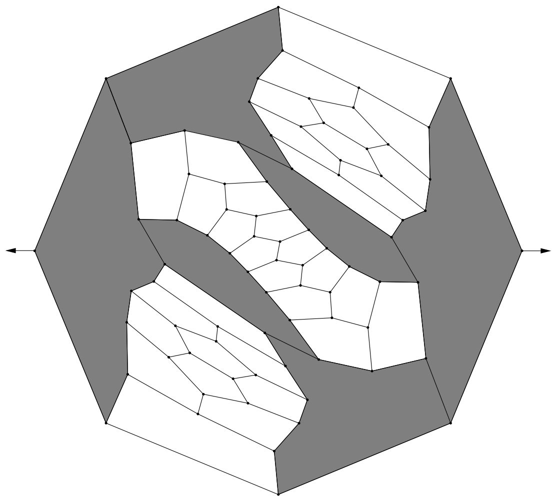
6, C_2;12,24



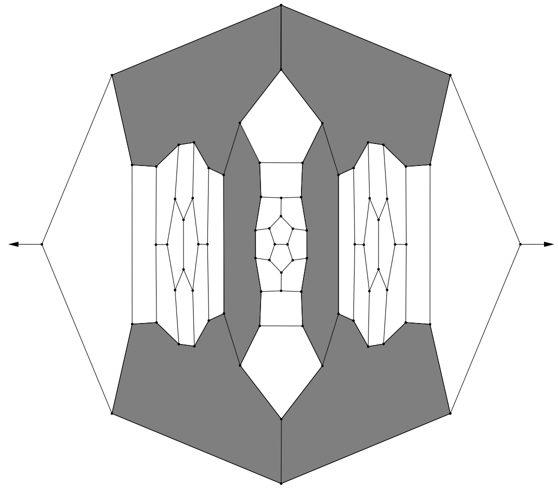
6, C_{2v};14,22



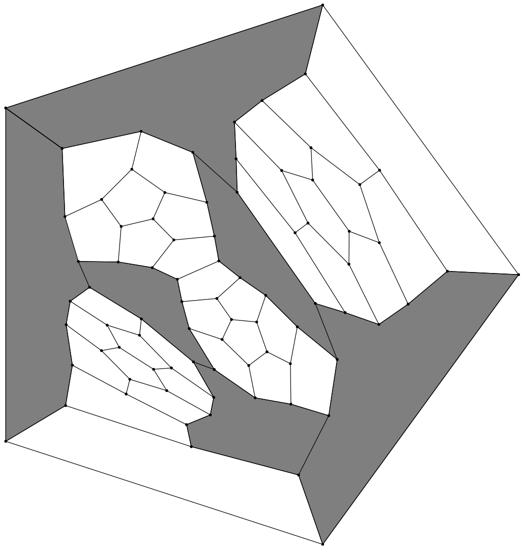
6, C_s;13,23



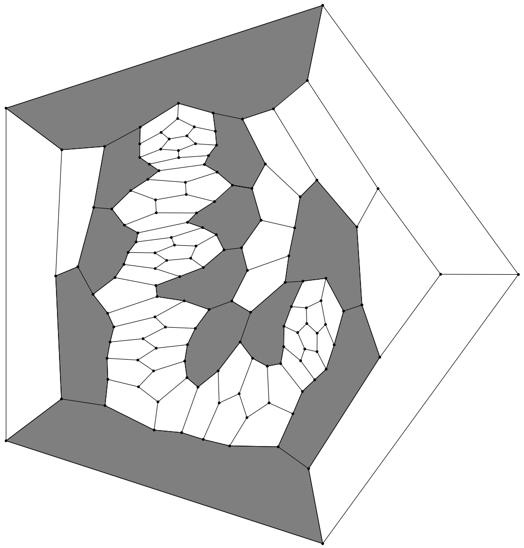
6, C_2;14,22



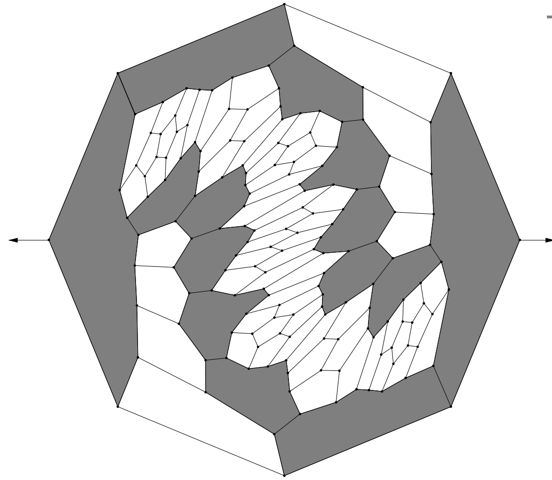
6, C_{2v};12,24



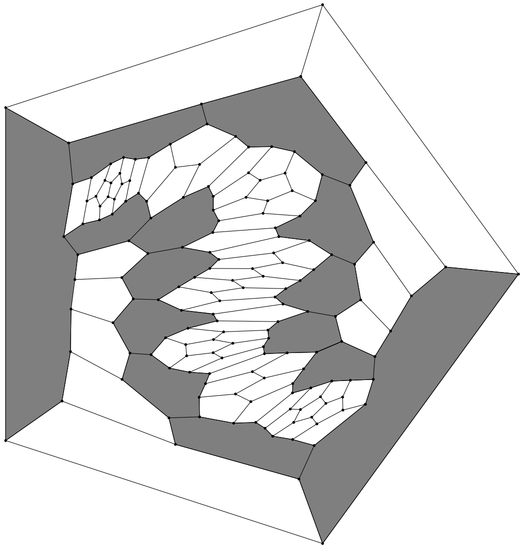
6, C_1;15,21



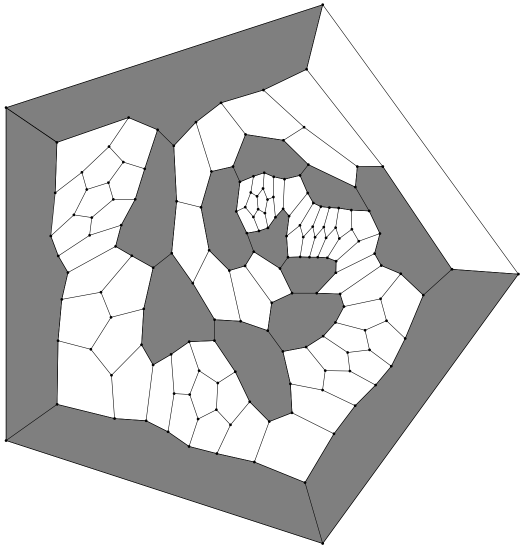
12, C_1;11,49



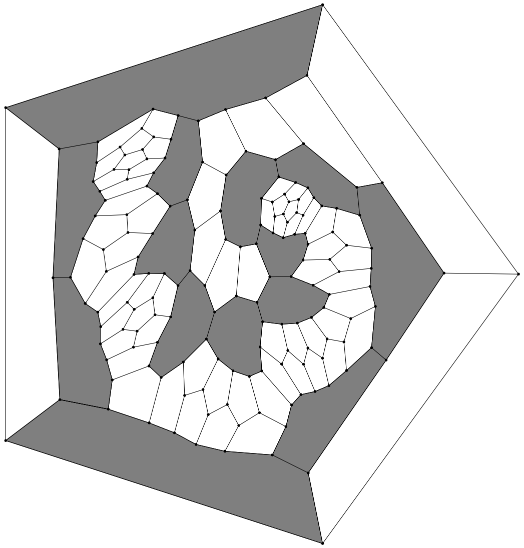
14, C_2;58,10



14, C_1;11,57



14, C_1;11,57



14, C_1;11,57

All parameters (p, q)

(p, q)	n	maps
$(p \geq 3, 4)$	p	$1(Prism_p)$
$(3, 6)$	2	1
$(4, 5)$	4	1
$(4, 6)$	$3, 4$	2
$(4, 7)$	4	1
$(4, 8)$	$2, 4$	2
$(4, q > 8)$	4	1
$(6, 5)$	12	4(full.)

(p, q)	n	maps
$(5, 5)$	$5, 6$	3(Dode.)
$(5, 6)$	$5, 6, 8, 10$	5(full.)
$(5, 7)$	$4, 10, 12, 16, 20$	10(azu.)
$(5, 8)$	≥ 3	≥ 16
$(5, 9)$	≥ 6	≥ 7
$(5, 10)$	≥ 2	≥ 2
$(5, q > 10)$	≥ 2	?
$(7, 5)$	≥ 28	≥ 2(azu.)

IV. Generalizations

Several rings

A $M_{n_1,\dots,n_t}(p,q)$ denotes a 3-valent plane graph with p-gons and q-gons, where q-gons form t rings of length n_1, ..., n_t (equiv. each q-gon is adjacent exactly to two q-gons).

Theorem: *One has the equation*

$$(4-(4-p)(4-q))\sum_i n_i + (6-p)(x_1+x_2) = 4p,$$, where

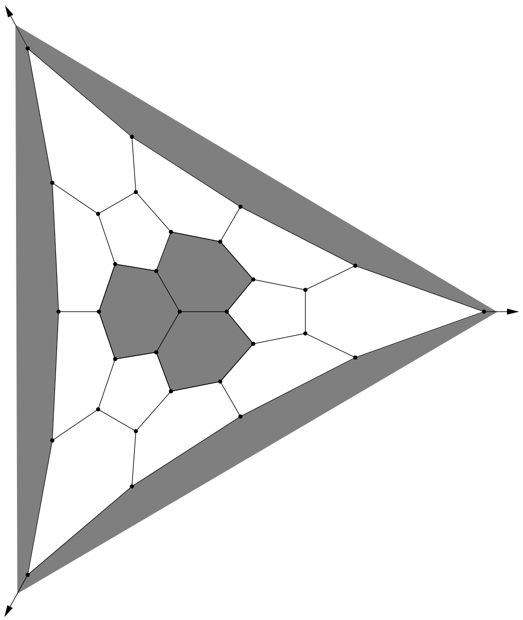
- x_1 *is the number of vertices incident to* 3 p*-gonal faces and*
- x_2 *the number of vertices incident to* 3 q*-gonal faces.*

➠ finiteness for $(4,q)$, $(5,6)$, $(5,7)$ but we have infinity for $(6,5)$ and, possibly, for $(5,q)$, $q\geq 8$.

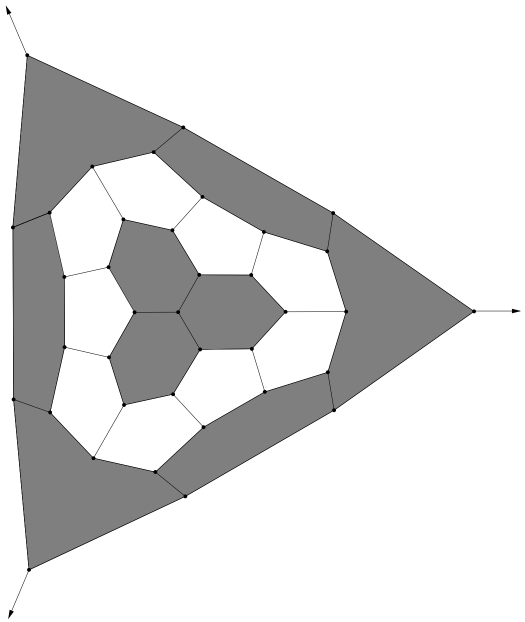
The case (p, q)=$(5, 6)$ (fullerenes)

All maps $M_{...}(5, 6)$ are:

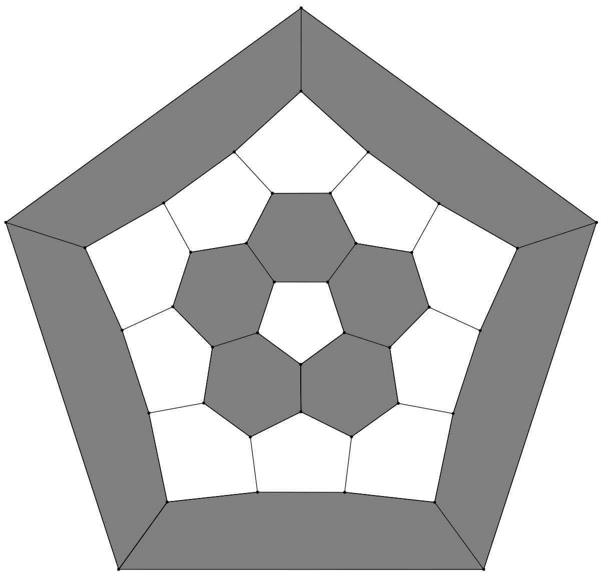
- five maps with one ring of 6-gons,
- following three maps with two rings of 6-gons:



D_{3h}; 32

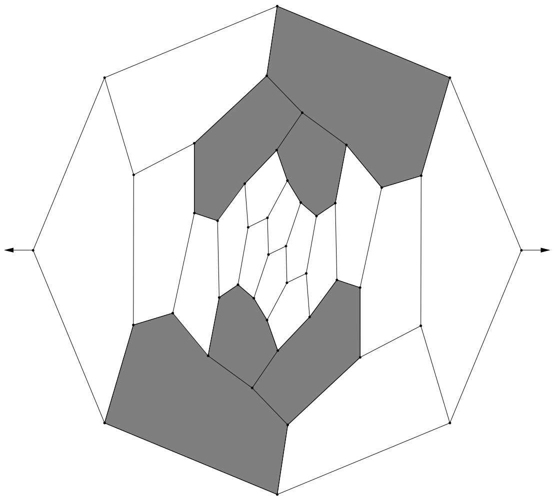


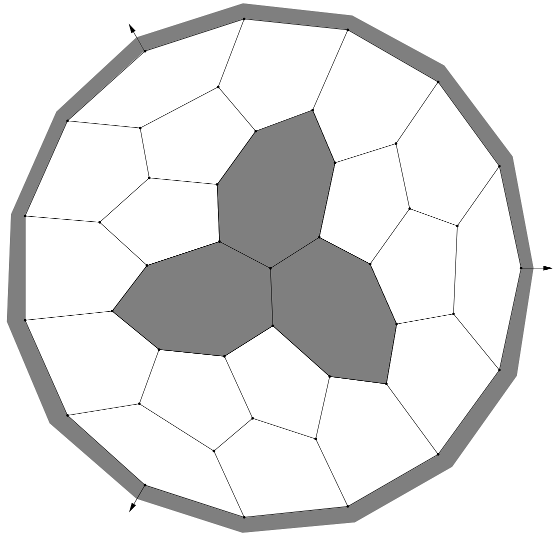
C_{3v}; 38

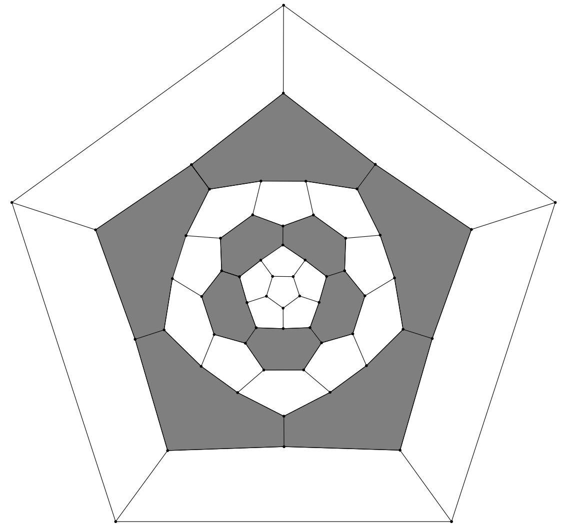


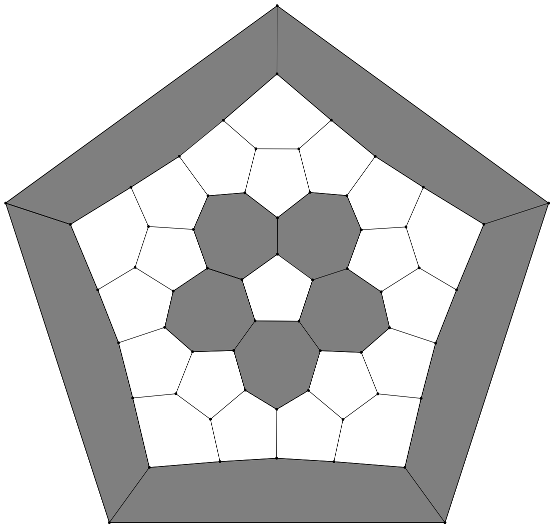
D_{5h}; 40

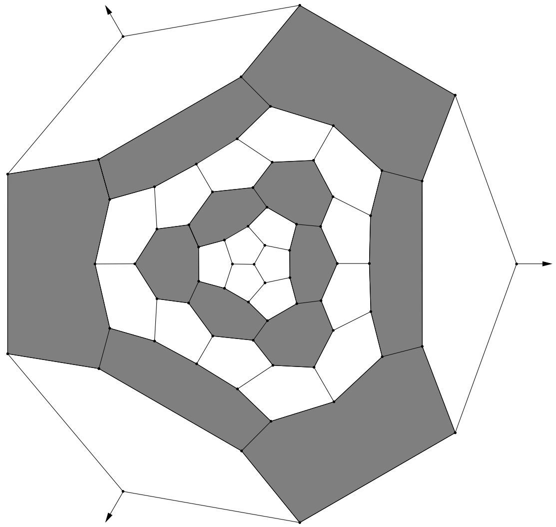
Two rings of 7-gons filled by 5-gons

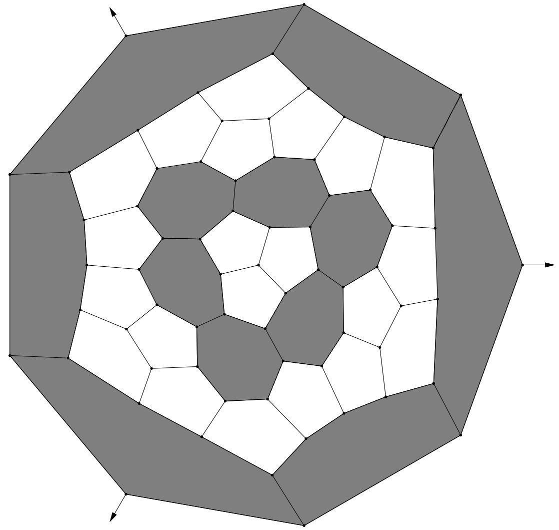

C_{2h}; 44


D_3; 44

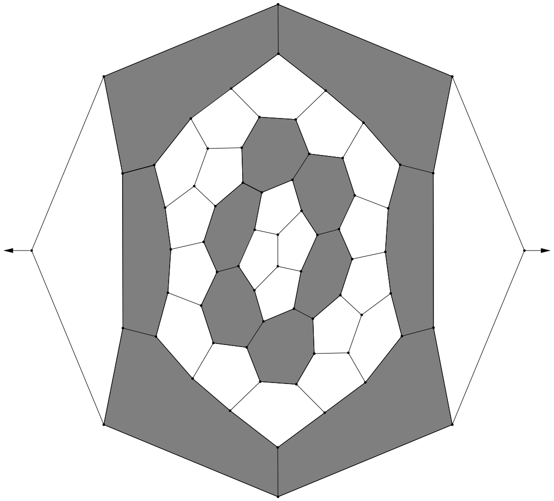

D_{5d}; 60


D_{5h}; 60

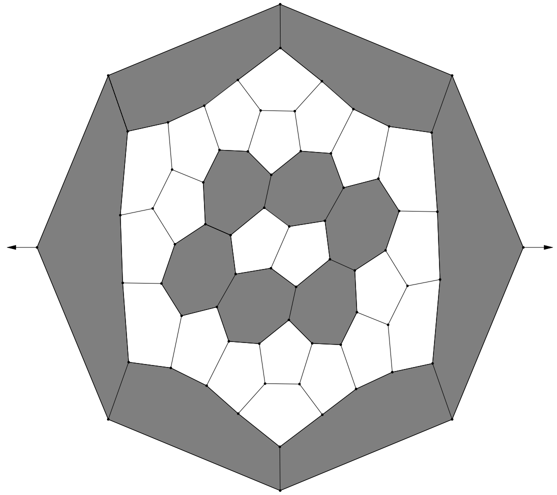

D_{3d}; 68


D_3; 68

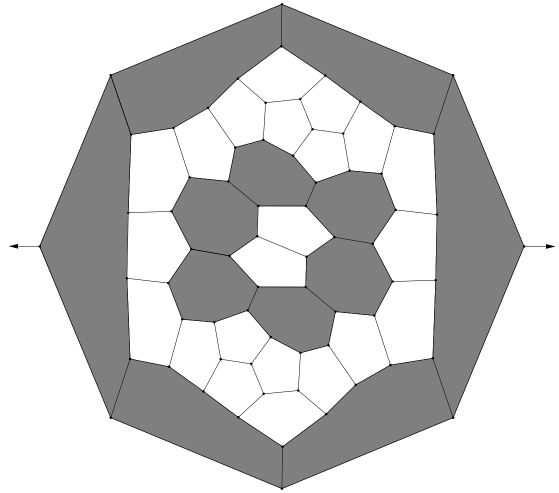
Two rings of 7-gons filled by 5-gons



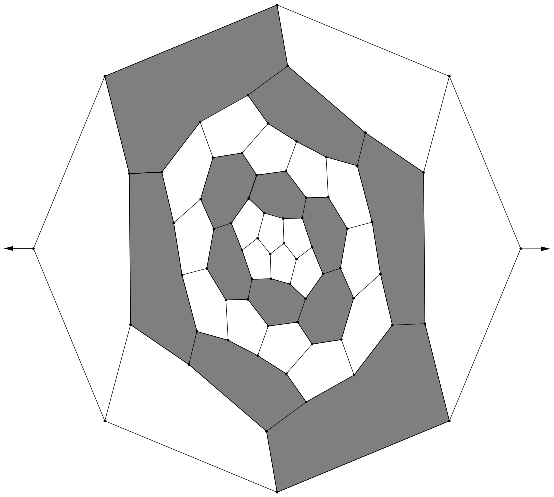
D_2; 68



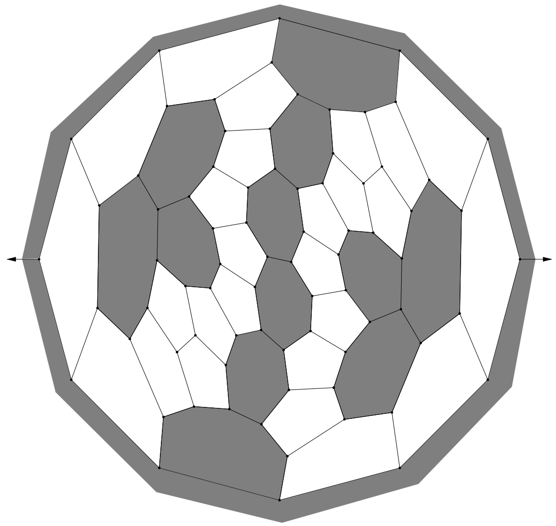
D_2; 68



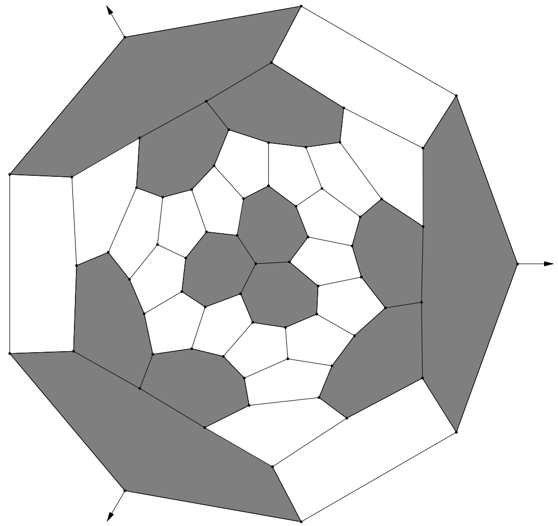
D_2; 68



D_2; 68

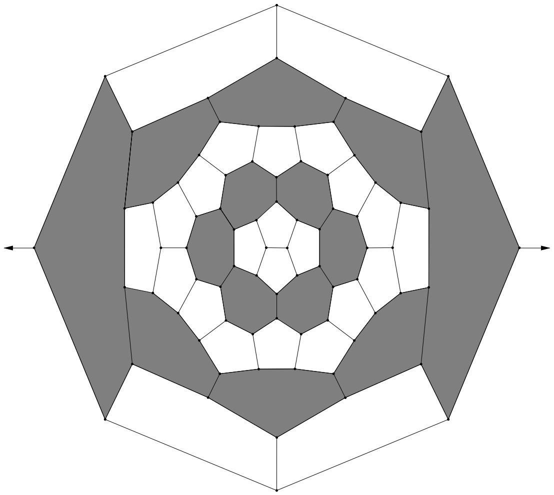


C_{2h}; 76

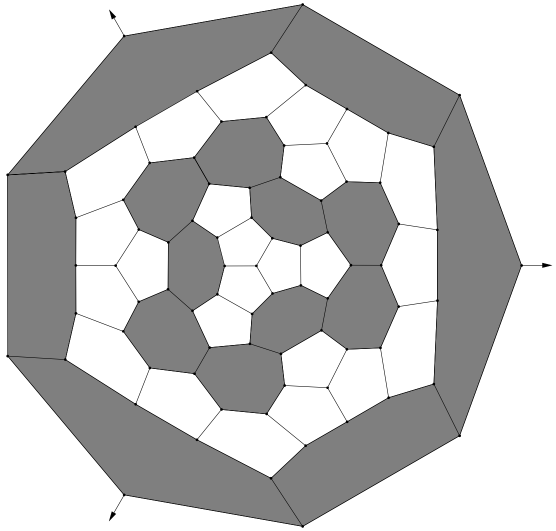


T; 68

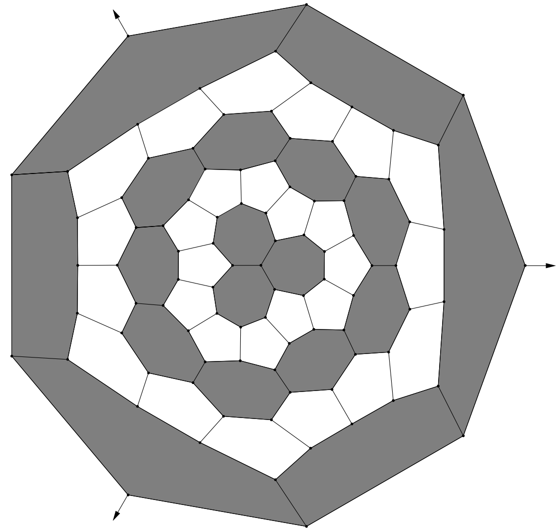
Remaining graphs $M_{\ldots}(5,7)$ (azulenoids)



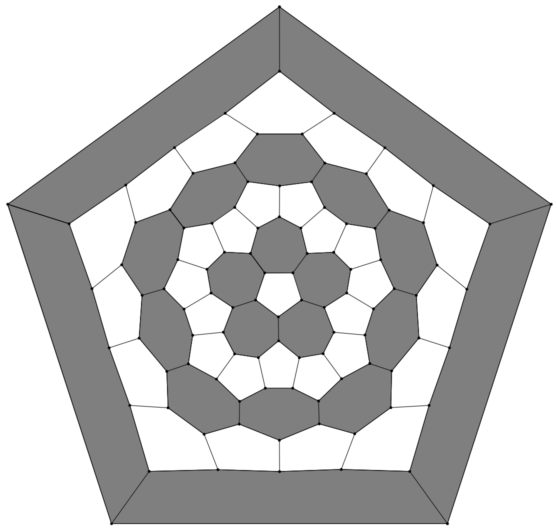
C_{2v}; 76



C_{3v}; 80



C_{3v}; 92

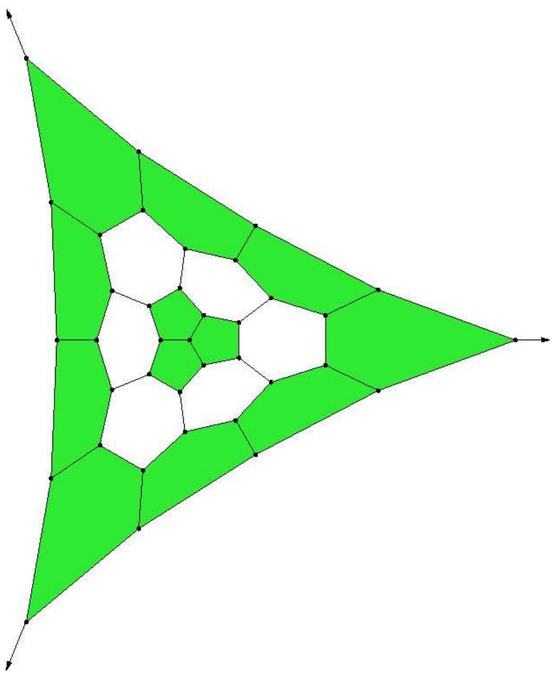


D_{5d}; 100

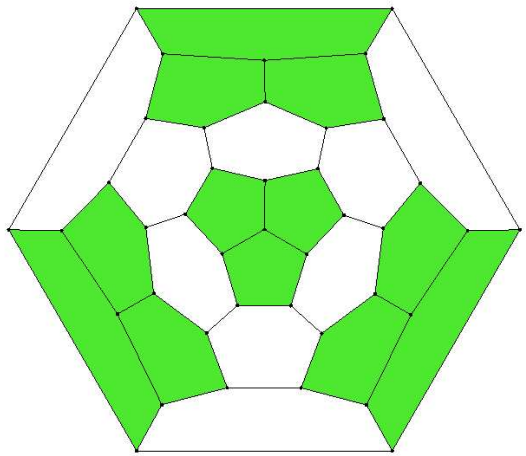
The case (p, q)=$(6, 5)$ (fullerenes)

All maps $M_{...}(6, 5)$ are:

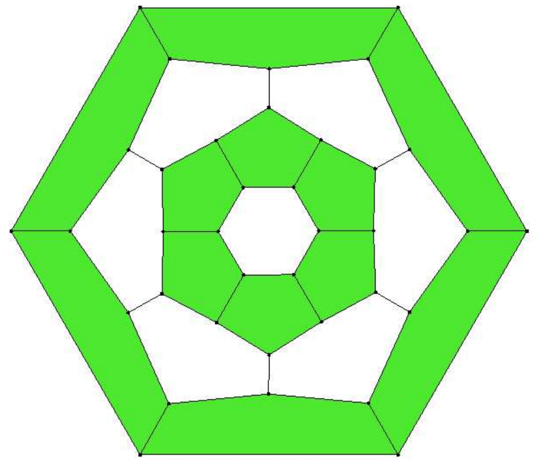
- four maps with exactly one ring of 5-gons,
- the maps:



special map



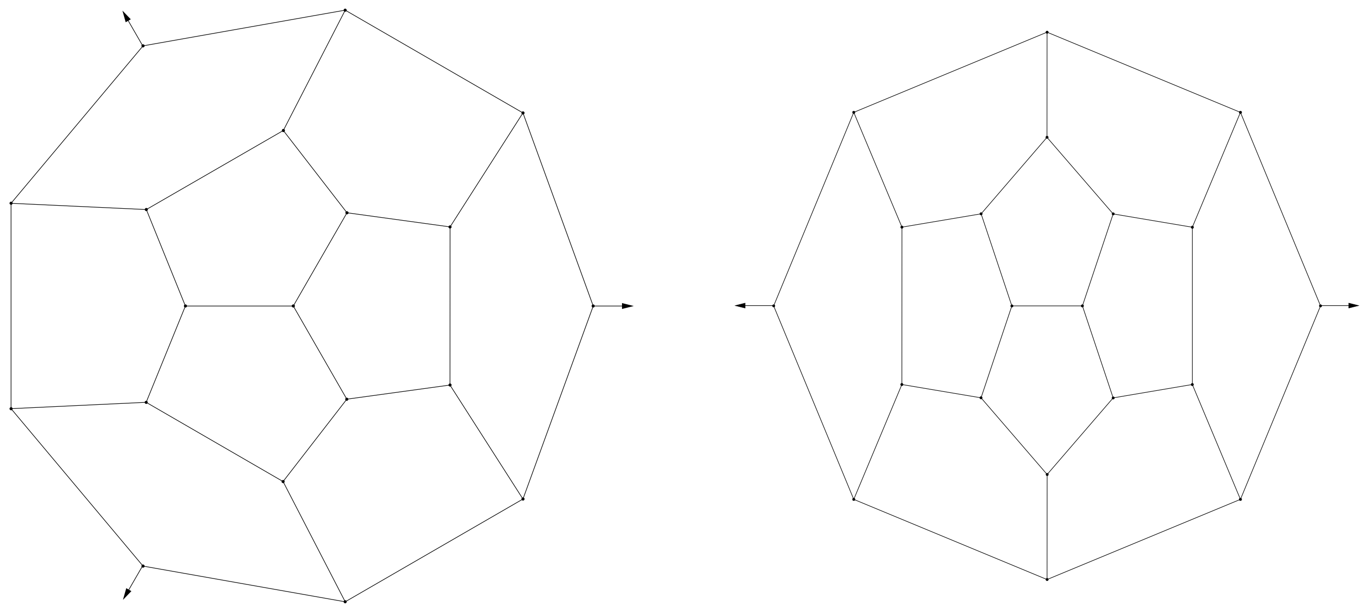
infinite family: 4 triples of pentagons



infinite family: $t \geq 1$ concentric 6-rings of hexagons

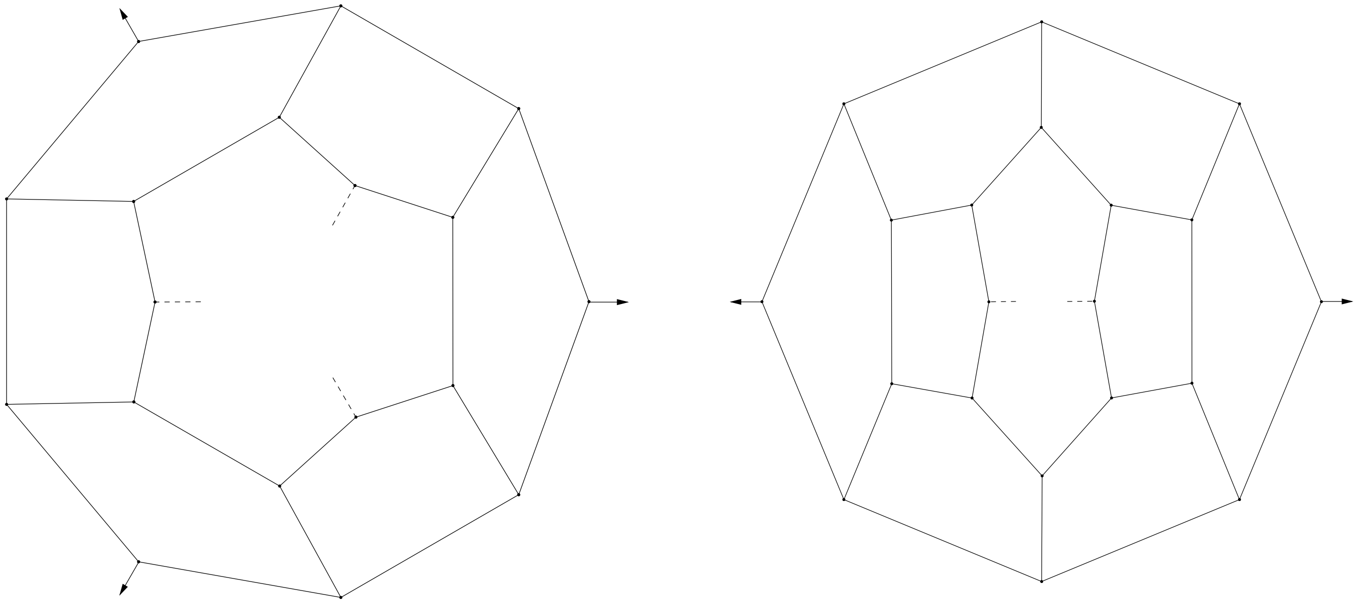
Infinite families

For any $t \geq 0$, there exists a map $M_{3,\ldots,3}(5,8)$ (with t 3-rings of 8-gons) and a map $M_{2,\ldots,2}(5,10)$ (with t 2-rings of 10-gons)



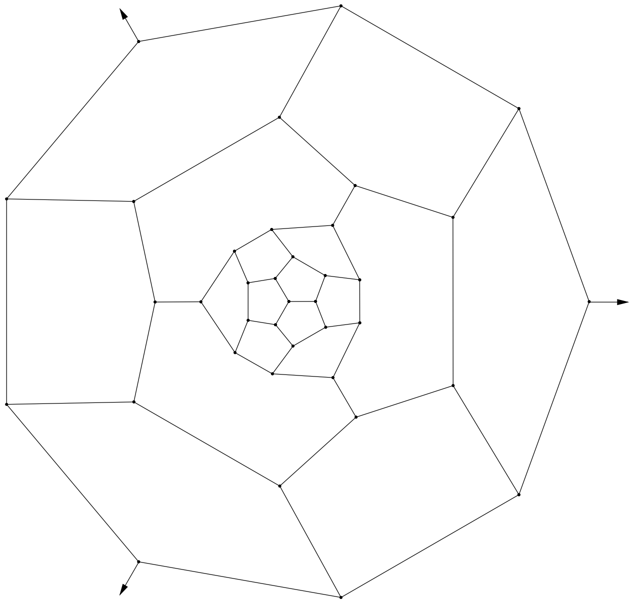
Infinite families

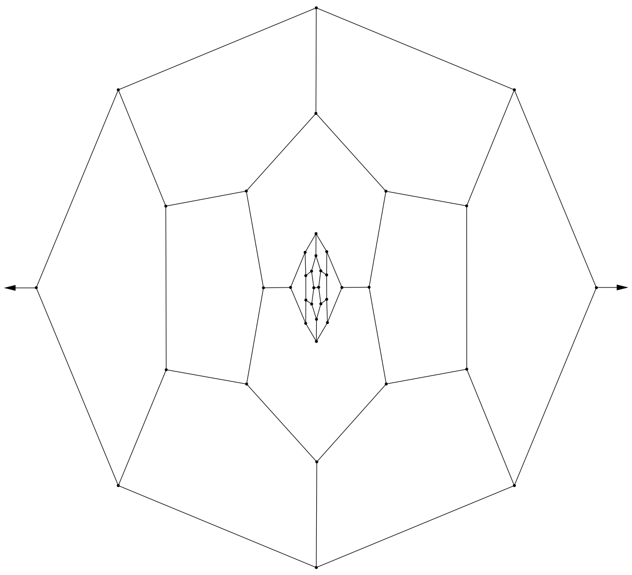
For any $t \geq 0$, there exists a map $M_{3,\ldots,3}(5,8)$ (with t 3-rings of 8-gons) and a map $M_{2,\ldots,2}(5,10)$ (with t 2-rings of 10-gons)



Infinite families

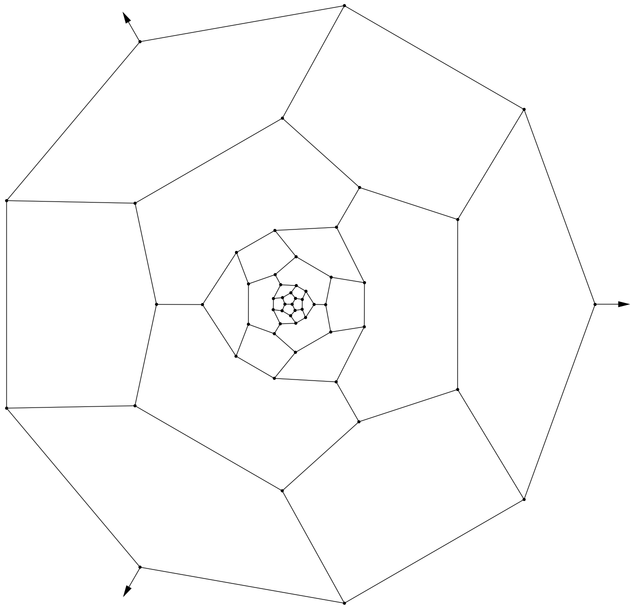
For any $t \geq 0$, there exists a map $M_{3,\ldots,3}(5,8)$ (with t 3-rings of 8-gons) and a map $M_{2,\ldots,2}(5,10)$ (with t 2-rings of 10-gons)

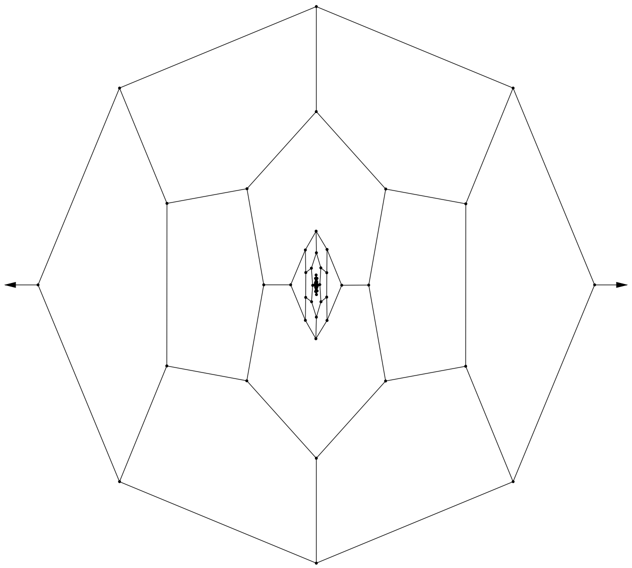




Infinite families

For any $t \geq 0$, there exists a map $M_{3,\ldots,3}(5,8)$ (with t 3-rings of 8-gons) and a map $M_{2,\ldots,2}(5,10)$ (with t 2-rings of 10-gons)

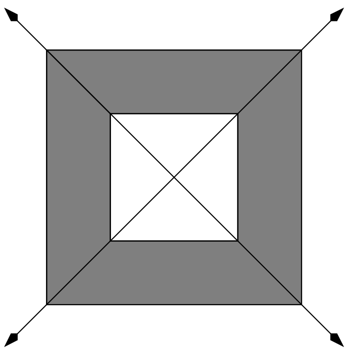




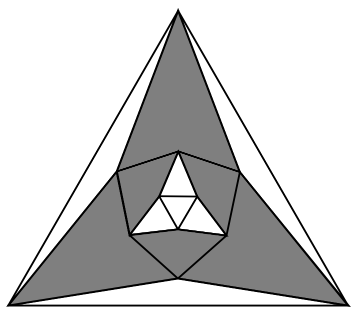
k-valent maps

A $M_n^k(p,q)$ denotes a k-valent map with p-gons and q-gons only, where q-gons form a ring of length n.

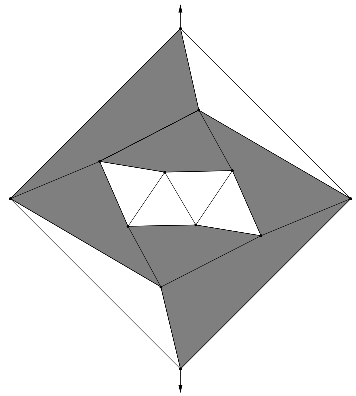
- The only $M_n^4(p,3)$ is p-gonal antiprism.
- All $M_n^4(3,4)$ are:



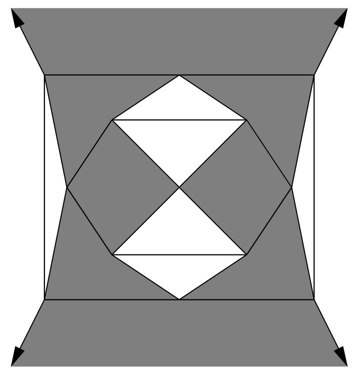
D_{4h}; 10



D_{3d}; 12



D_2; 12



D_{2d}; 14

There is only one other $M_{...}^4(3,4)$; it has two rings of 4-gons, 14 vertices and symmetry D_{4h}.