Polycycles and their boundaries

Michel Deza

Ecole Normale Superieure, Paris, and JAIST, Ishikawa

Mathieu Dutour Sikiric

Rudjer Boskovic Institute, Zagreb

and Mikhail Shtogrin

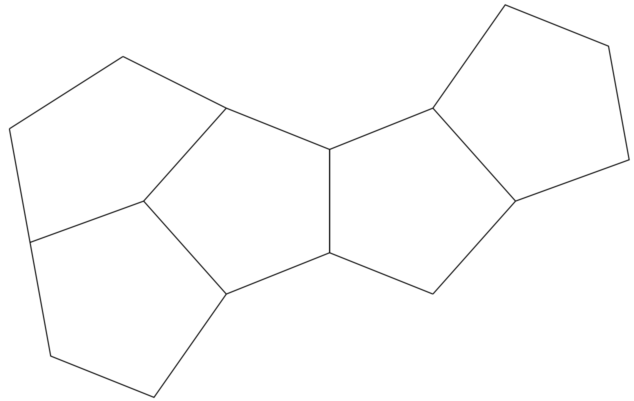
Steklov Institute, Moscow

I. $(p, 3)$-polycycles

Polycycles

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

- all interior faces are (combinatorial) p-gons,
- all interior vertices are of degree 3,
- all boundary vertices are of degree 2 or 3.



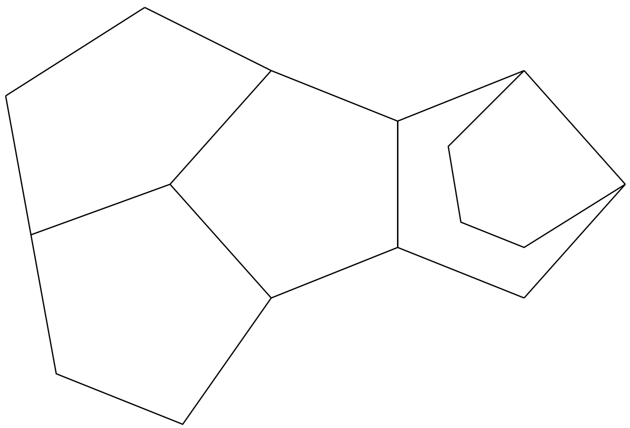
In more general (p, q)-polycycle, interior vertices have degree q and boundary ones are of degree $2, \dots, q$.

Theorem

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

Theorem

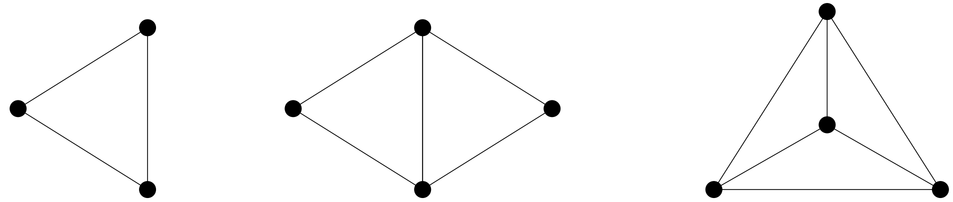
A $(p, 3)$*-polycycle is determined by its skeleton with the exception of the Platonic solids, for which any of their faces can play role of exterior one*



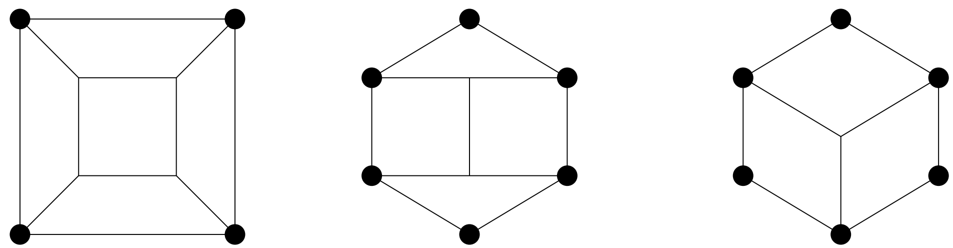
an unauthorized plane embedding

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

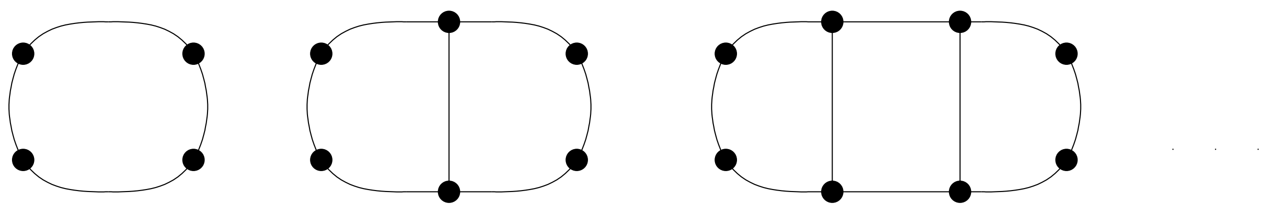
(i) Any $(3,3)$-polycycle is one of the following 3 cases:



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



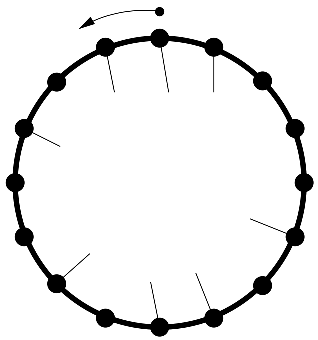
or belong to the following infinite family of $(4,3)$-polycycles:



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.

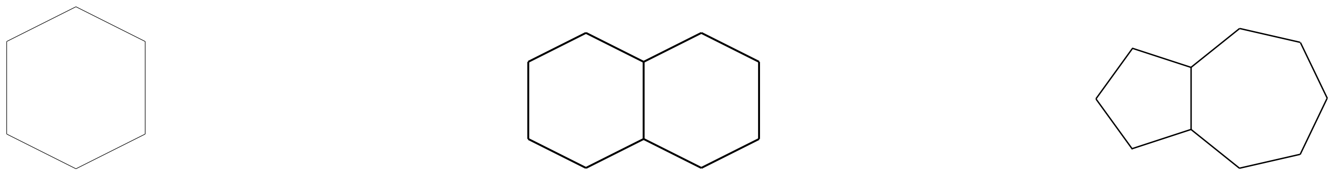


Associated sequence is 3323223233232223

- 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.

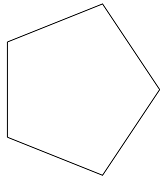


benzene C_6H_6 naphtalene $C_{10}H_8$ azulene $C_{10}H_8$

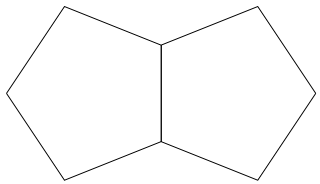
Algorithm for enumerating $(p, 3)$-polycycles with n p-gons:

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

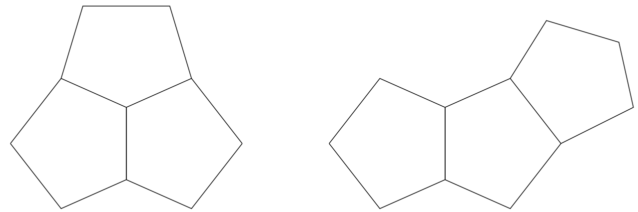
Enumeration of small $(5,3)$-polycycles



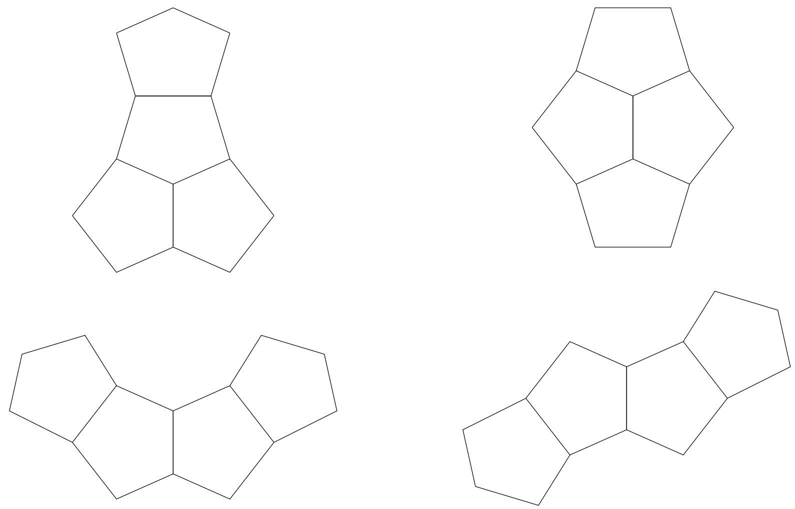
$n = 1$



$n = 2$



$n = 3$

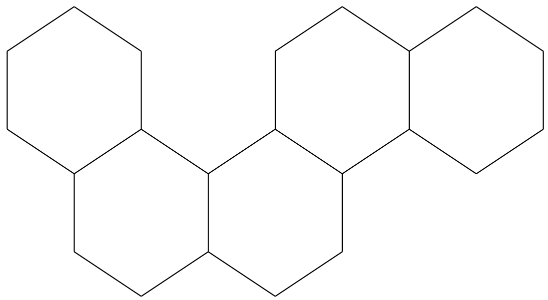


$n = 4$

n		n		n	
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

What boundary says about its filling(s?)

- The boundary of a $(p,3)$-polycycle defines it if $p=3,4$.
- A $(6,3)$-polycyle is of lattice type if its skeleton is a partial subgraph of the skeleton of the partition $\{6^3\}$ of the plane into hexagons. Such $(6,3)$-polycycles are uniquely defined by their boundary sequence.



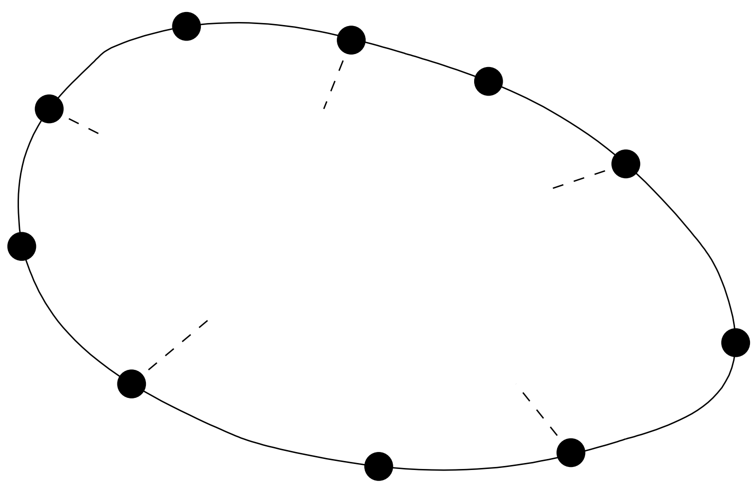
- From Euler formula, for any $(p,3)$-polycycle, its boundary defines uniquely the number f_p of p-gons:
  If $p\neq 6$, then $f_p=\frac{v_2-v_3+5}{p-6}$ and $v_{int}=\frac{2(v_2-p)-(p-4)v_3}{p-6}$.
  If $p=6$, then f_6 is also defined uniquely and $v_2=6+v_3$.

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.

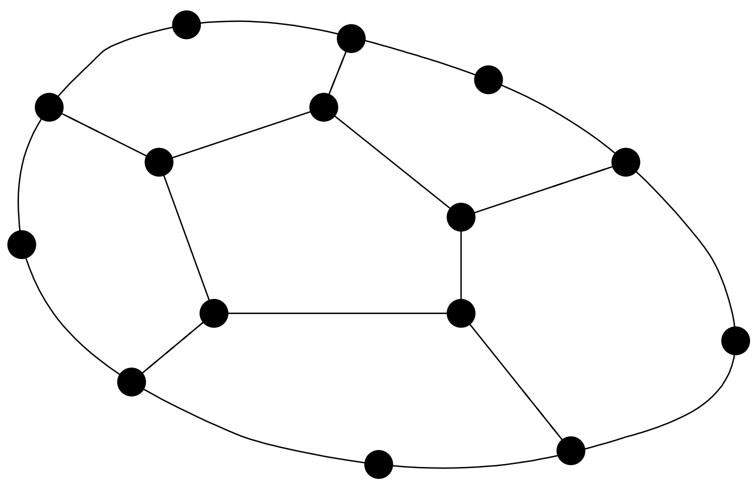
Remind, that the cases $p = 3$ or 4 are trivial.
Let $p = 5$; consider, for example, the sequence 2323232323



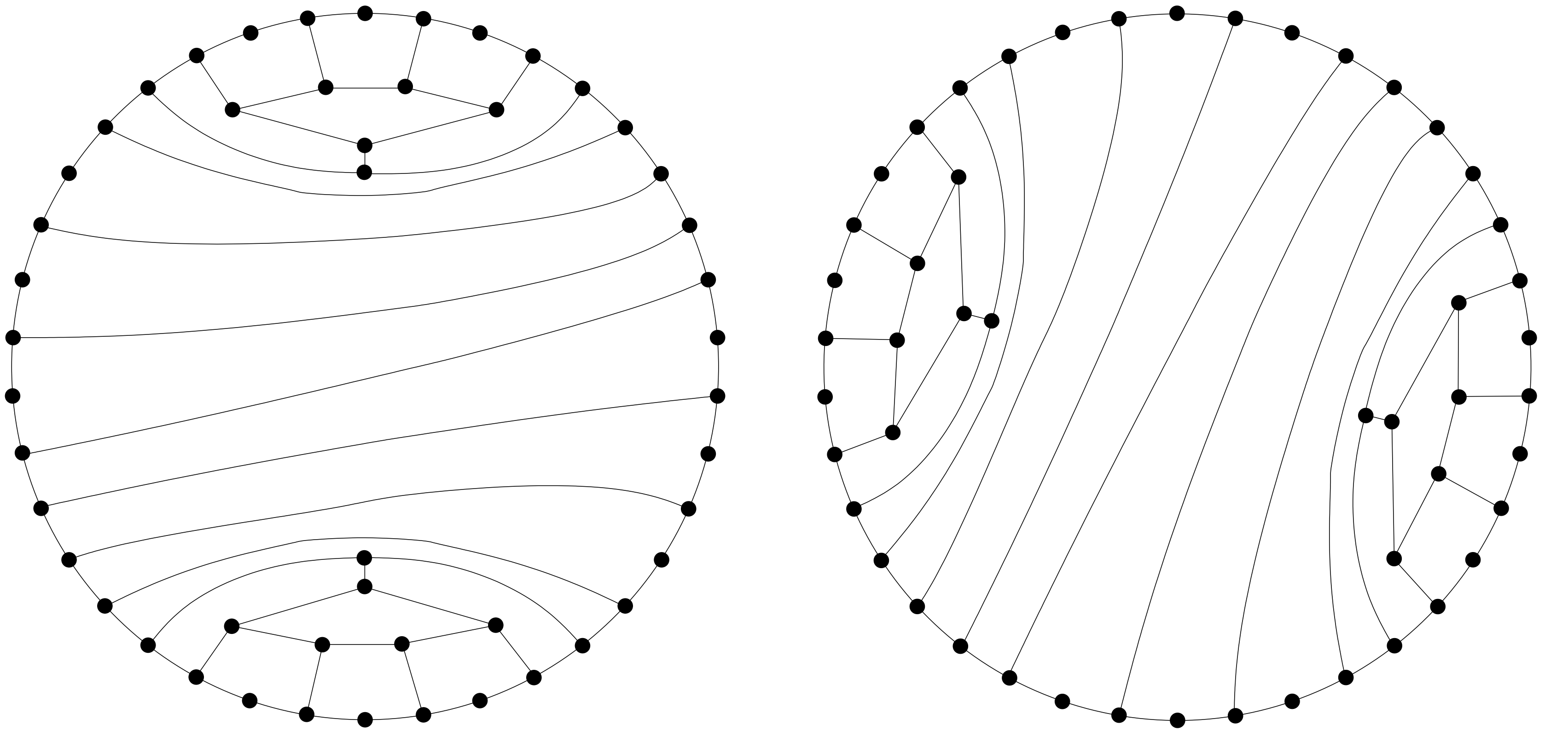
The filling problem

- 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

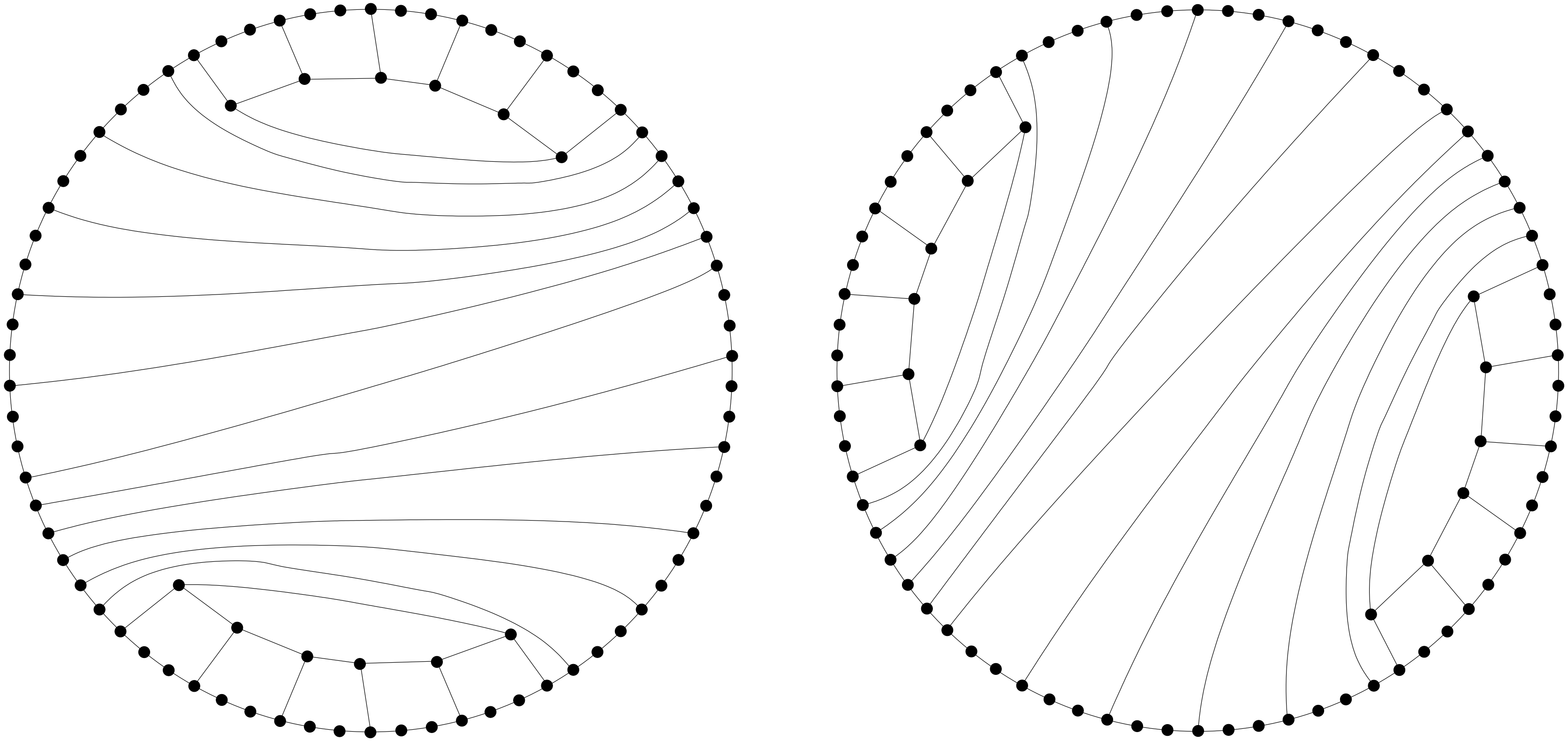


2 equi-boundary $(5,3)$-polycycles



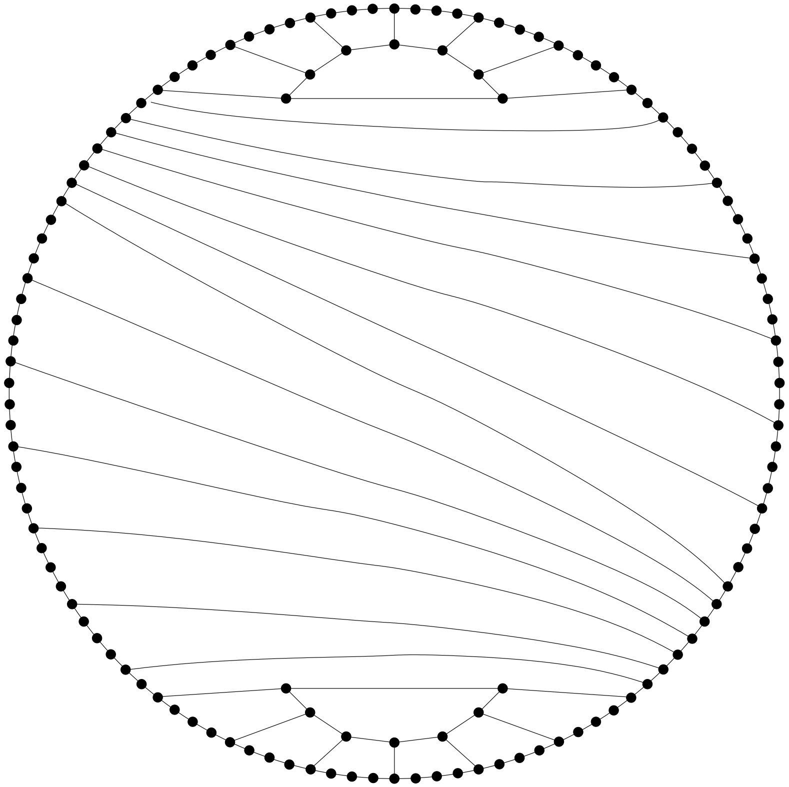
Boundary sequence: 12, 26 vertices of degree 2, 3, resp.
Symmetry groups: of boundary: C_{2v}, of polycycles: C_2.
Fillings: 20 pentagons, 12 interior points.
It is unique ambiguous boundary with $f_5 \leq 20 = 4 \times 5$.

2 equi-boundary $(6,3)$-polycycles



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.
It is unique ambiguous boundary with $f_6 \leq 24 = 4 \times 6$.

Ambiguous boundary 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.

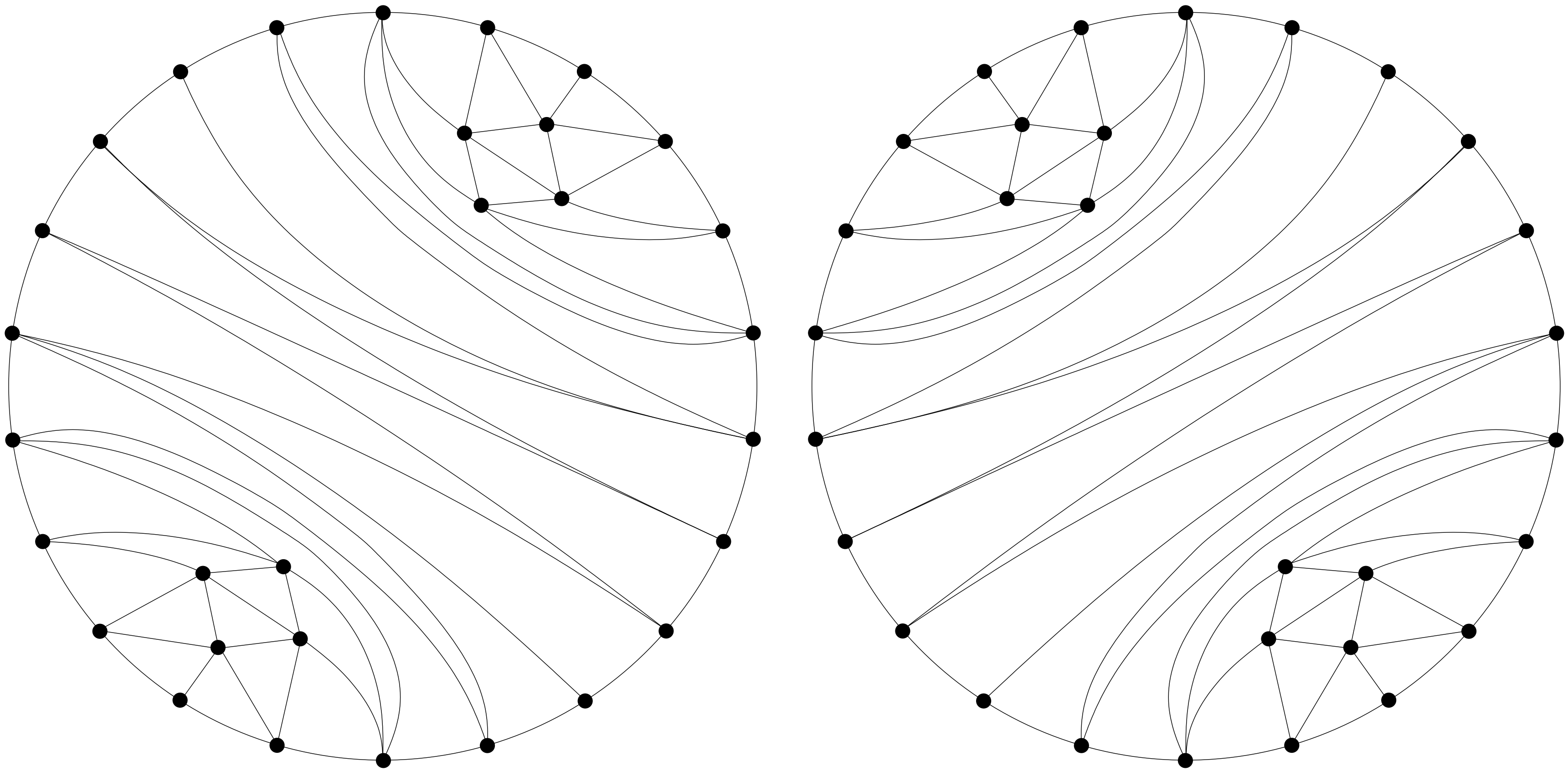
Symmetry groups are:
of boundary: C_{2v},
of polycycles: C_2.

This boundary admits two isomorphic $(p,3)$-fillings (having $4p$ p-gons and $2p$ interior 3-valent vertices).
Boundaries, admitting two non-isomorphic $(p,3)$-fillings, can be obtained by adding one p-gon.

Equi-boundary pairs of $(p, 3)$-polycycles

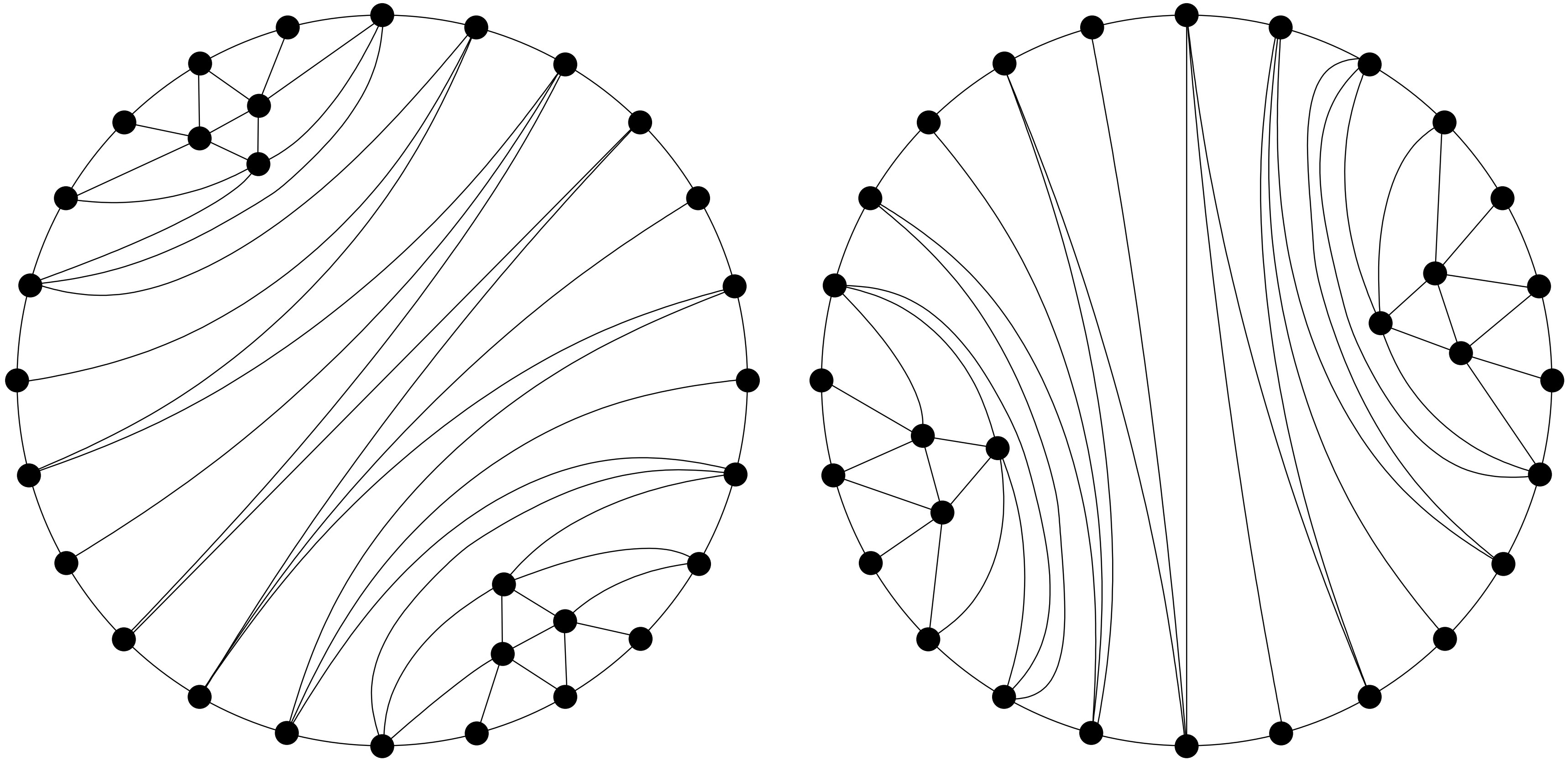
- M. Zheng (c. 2000, unpublished): the original example - two equi-boundary $(6, 3)$-polycycles with 25 hexagons.
- G.Brinkmann, O.Delgado-Friedrichs and U. von Nathusius (2004): equi-boundary $(p, 3)$-polycycles have the same number f_p of p-gons.
  So, let $N_p(k)$ be the number of such pairs with k p-gons.
- M.Deza, M.Shtogrin and M.Dutour (2005):
  proved $N_p(k) > 0$ for $k \geq 4p \geq 20$, and
  conjectured $N_p(k) = 0$ for $k < 4p$.
  The conjecture holds for $p = 5$; moreover,
  $N_5(k) = 1, 3, 17, \geq 17$ for $k = 20, = 21, = 22, \geq 23$.
- X.Guo, P.Hansen and M.Zheng (2002): the conjecture holds for $p = 6$; moreover, $N_6(k) = 1, \geq 1$ for $k = 24, \geq 25$.
  Zheng et al. found all $(6, 3)$-polycycles with ≤ 20 6-gons.

Equi-boundary $(3,5)$-fillings



Two different (but isomorphic as maps) $(3,5)$-fillings
of the same boundary $(43445544345)^2$
(by 36 triangles and 30 int. vertices).

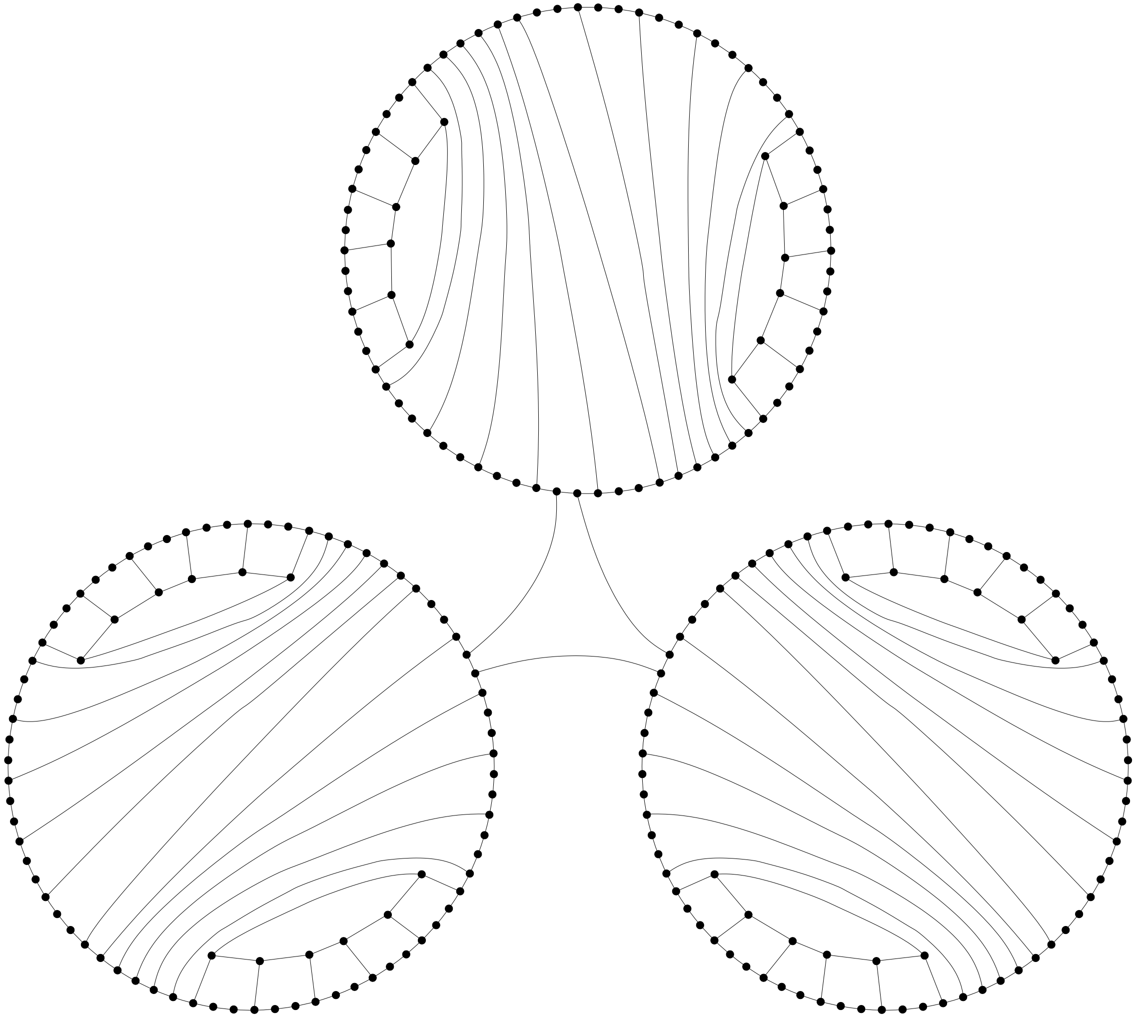
Equi-boundary $(3,5)$-fillings



Two non-isomorphic $(3,5)$-fillings of the same boundary $(34345)^2 5^2 (34345)^2 5^2$ (by 34 triangles and 30 int. vertices). Their symmetry is C_2 as of the boundary. This boundary might be minimal for the number f_3 of triangles and/or v_{int}.

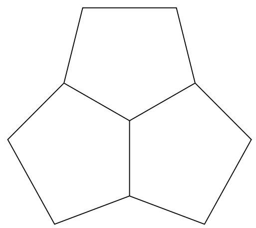
Many equi-boundary $(p, 3)$-fillings

8 $(6, 3)$-fillings come by two fillings of those 3 components; same aggregating gives arbitrarily large number for $p \geq 6$.

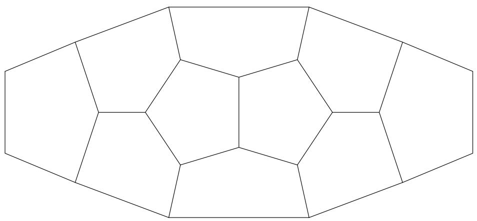


$n+1$ equi-boundary $(5,3)$-fillings

Theorem: the boundary $223^{5n+1}223^{5n+3}223^{5n+1}223^{5n+3}$ admits exactly $n+1$ different $(5,3)$-fillings (by $20n+6$ pentagons and $20n+2$ interior vertices).
Each such k-th filling, $0 \le k \le n$, is obtained by gluing two (elementary $(5,3)$-polycycles) E_1 and adding to the 4 open edges (i.e., with 2-valent end-vertices) of $E_1 + E_1$, respectively, chains of k, $n-k$, k and $n-k$ (elementary $(5,3)$-polycycles) C_1.



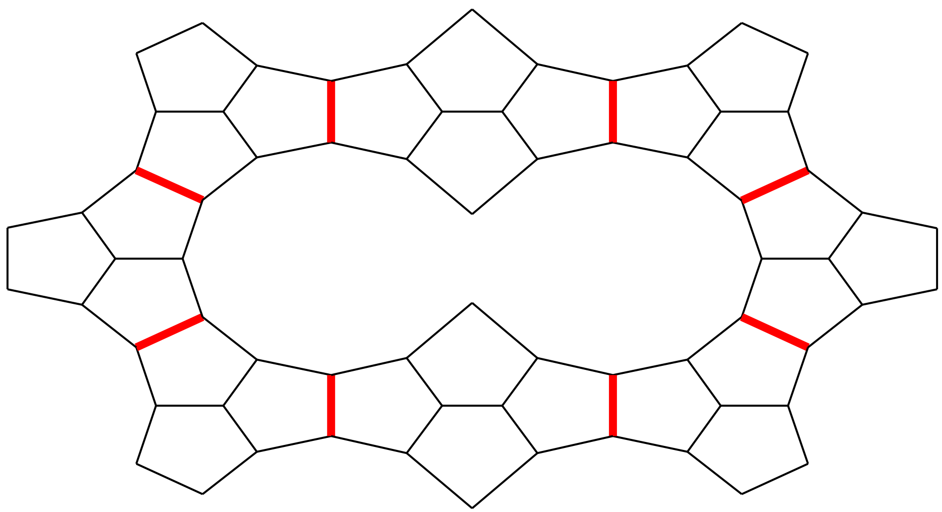
E_1: $(223)^3$



C_1: $(223333)^2$

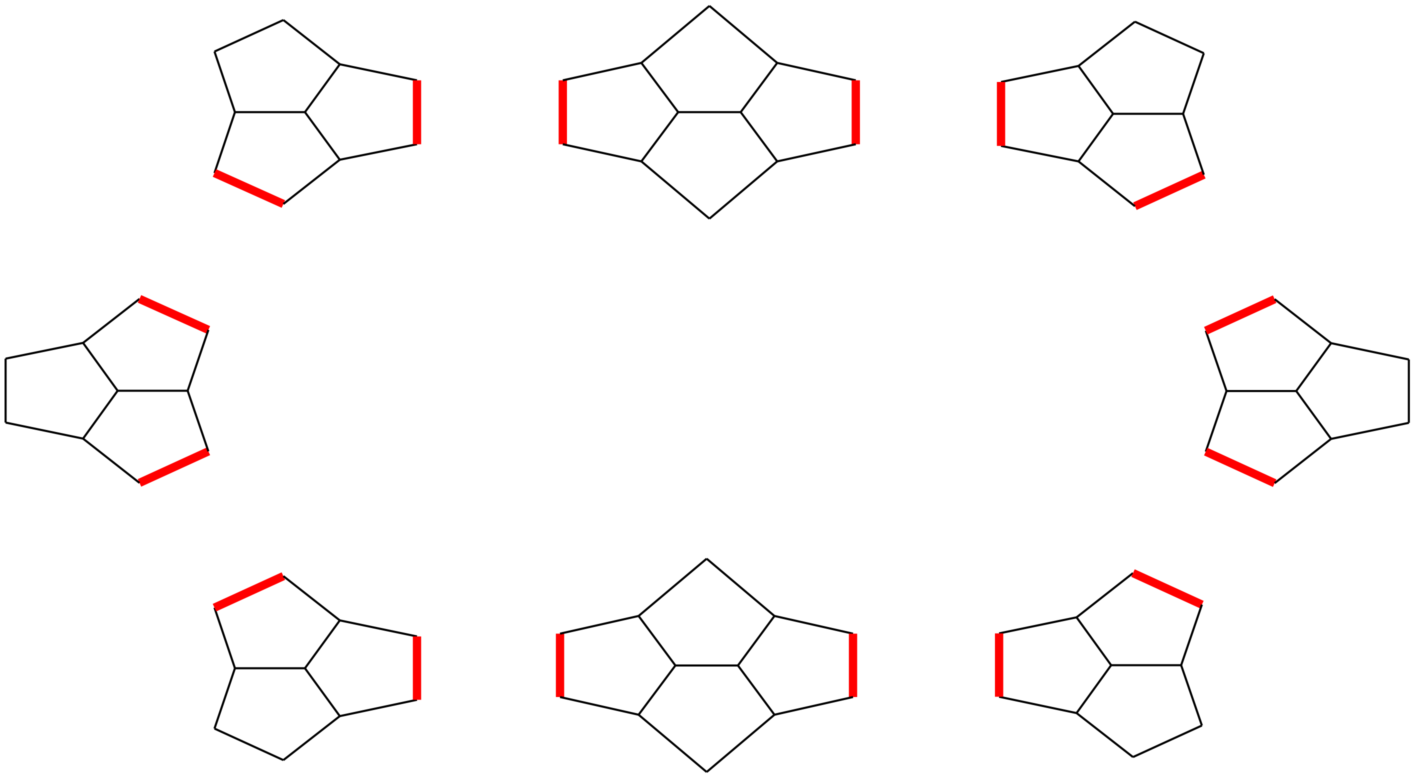
Decomposition theorem

- Theorem: Any (R, q)-polycycle is uniquely decomposed into elementary (R, q)-polycycles along its bridges.
- In other words, any (R, q)-polycycle is obtained by gluing some elementary (R, q)-polycycles along open edges.



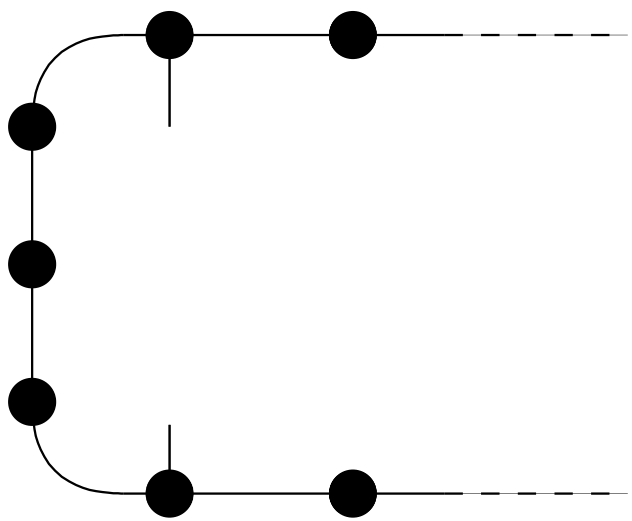
Decomposition theorem

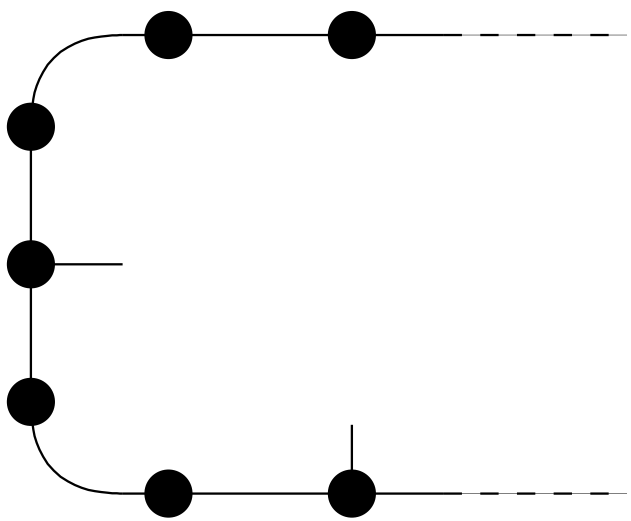
- Theorem: Any (R, q)-polycycle is uniquely decomposed into elementary (R, q)-polycycles along its bridges.
- In other words, any (R, q)-polycycle is obtained by gluing some elementary (R, q)-polycycles along open edges.



Possible filling

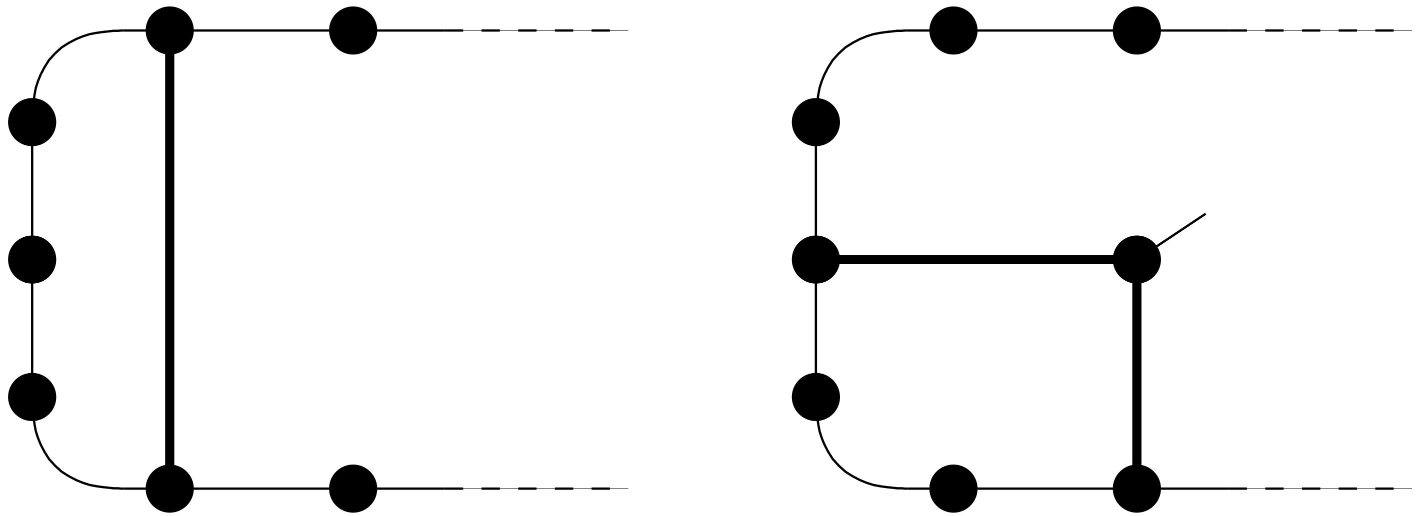
Let us illustrate the algorithm for the simplest case $p = 5$.
In some cases we can complete the patch directly.





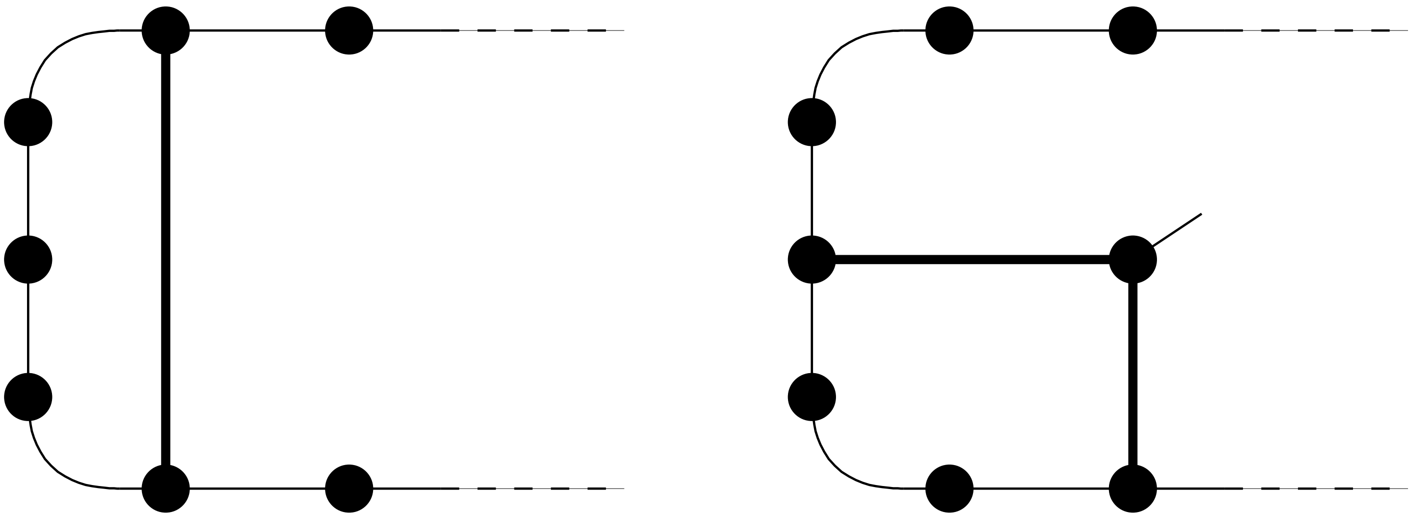
Possible filling

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



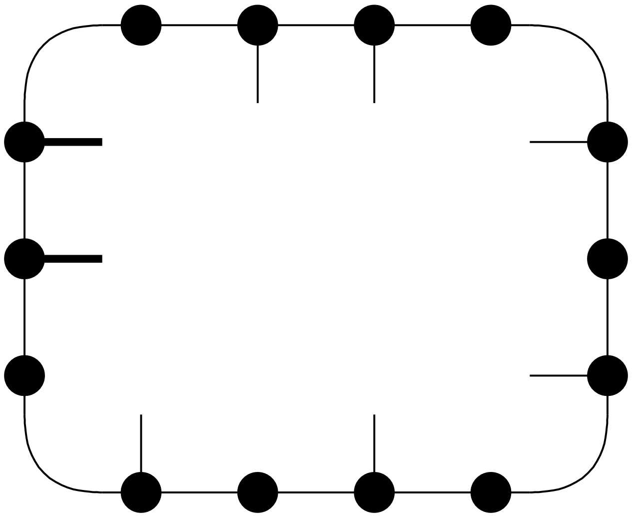
Possible filling

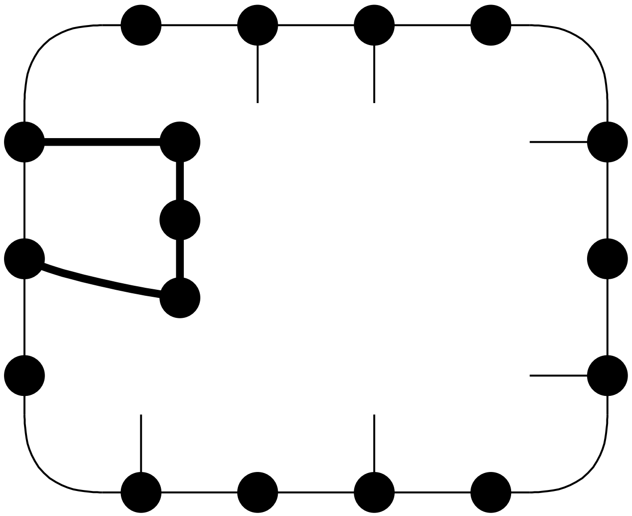
Let us illustrate the algorithm for the simplest case $p = 5$.
In some cases we can complete the patch directly.



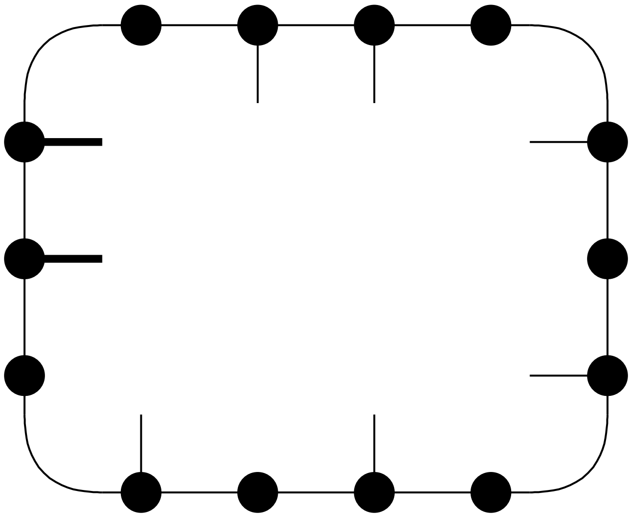
But in some cases more is needed:

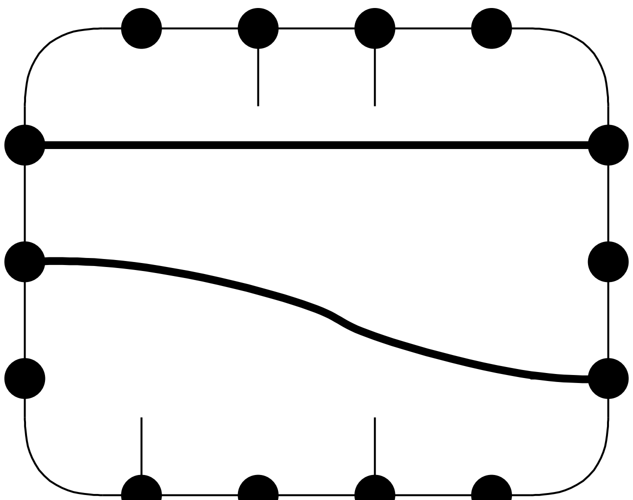
Different possible options



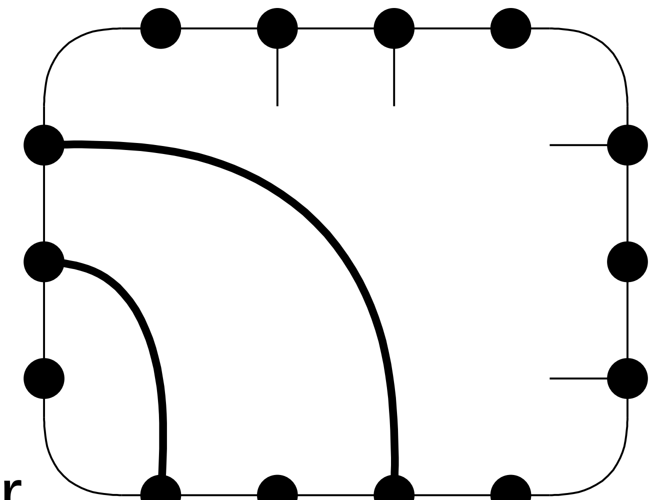


Different possible options

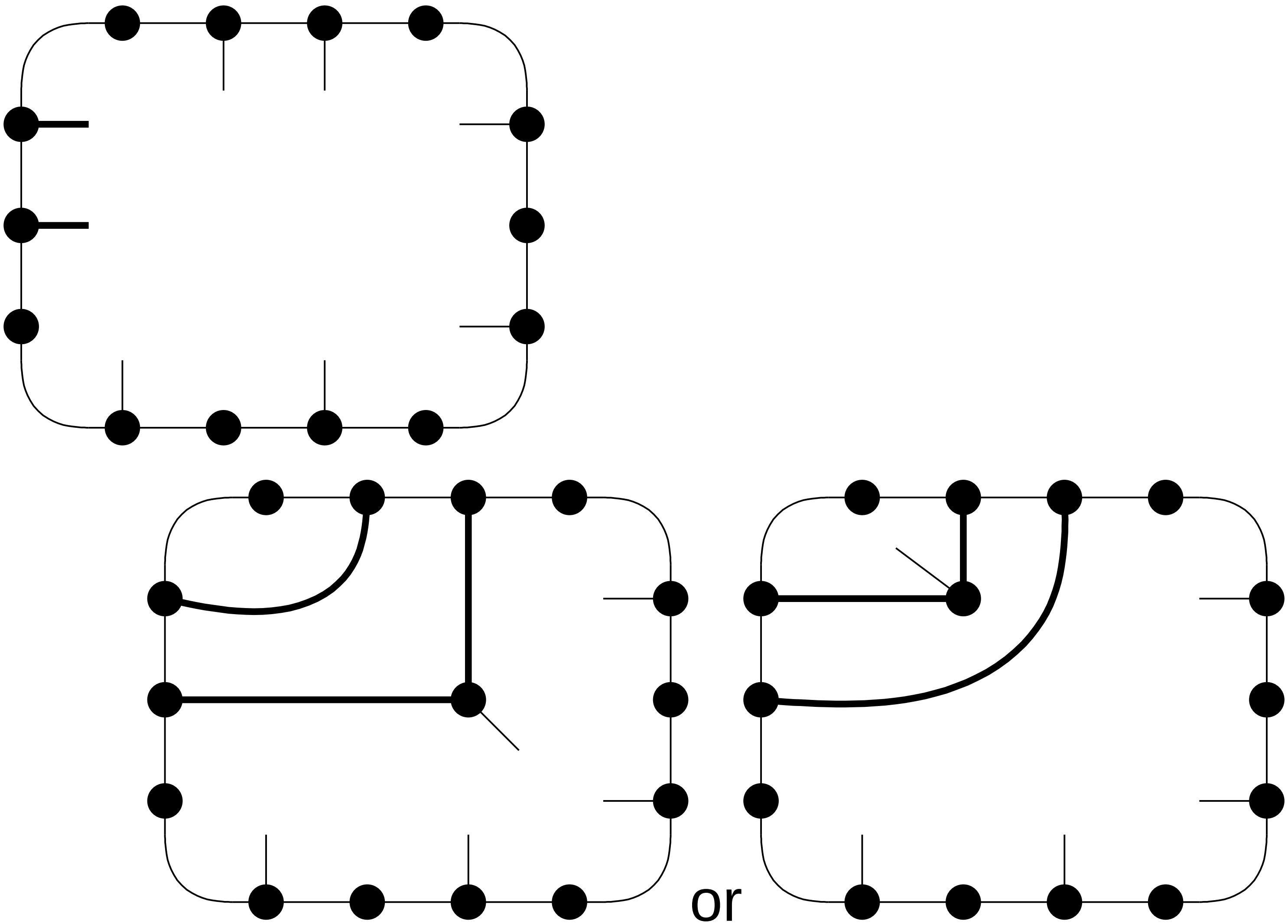




or



Different possible options



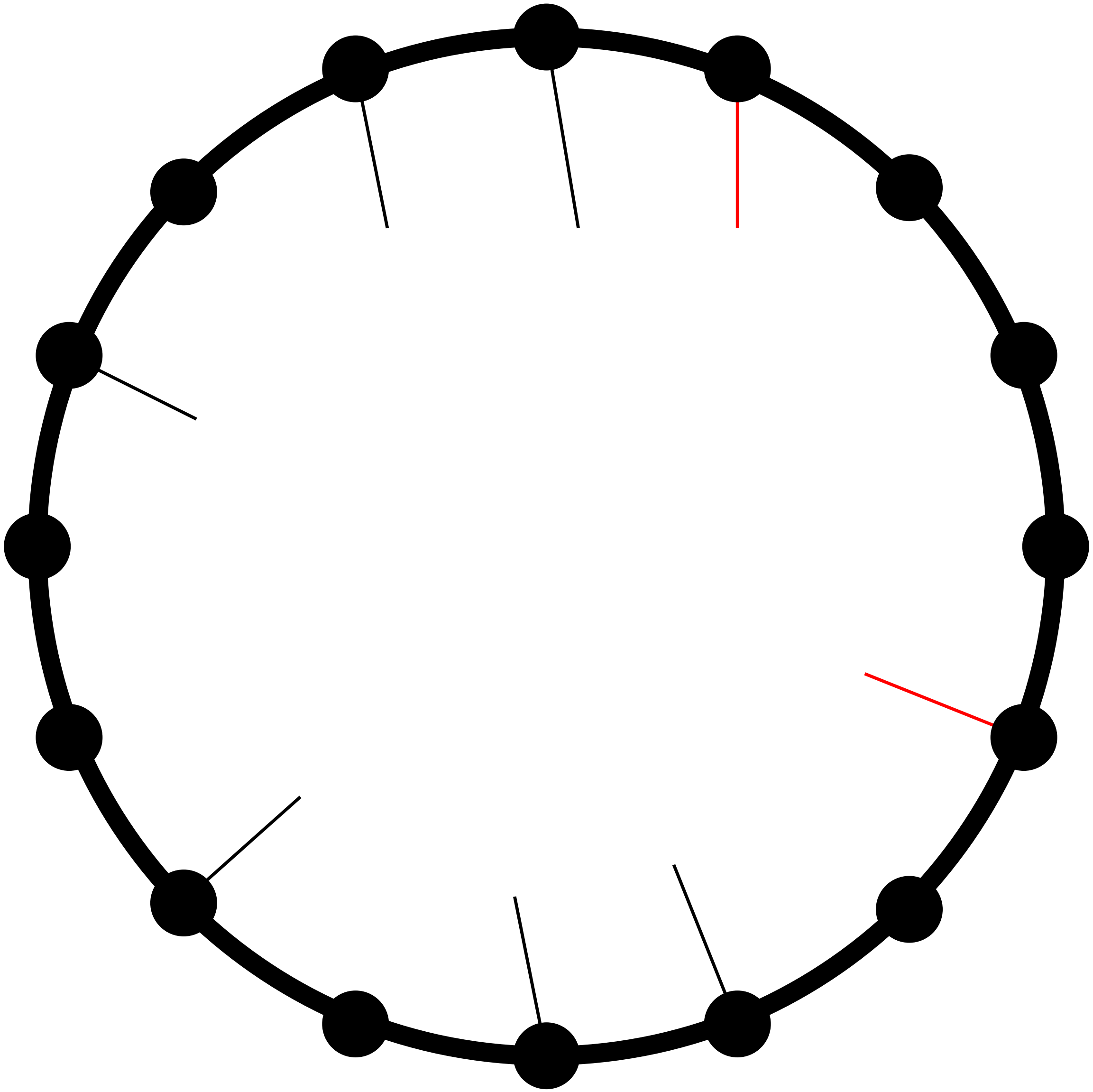
Algorithm

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:

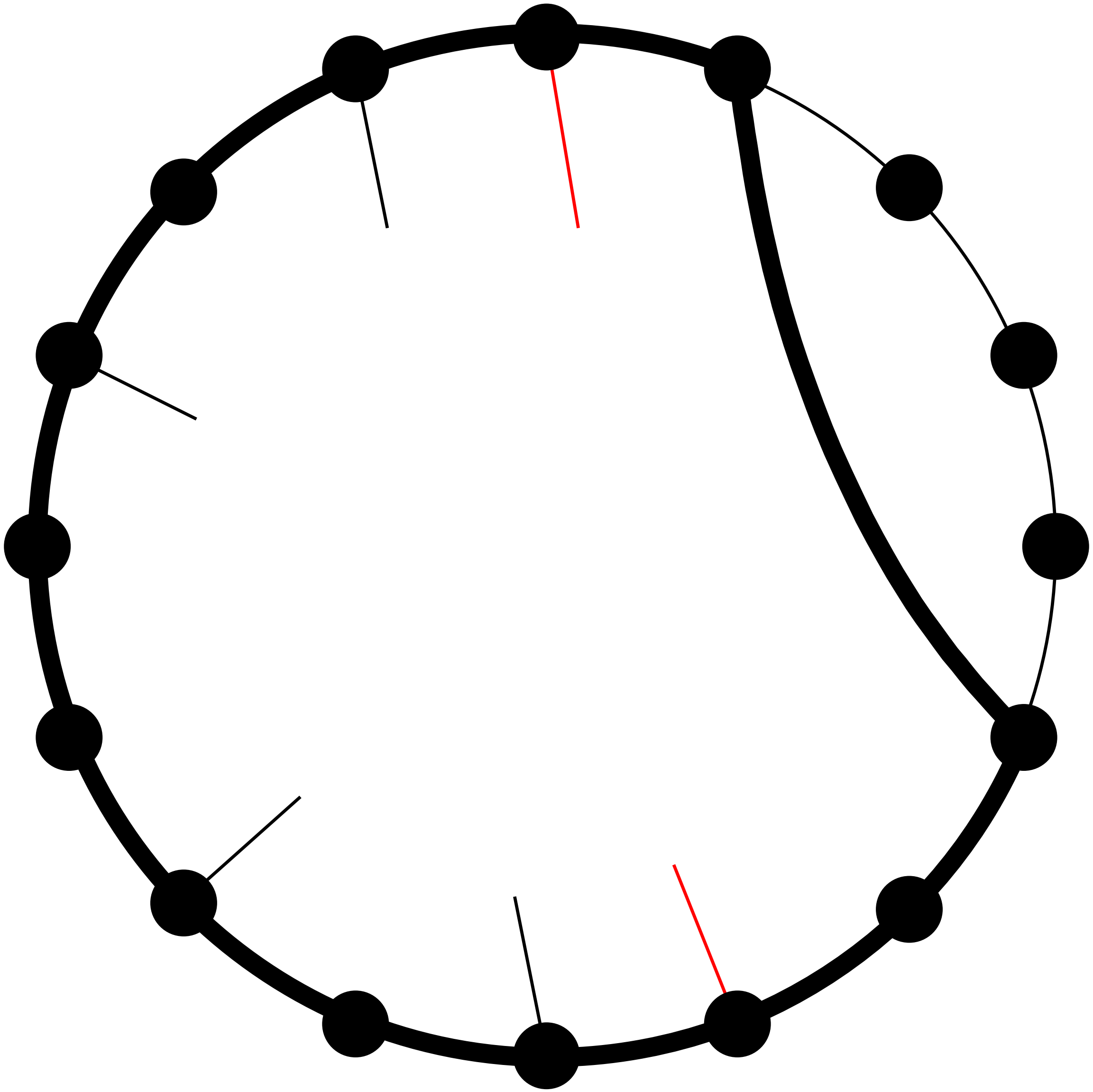
1. Take a pair of vertices of degree 3 on the boundary and consider all possible completions to form a p-gon.
2. Every possible case define another patch of faces. Depending on the choice, the patch will have one or more boundaries.
3. For any of those boundaries, reapply the algorithm.

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

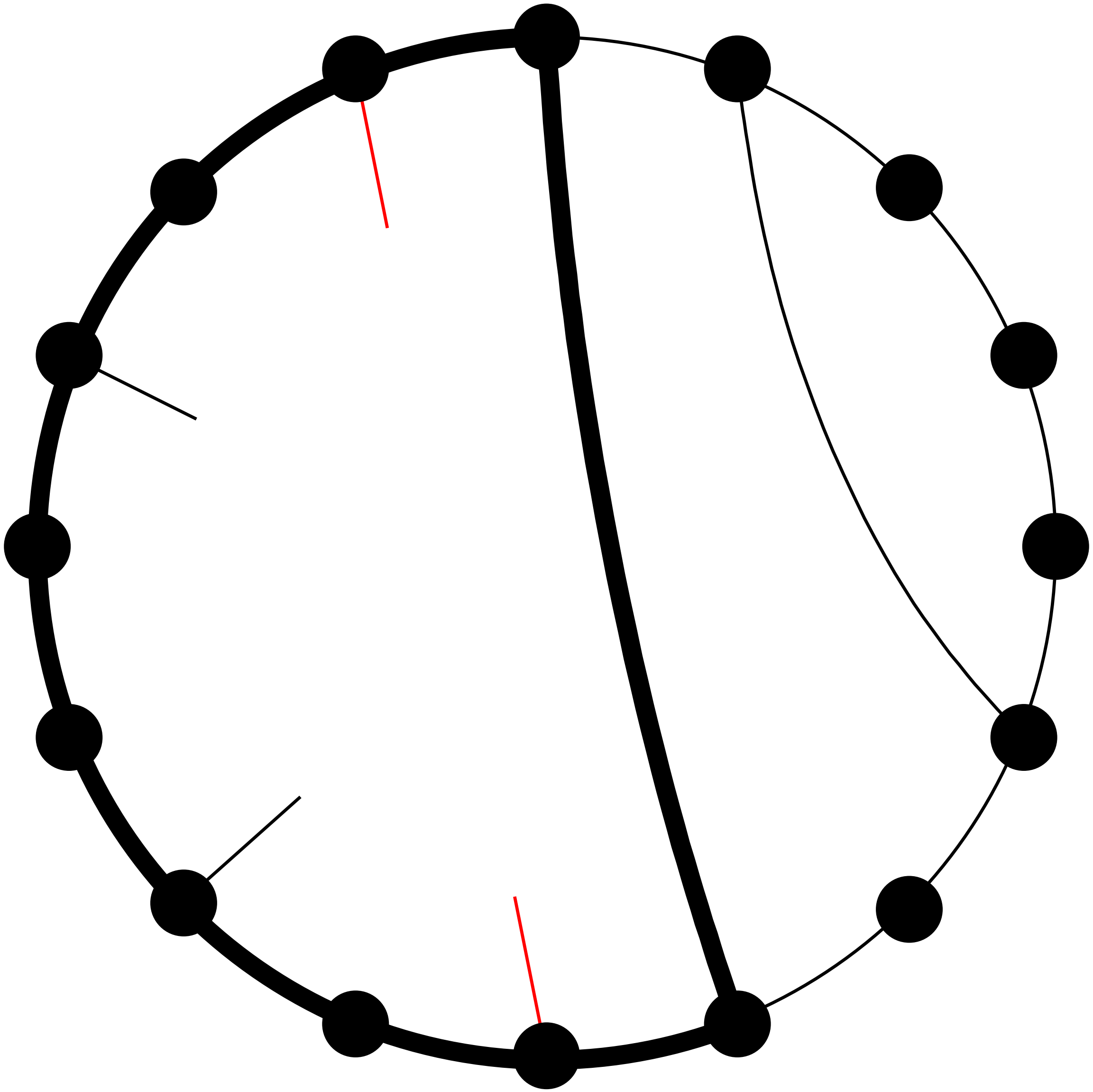
An example of a search



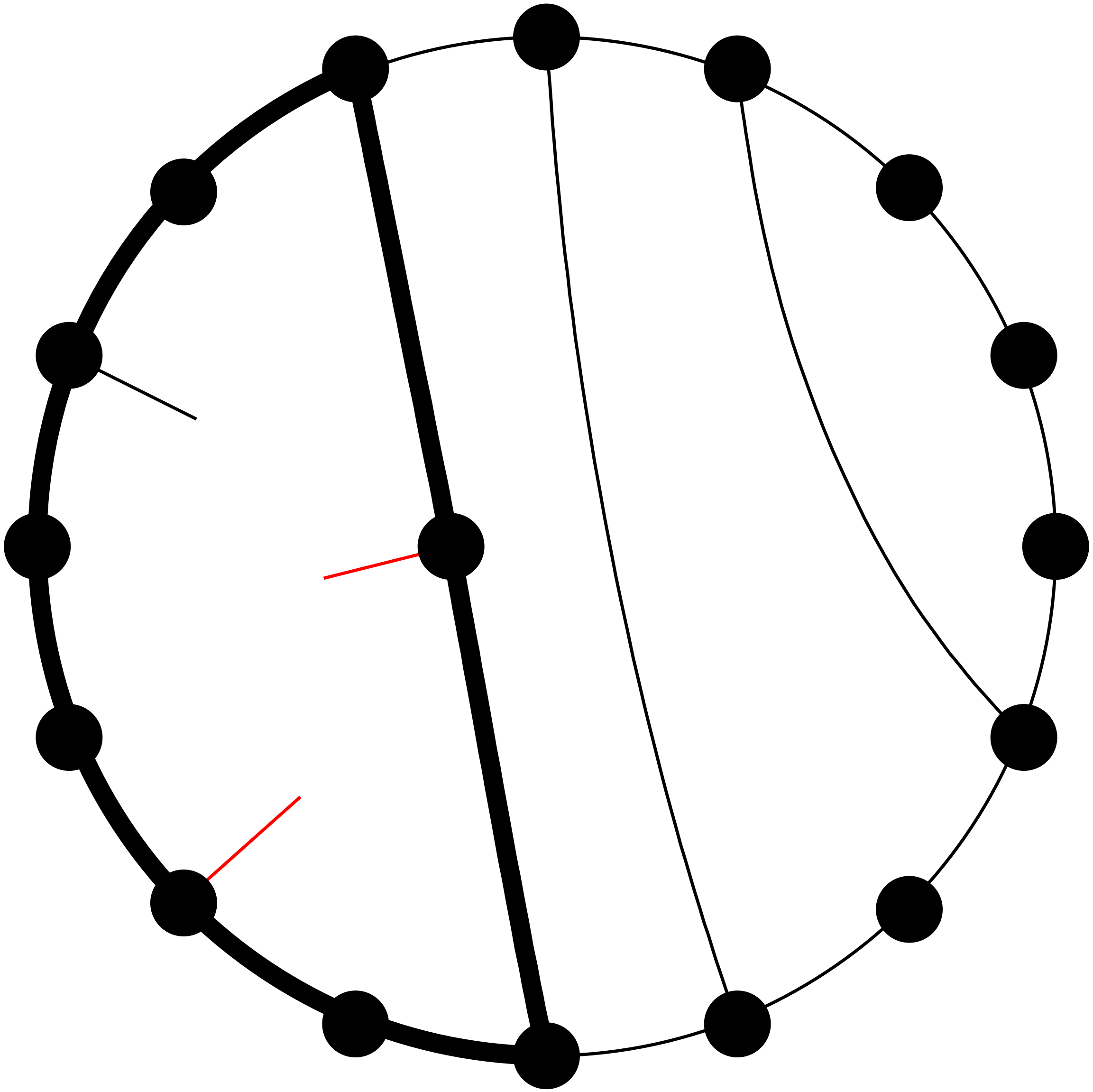
An example of a search



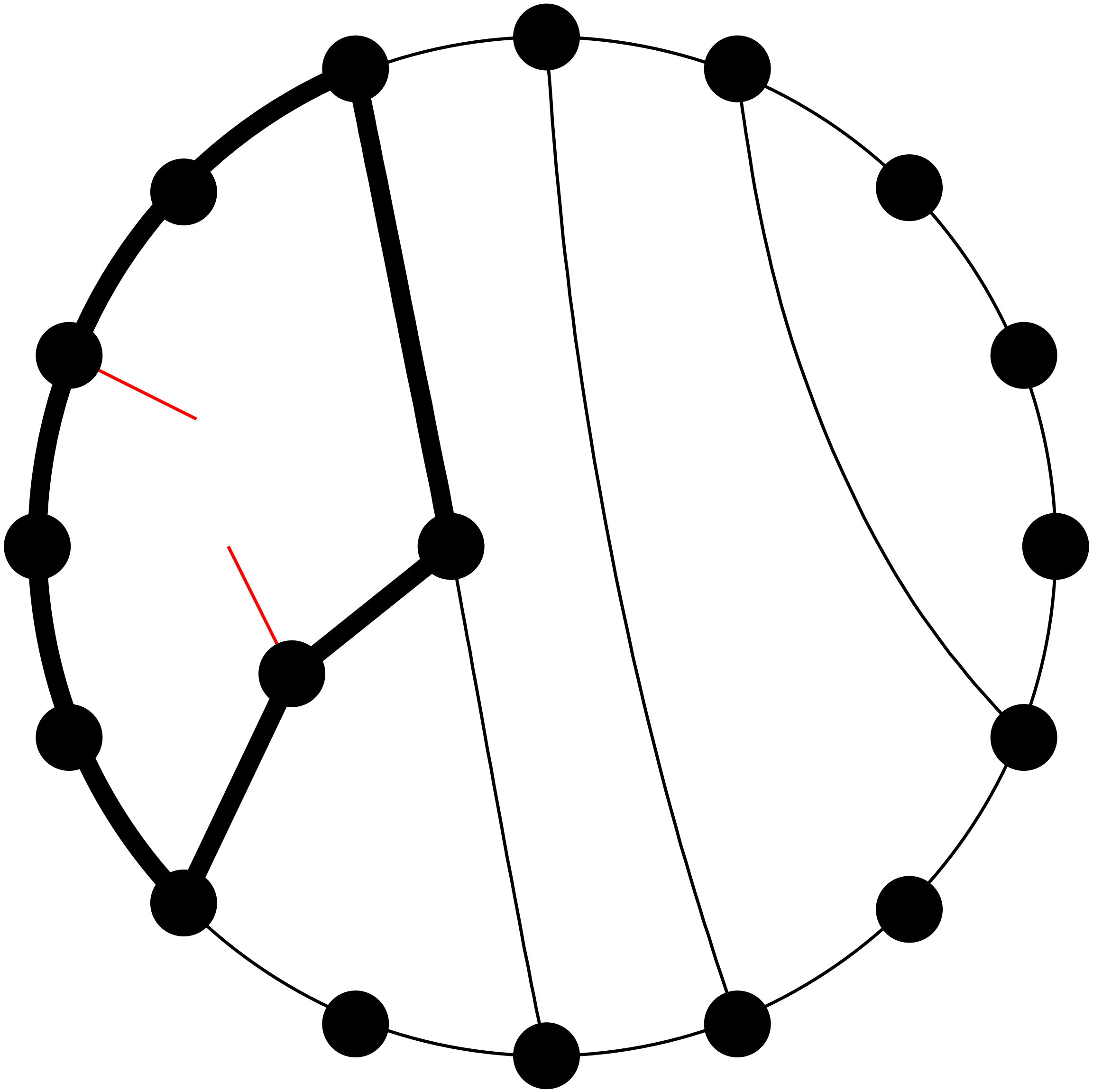
An example of a search



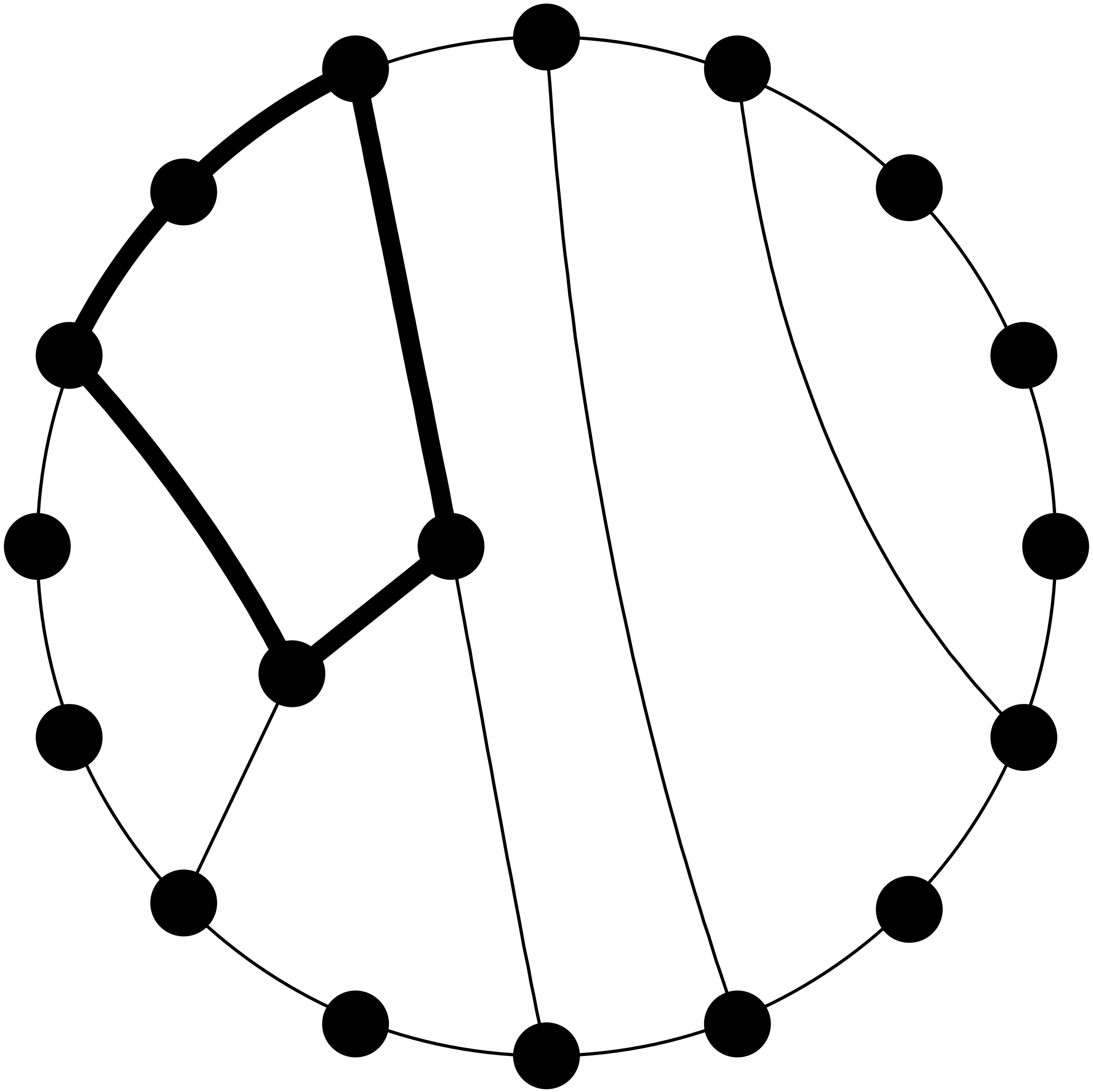
An example of a search



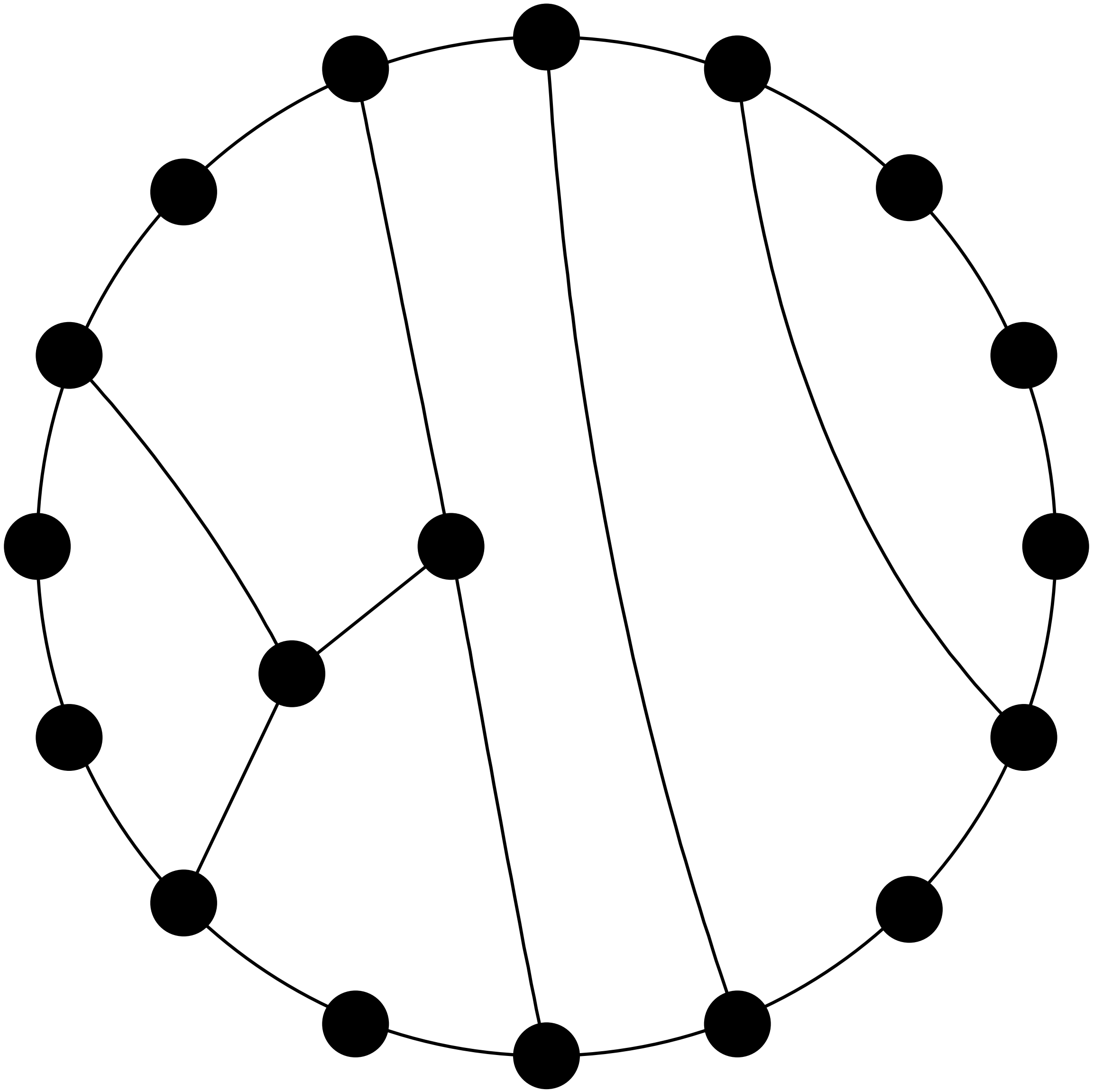
An example of a search



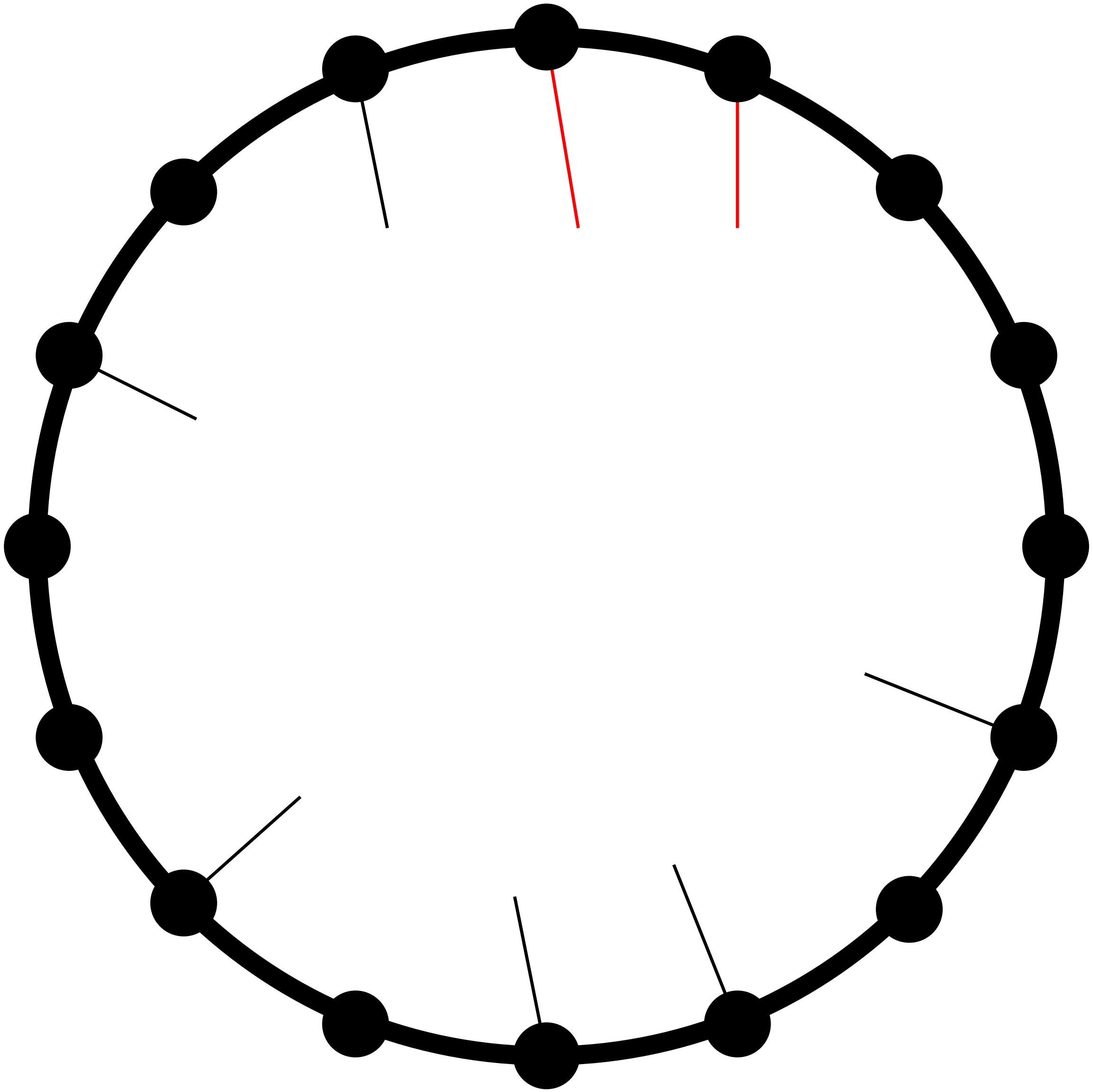
An example of a search



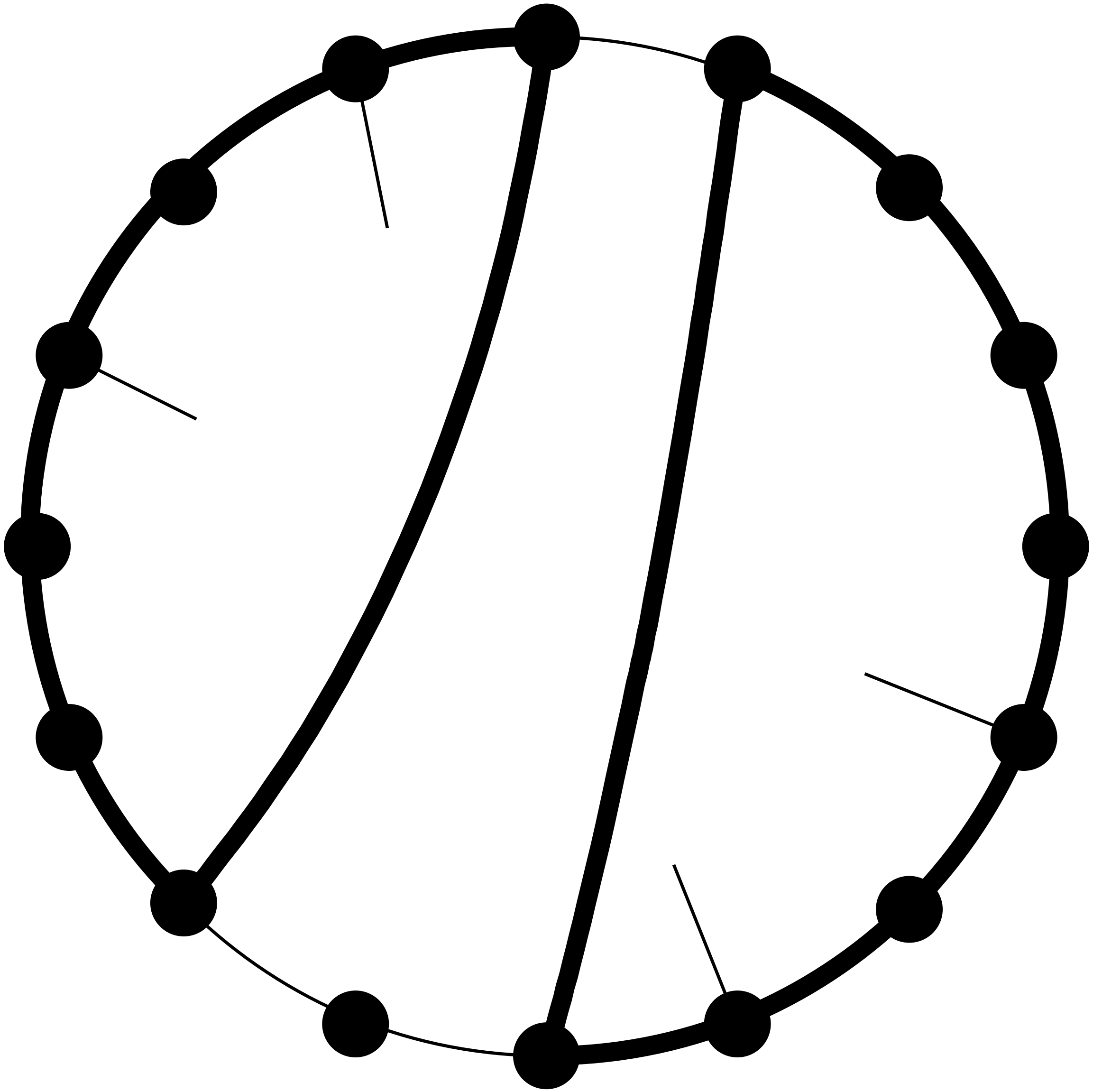
An example of a search



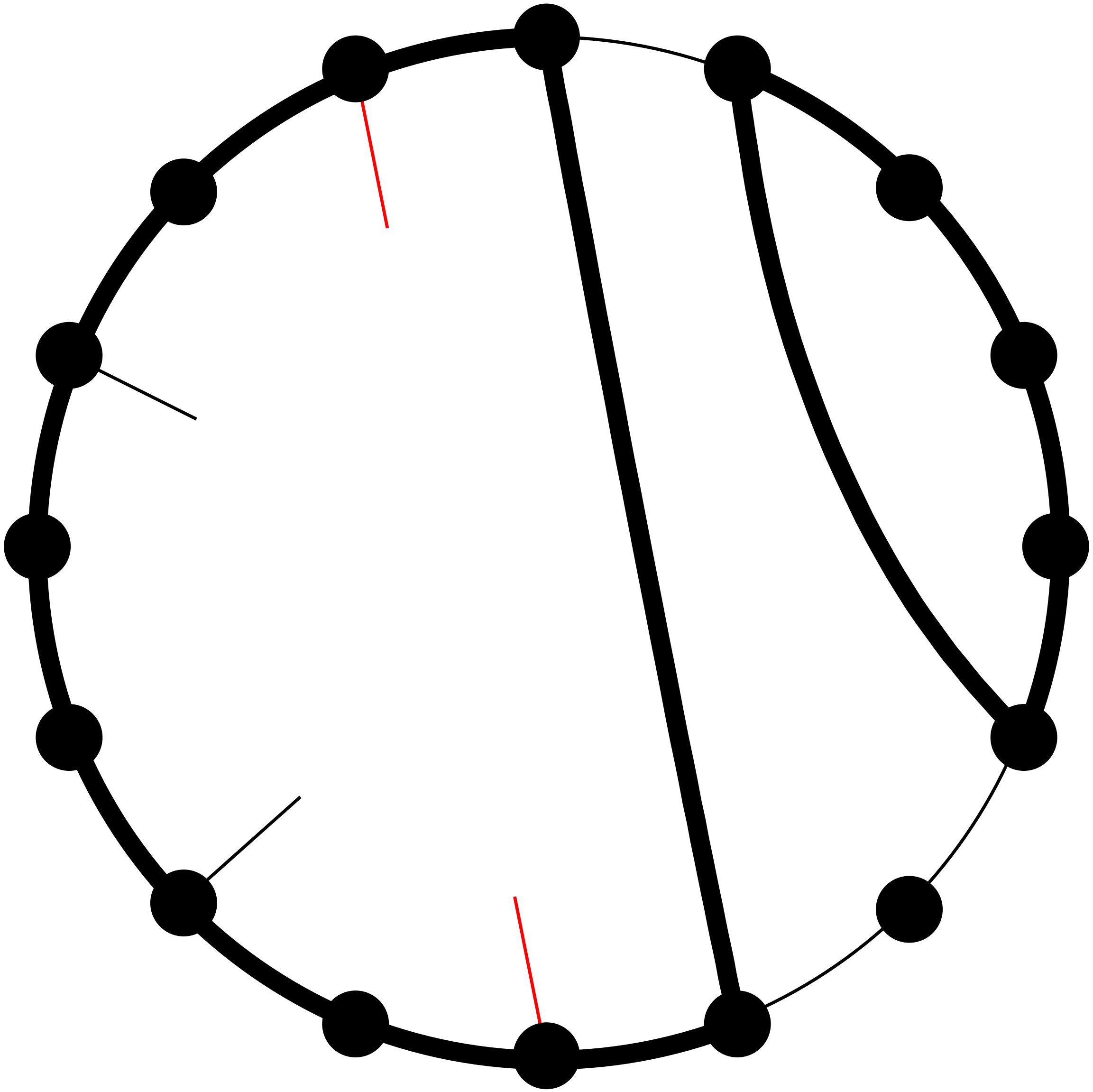
Another possible search



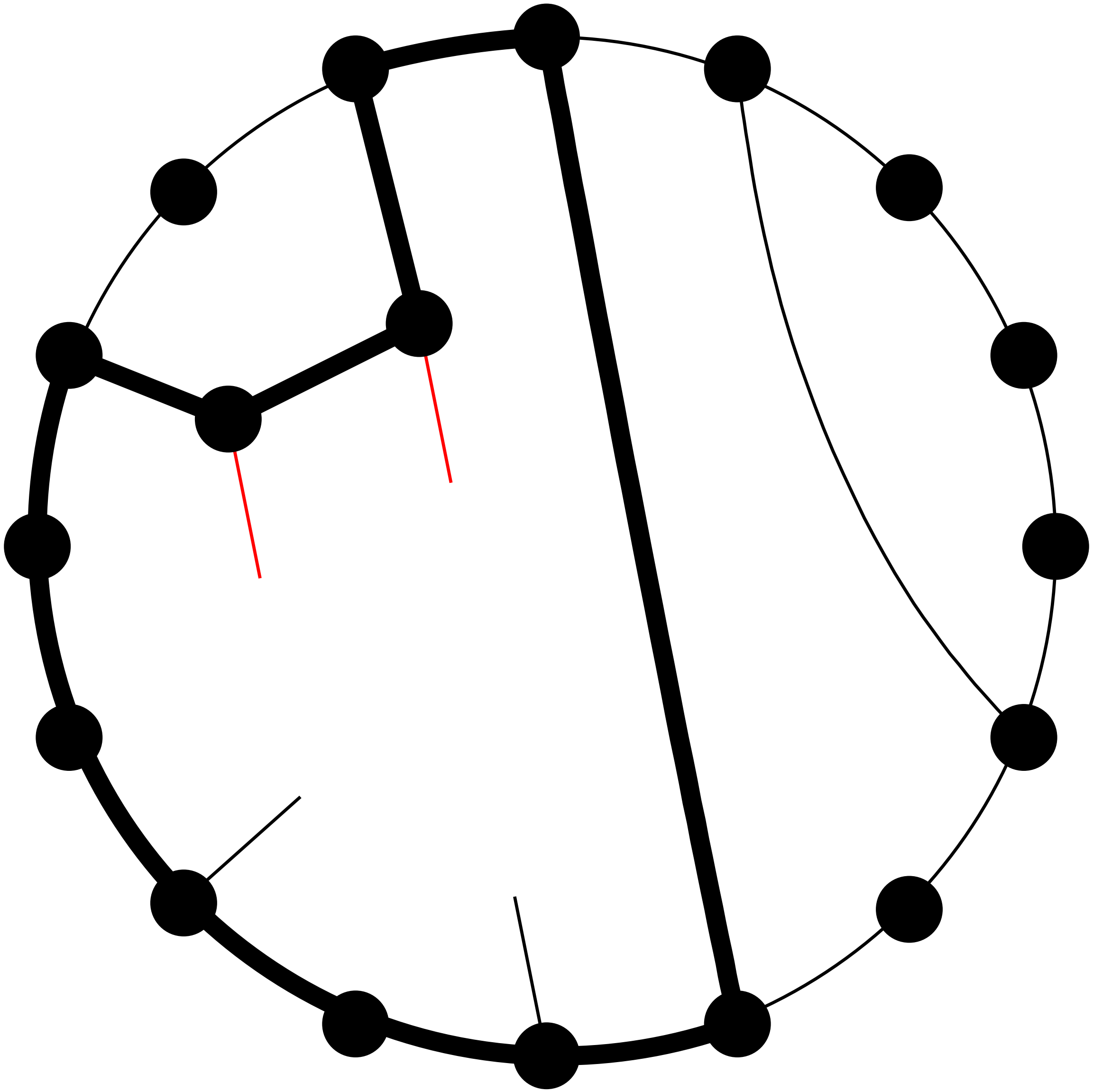
Another possible search



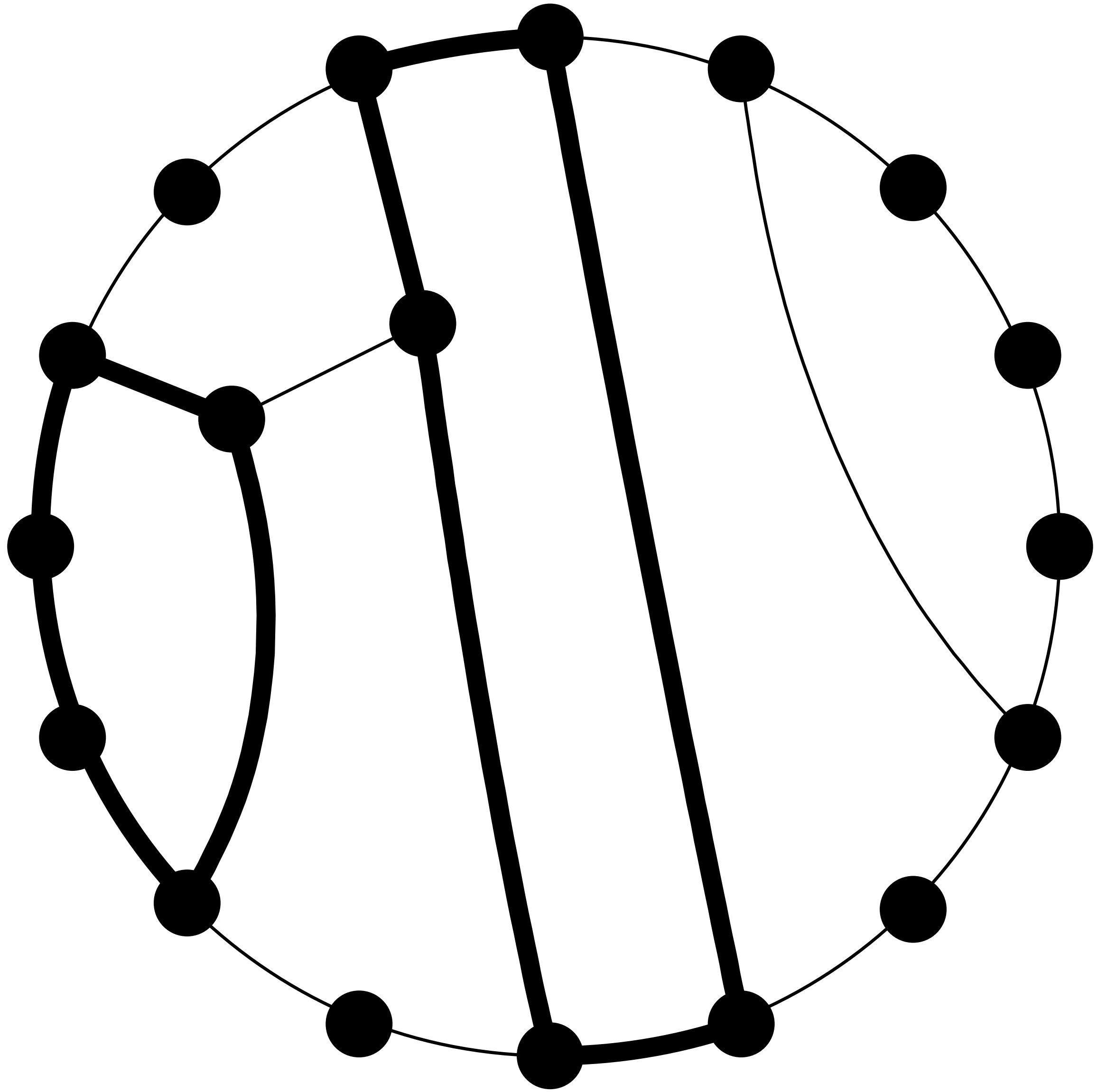
Another possible search



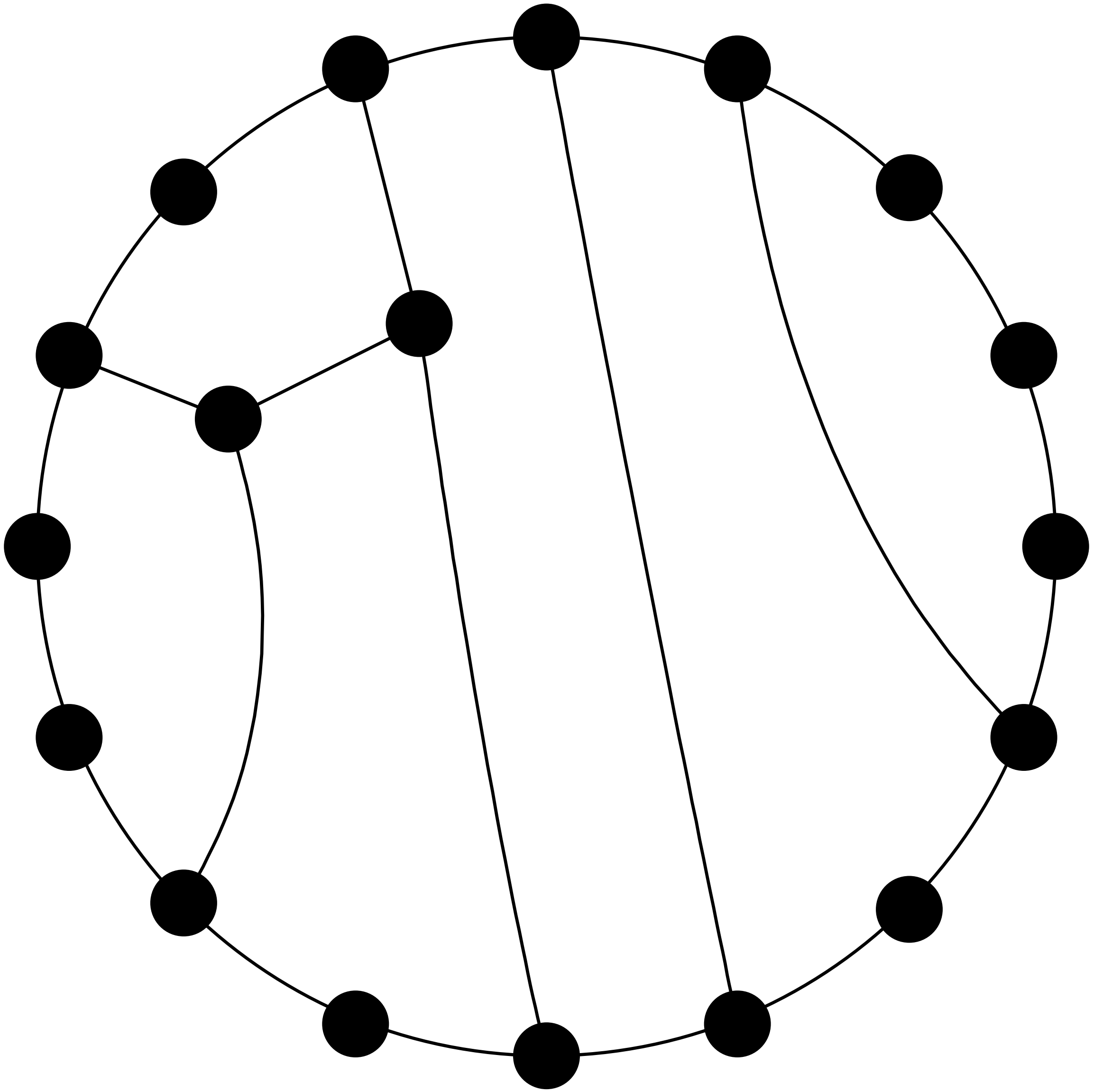
Another possible search



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.

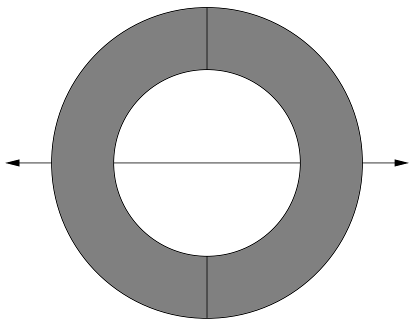
Classification theorem

Main Theorem

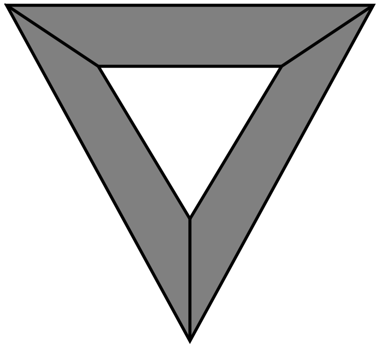
Besides the cases (p,q)=$(7,5)$ *and* $(5,q)$ *with* $q \geq 8$, *all such maps are known;*

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

If $p = 3$, two possibilities:



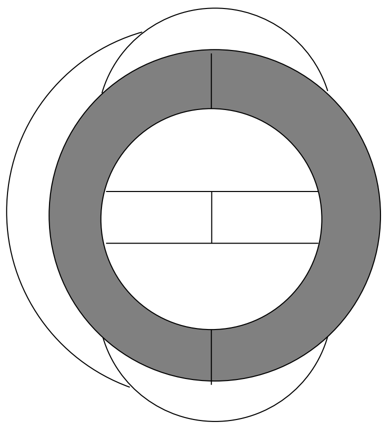
$M_2(3,6)(D_{2h})$



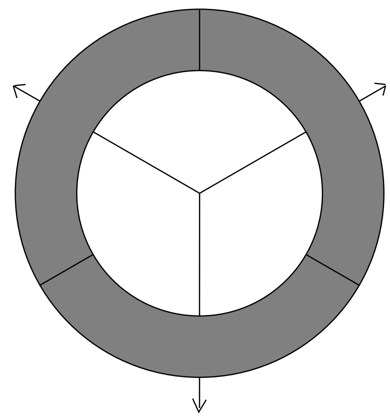
$M_3(3,4)(D_{3h})$

Case $p = 4$

If $p = 4$, two possibilities:

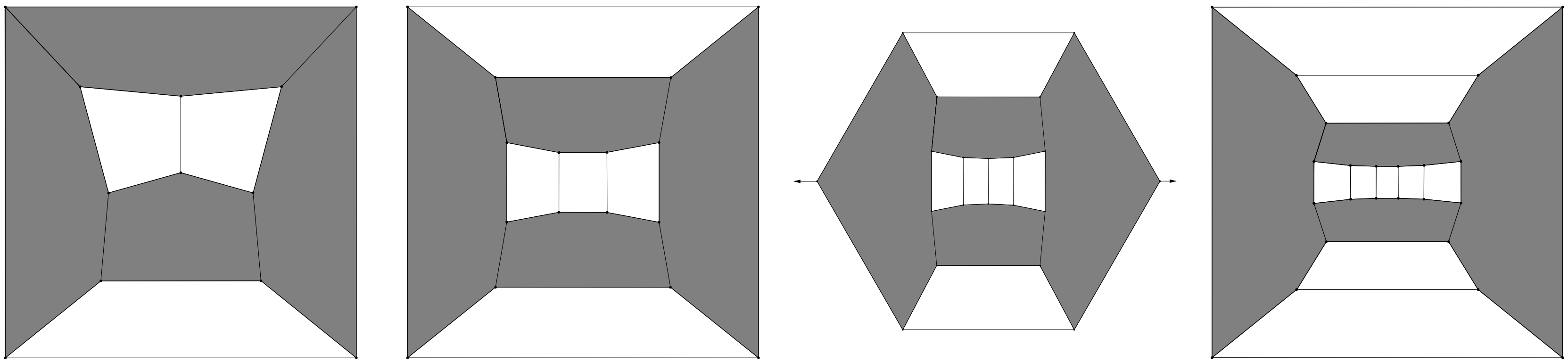


$M_2(4,8)(D_{2h})$



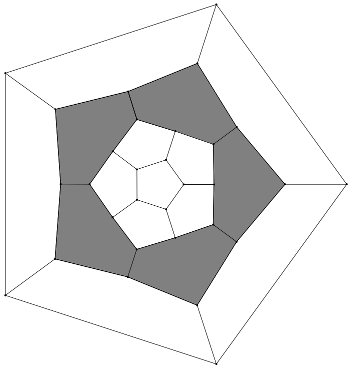
$M_3(4,6)(D_{3h})$

and an infinite serie

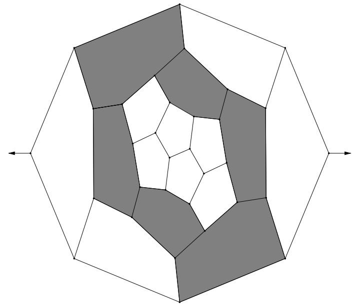


Case $p = 5$

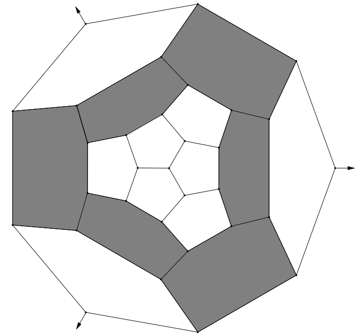
- If $q = 5$, then this is Dodecahedron
- If $q = 6$, then five possibilities:



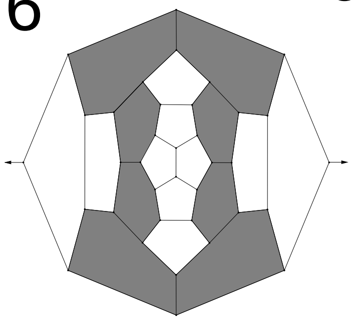
5, D_{5h};6,6



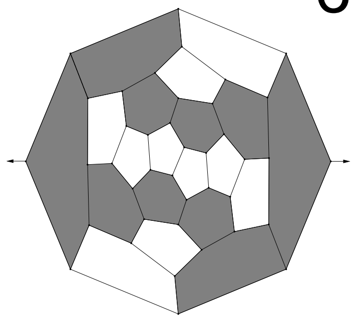
6, D_2;6,6



6, D_{3d};6,6



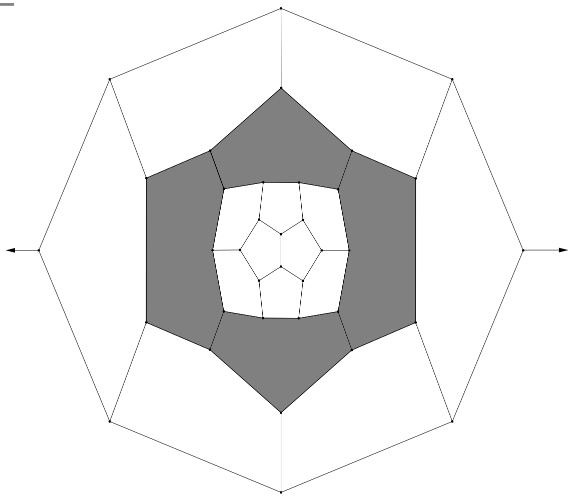
8, D_{2d};6,6



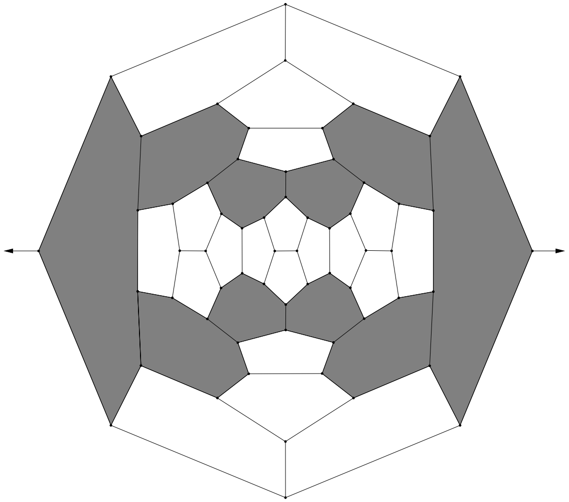
10, D_2;6,6

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

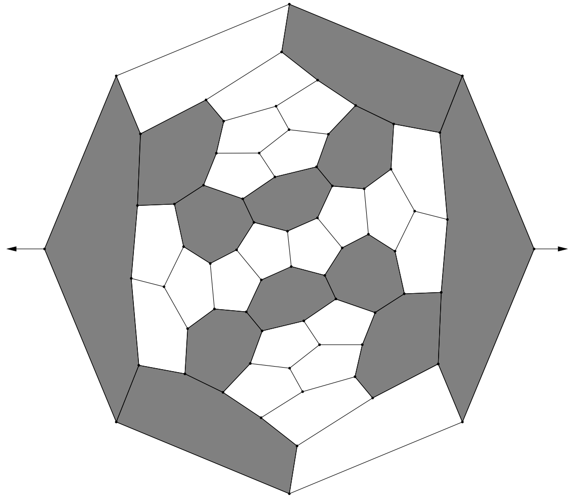
All $M_n(5,7)$



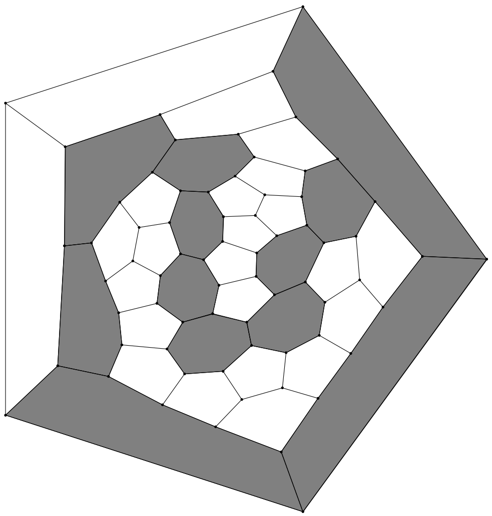
4, D_{2d};8,8



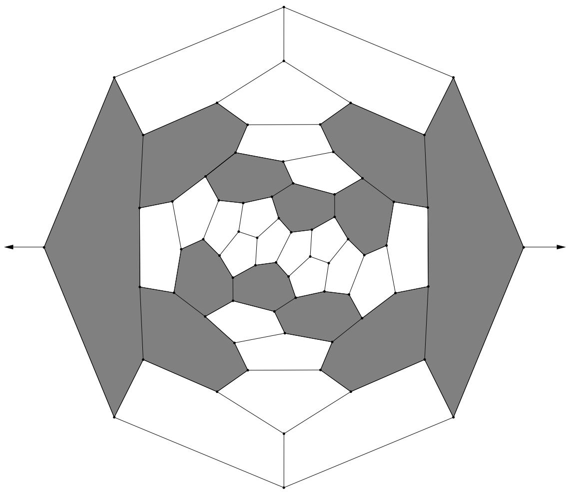
10, C_{2v};12,10



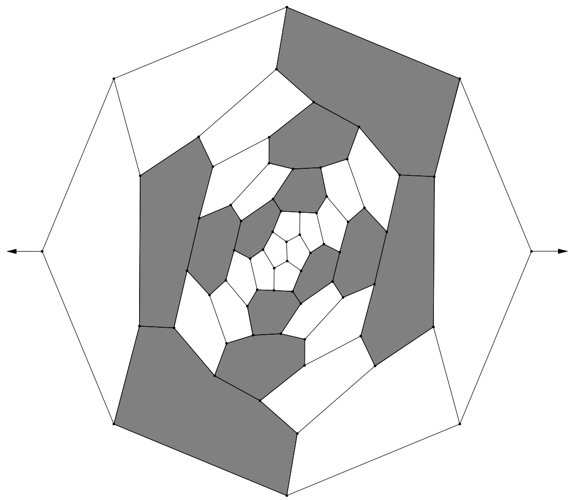
12, C_2;10,14



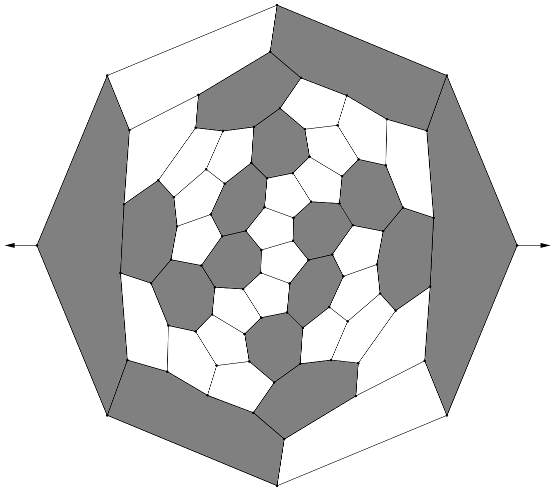
12, C_1;13,11



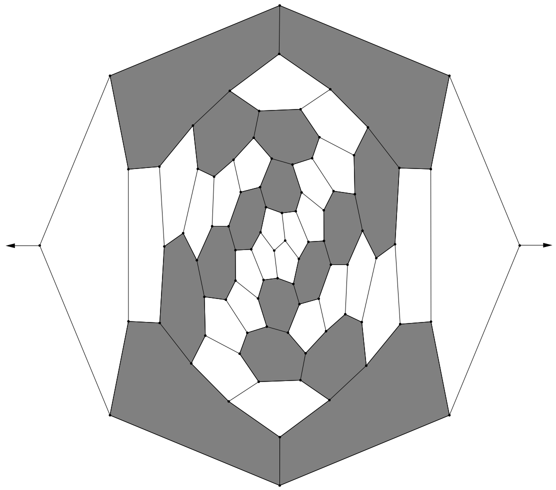
12, D_2;12,12



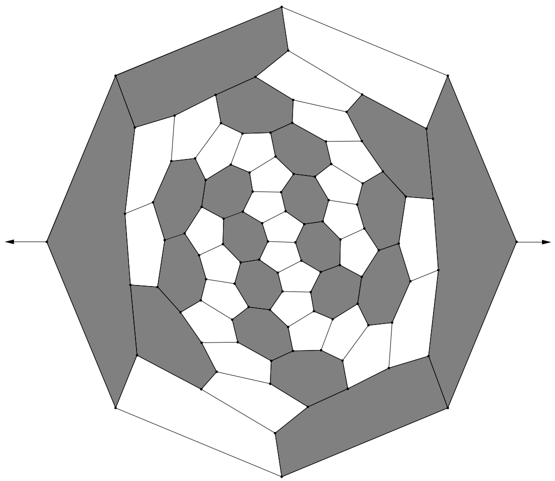
12, S_4;12,12



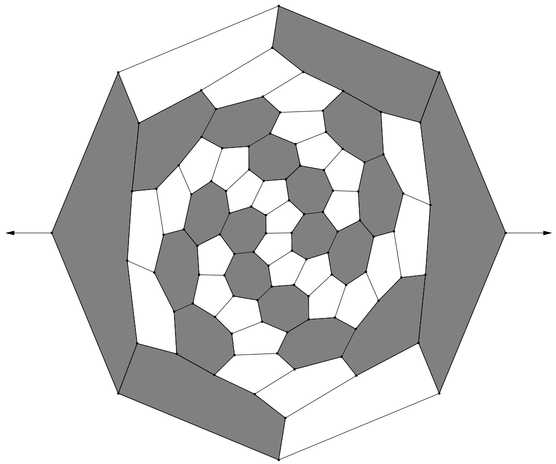
16, D_2;14,14



16, D_2;14,14



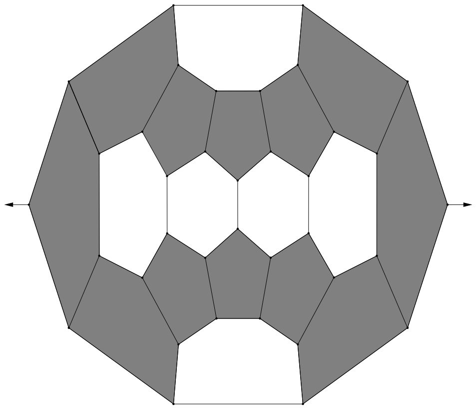
20, D_2;16,16



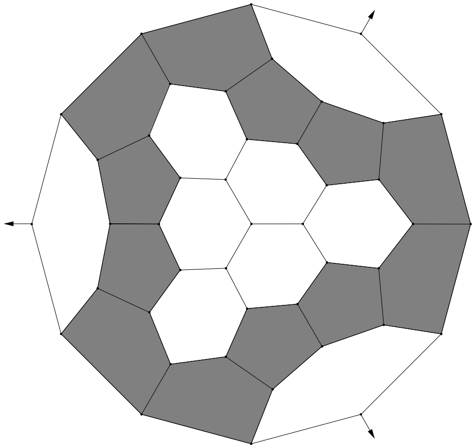
20, C_2;16,16

Case $p = 6$

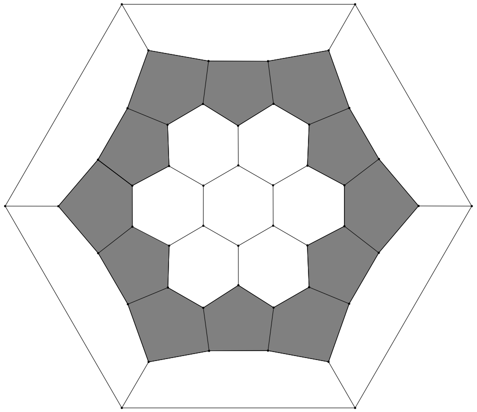
If $p = 6$, then $q = 5$. There are four possibilities:



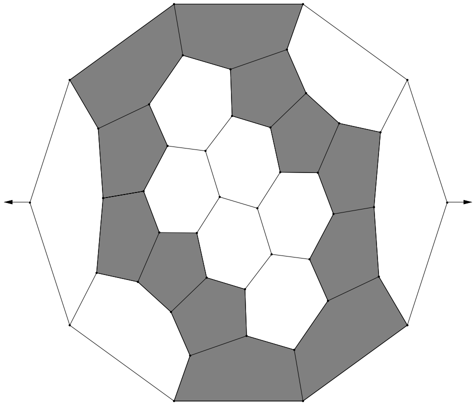
12, D_{2d};4,4



12, D_{3d};6,6



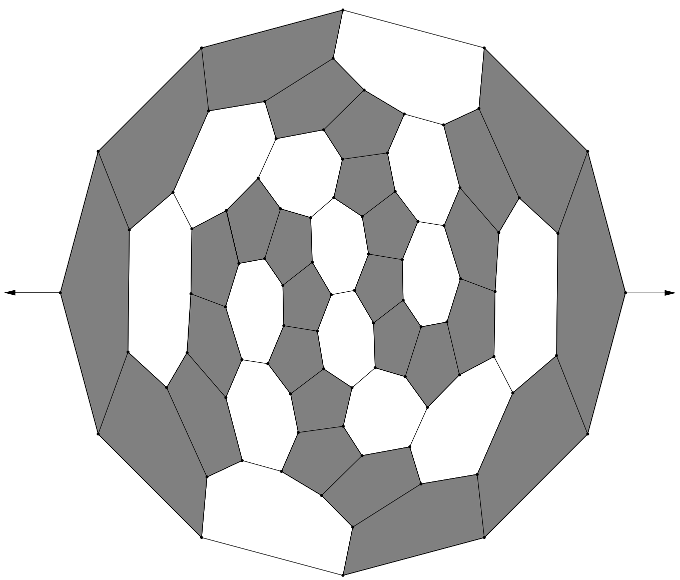
12, D_{6d};7,7



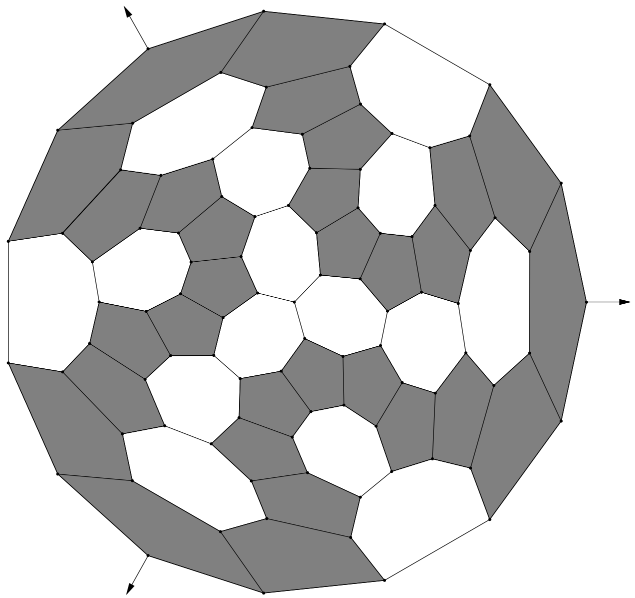
12, D_2;6,6

Two remaining undecided cases

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



28, D_2;8,8



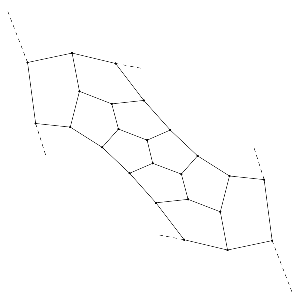
30, D_3;9,9

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

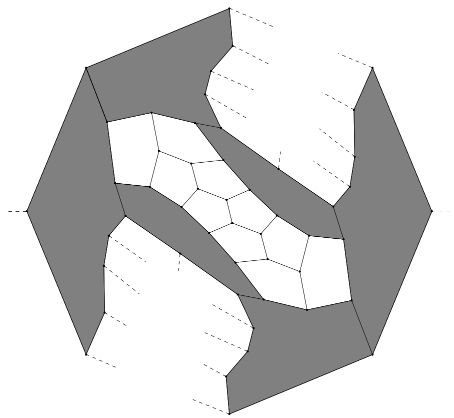
- Hadjuk and Soták found an infinity of maps $M_n(7, 5)$,
- Madaras and Soták found infinity of maps $M_n(5, q)$ for $q = 10$ and $q \equiv 2, 3 \pmod 5$, $q \geq 8$.

Enumeration techniques

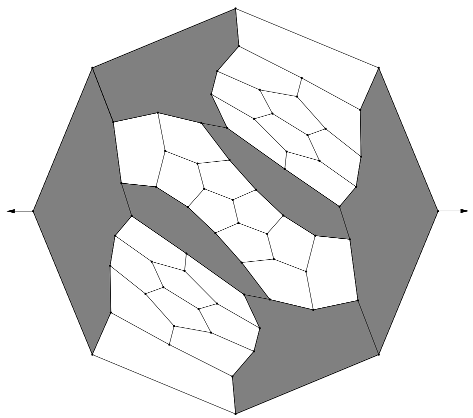
- Harmuth enumerated all 3-valent plane graphs with at most 84 vertices, faces of gonality 5 or 7 and such that every faces of gonality 7 is adjacent to two faces of gonality 7 (i.e. 7-gons are organised into disjoint simple cycles). It gives all $M_n(5,7)$ with $n \leq 16$.
- Remaining case $17 \leq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



Generating patches

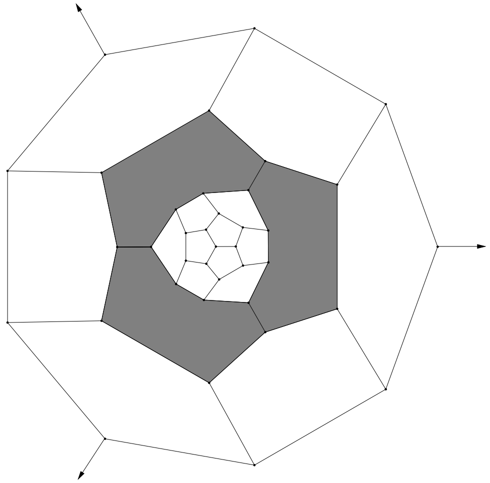


Adding ring of q gons

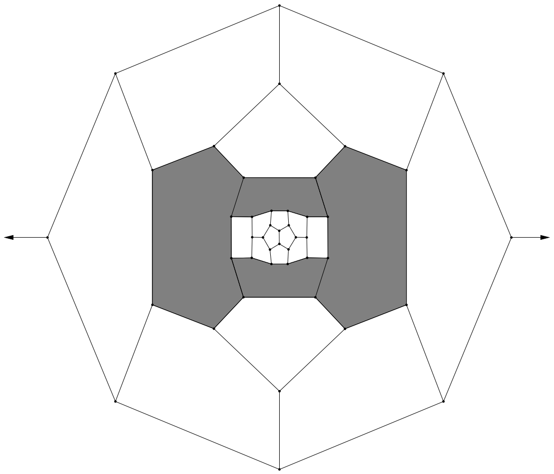


completing (if possible).

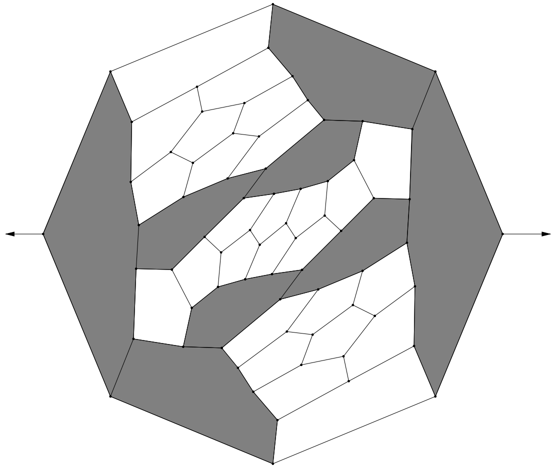
Known $M_n(5,8)$



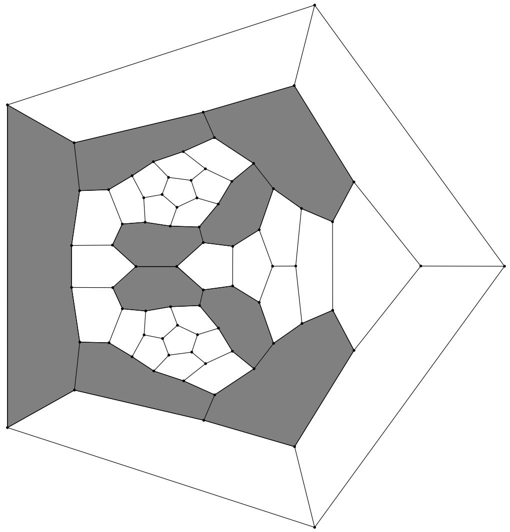
3, D_{3h};9,9



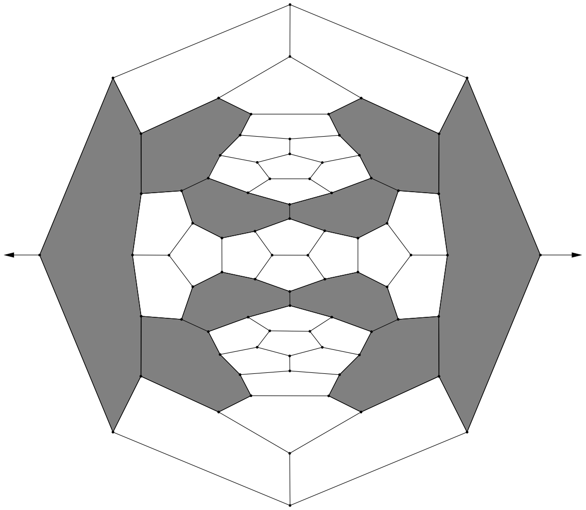
4, D_{2d};10,10



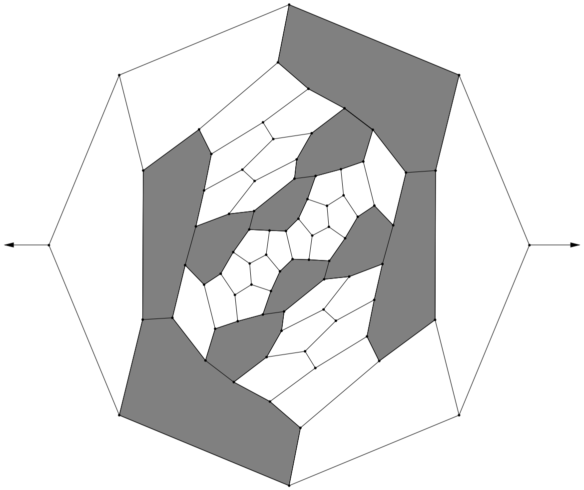
8, C_2;10,18



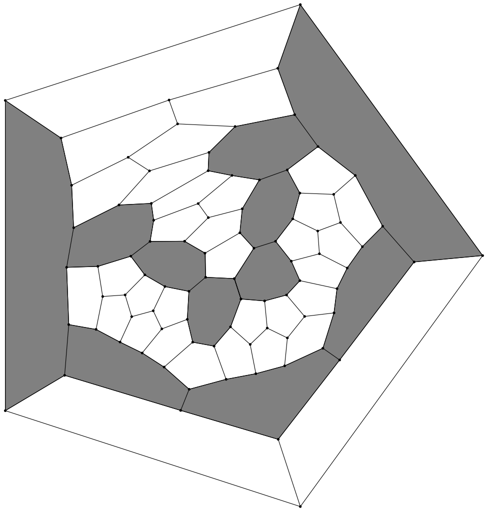
9, C_s;19,11



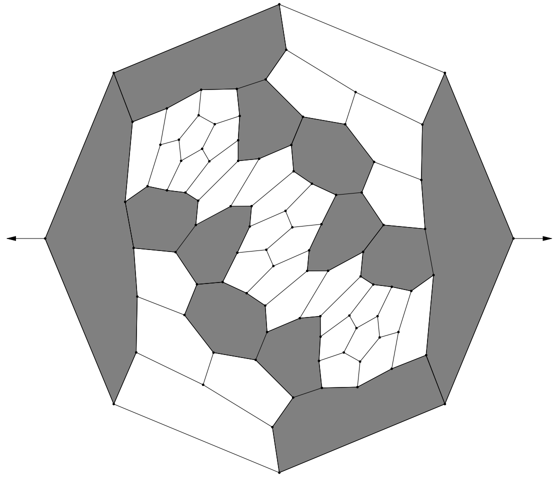
10, C_{2v};10,22



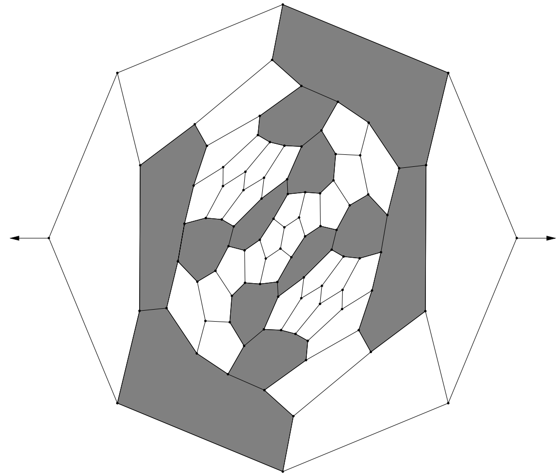
10, C_2;14,18



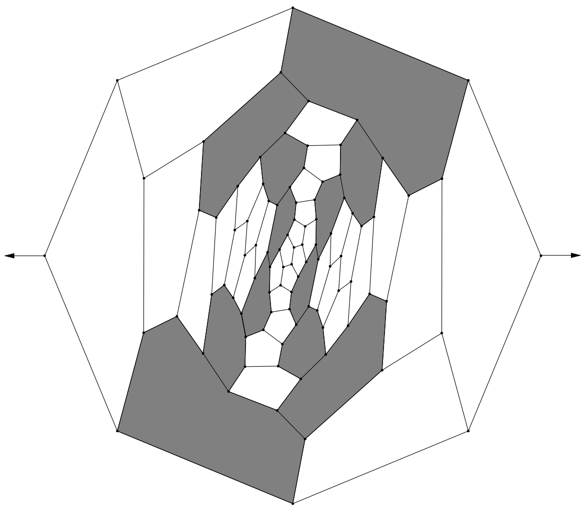
11, C_1;20,14



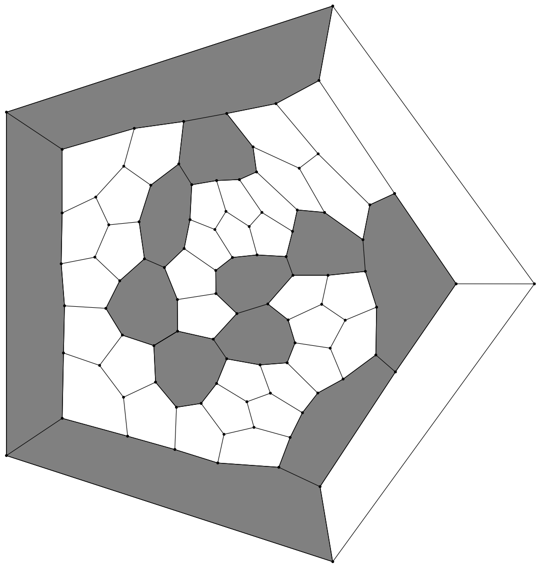
12, C_2;26,10



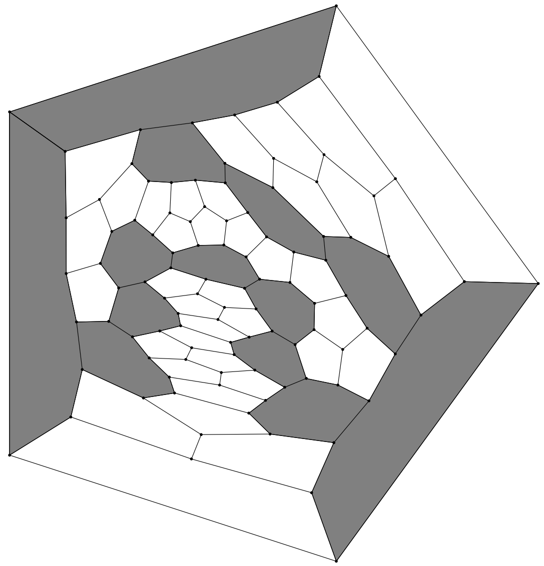
12, C_2;14,22



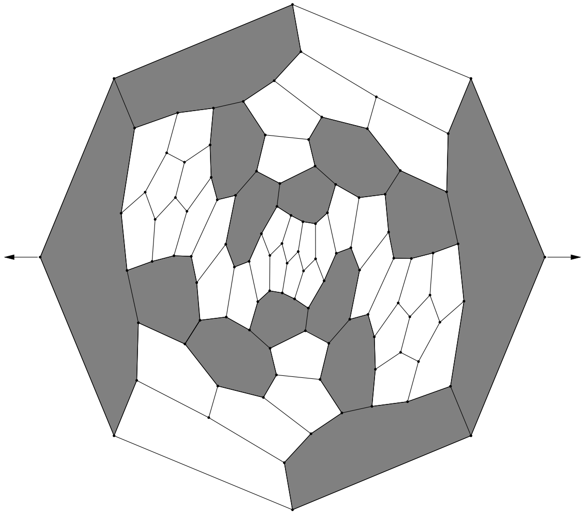
12, C_2;14,22



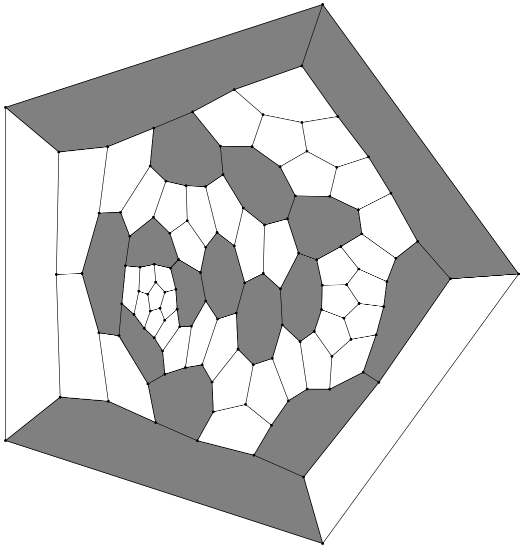
12, C_1;21,15



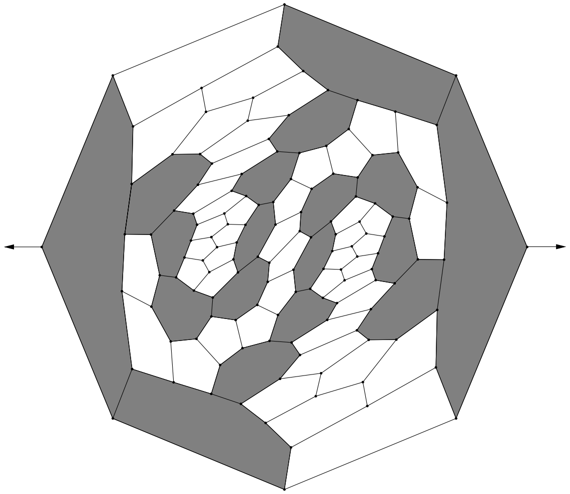
13, C_1;15,23



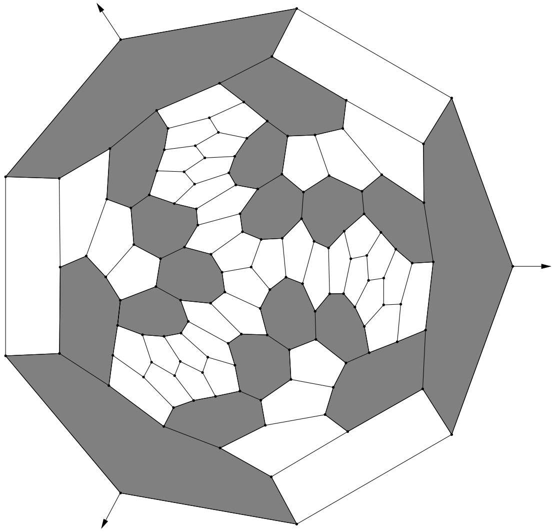
14, C_2;28,12



16, C_1;30,14

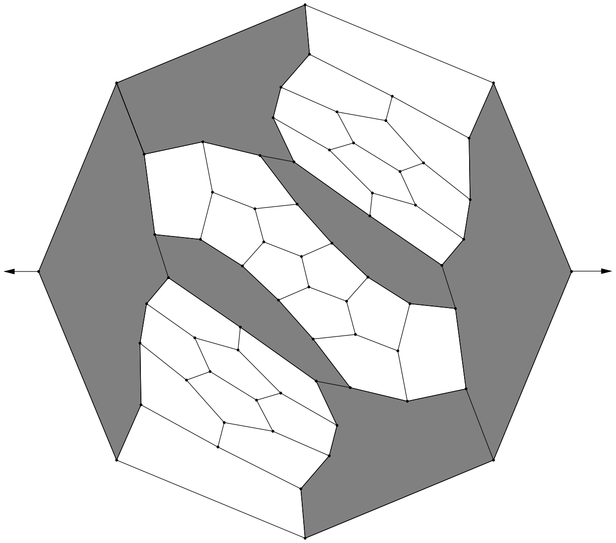


18, C_2;14,34

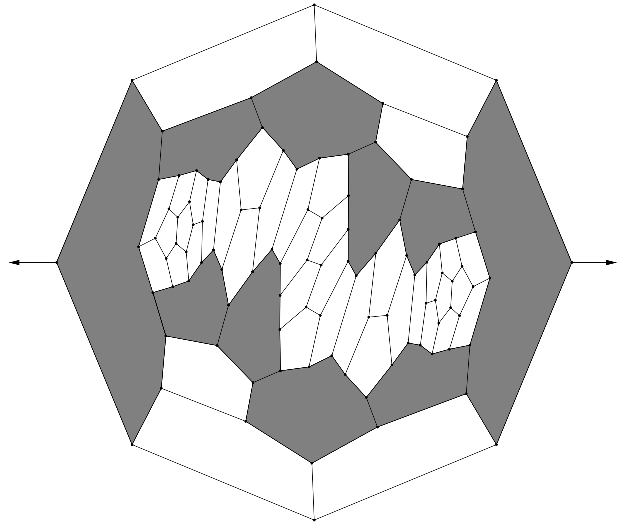


18, C_3;33,15

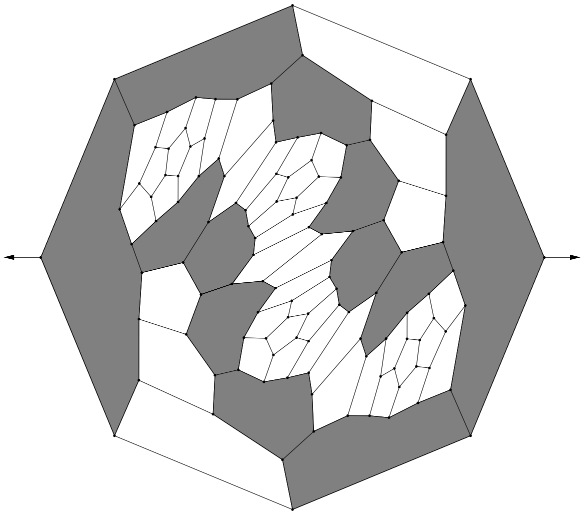
Known $M_n(5, 9)$



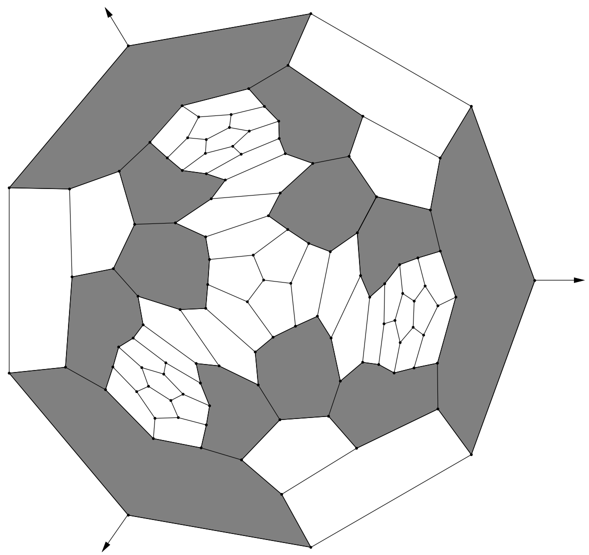
6, C_2;10,20



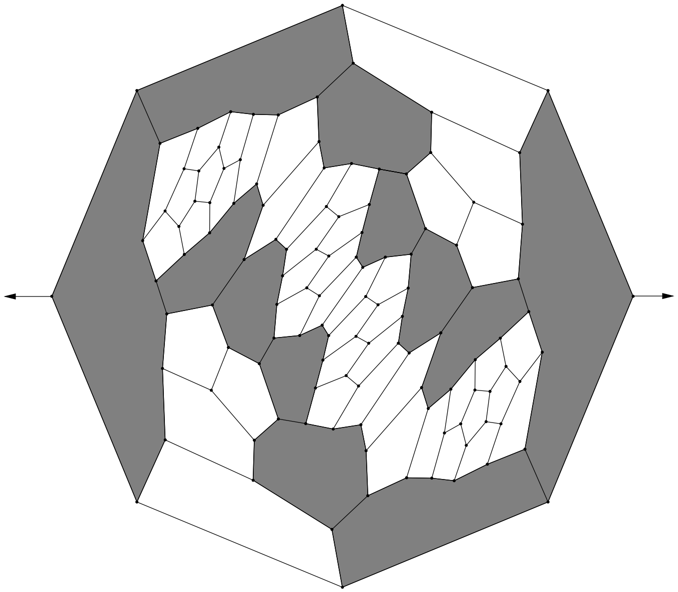
10, C_2;34,8



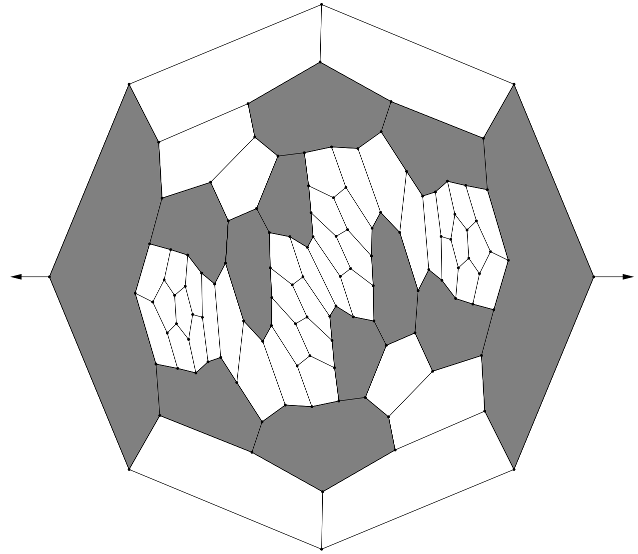
12, C_2;40,8



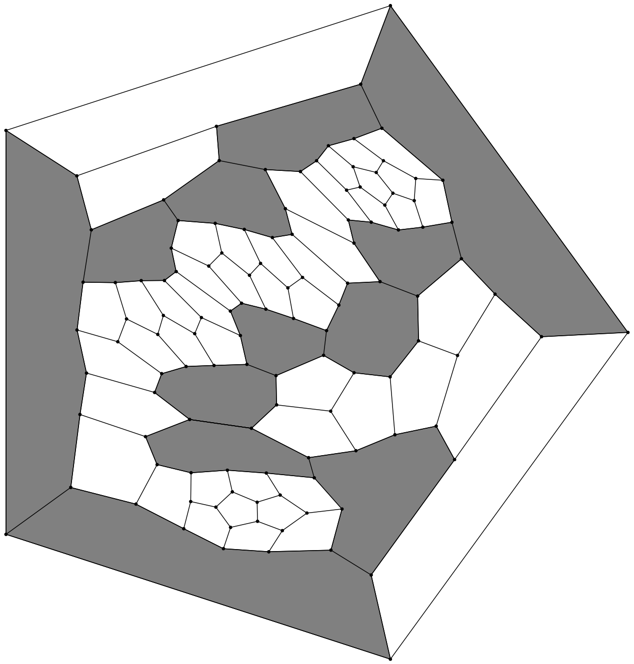
12, C_3;39,9



12, C_2;38,10

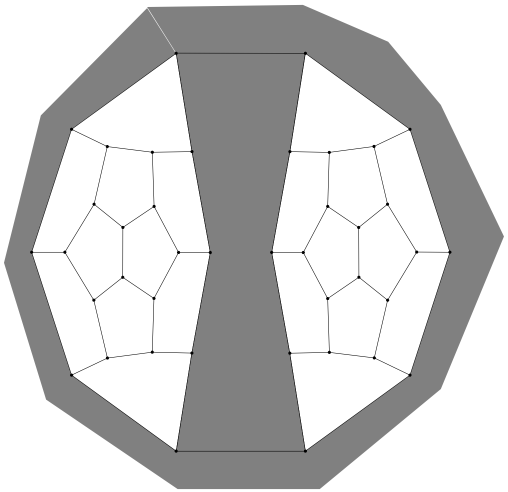


12, C_2;38,10

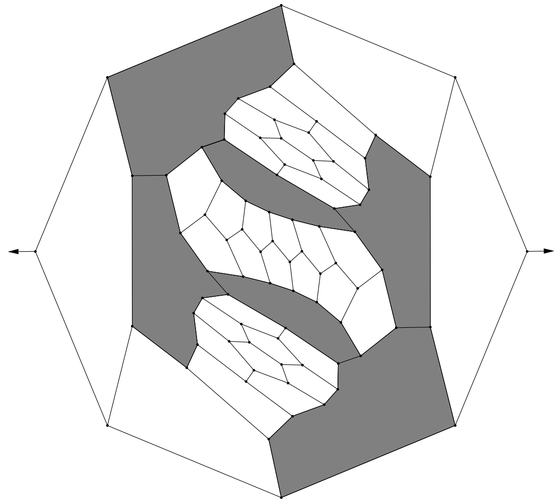


12, C_1;38,10

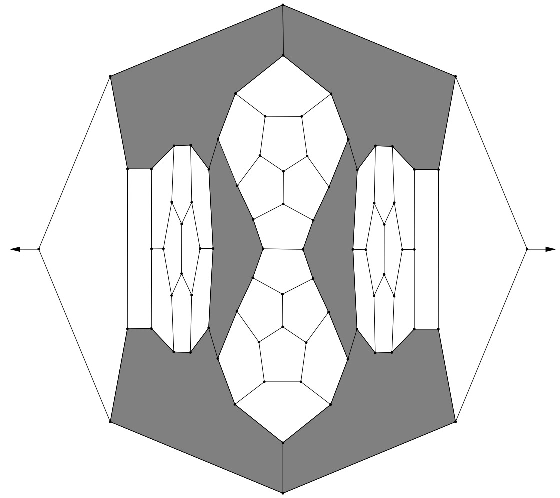
Known $M_n(5, 10)$



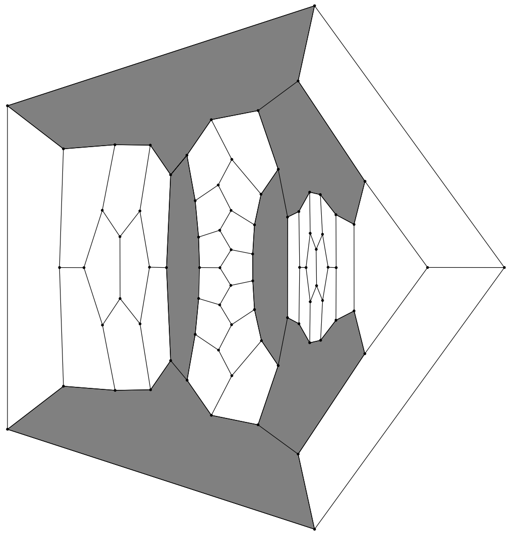
2, D_{2h};10,10



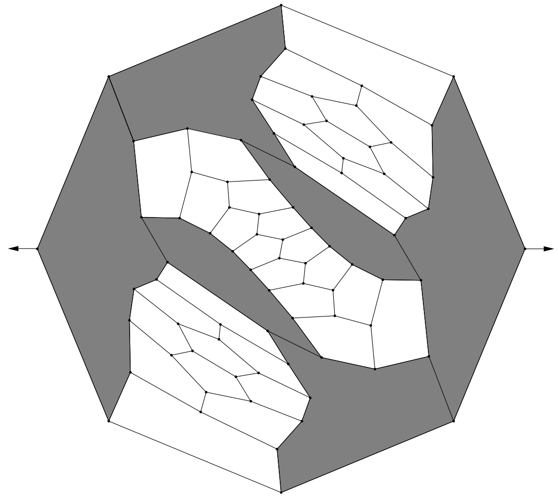
6, C_2;12,24



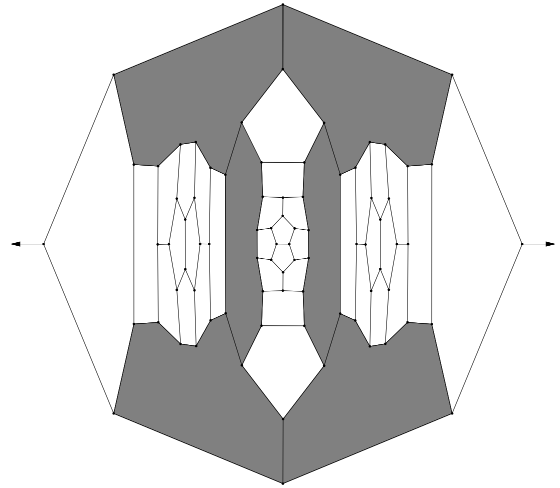
6, C_{2v};14,22



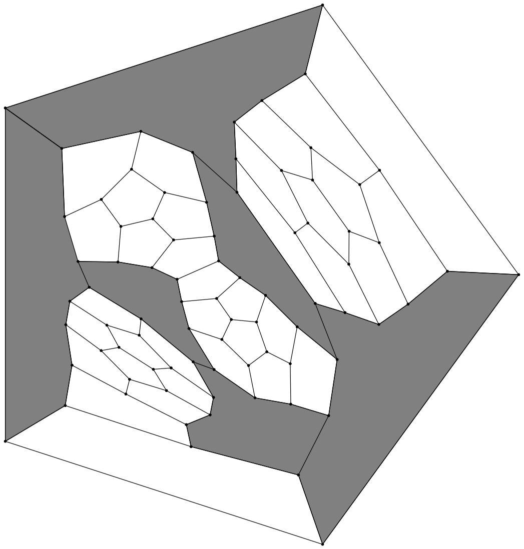
6, C_s;13,23



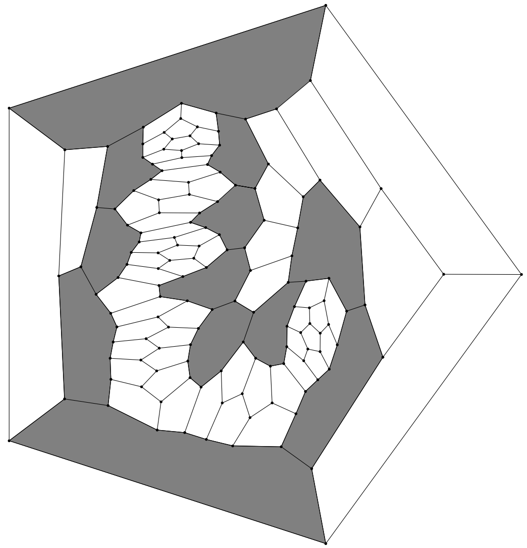
6, C_2;14,22



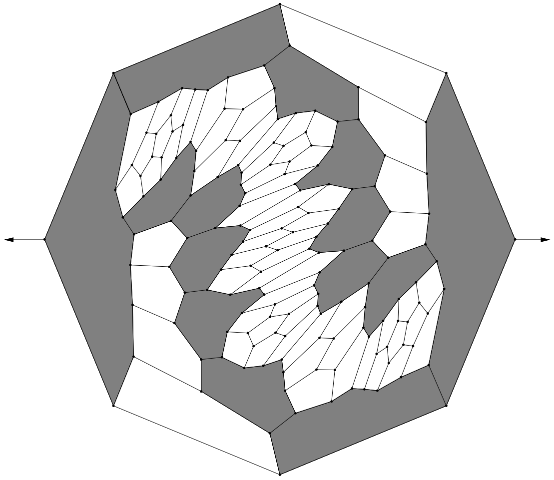
6, C_{2v};12,24



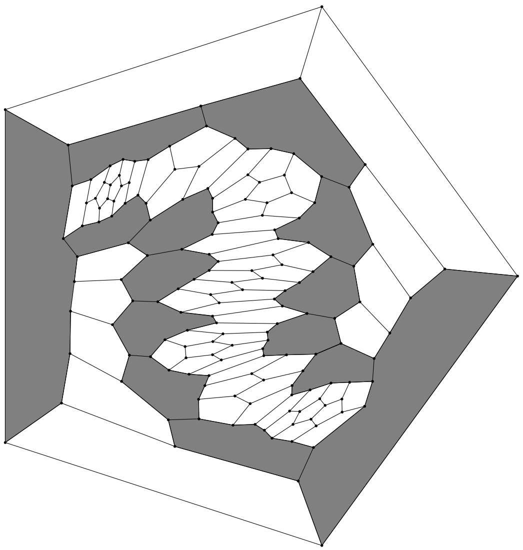
6, C_1;15,21



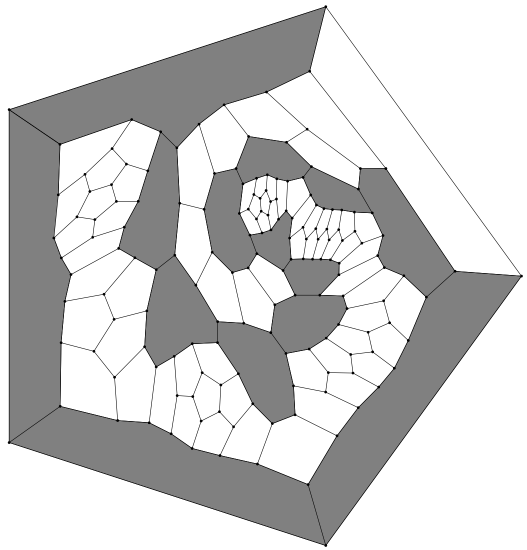
12, C_1;11,49



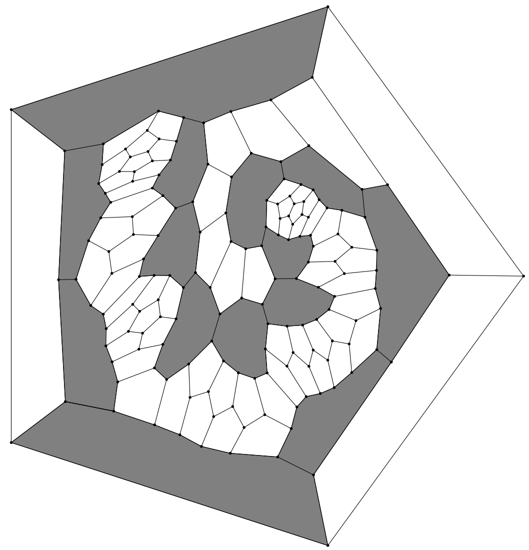
14, C_2;58,10



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 $n_1, \dots, n_t$ (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

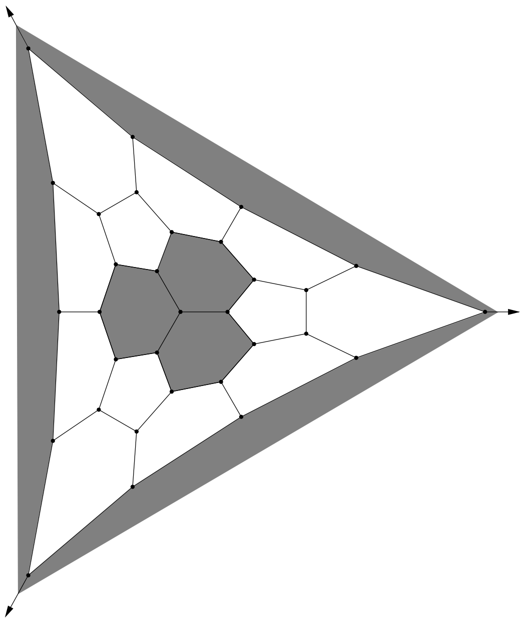
- x_1 *is the number of vertices incident to* 3 p*-gonal faces and*
- x_2 *the number of vertices incident to* 3 q*-gonal faces.*

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

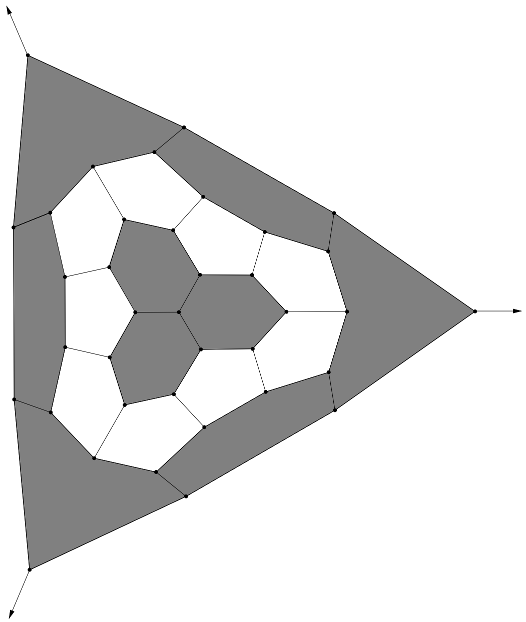
The case (p,q)=$(5,6)$ (fullerenes)

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

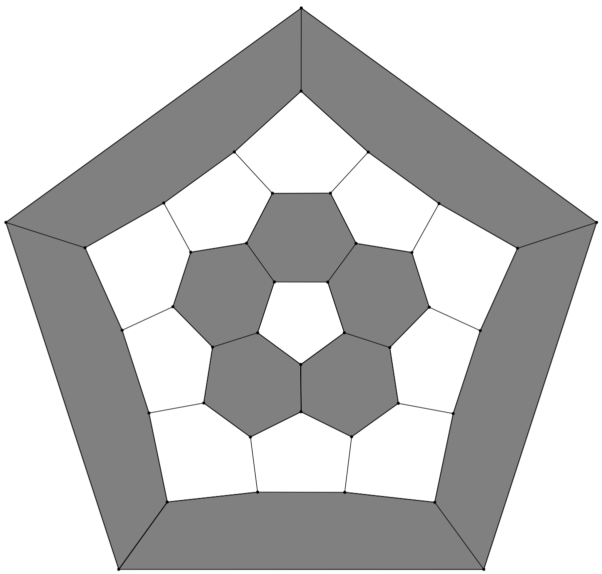
- five maps with one ring of 6-gons,
- following three maps with two rings of 6-gons:



D_{3h}; 32

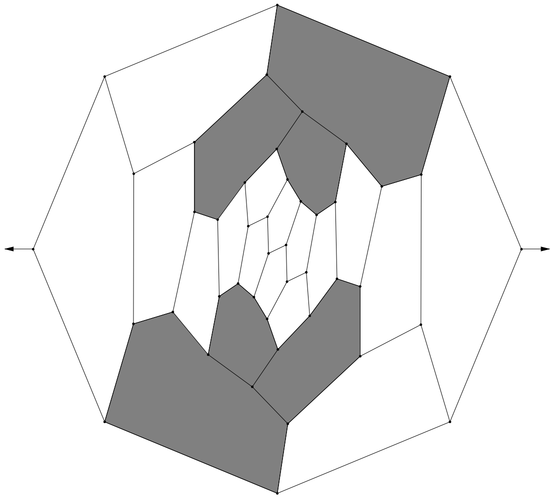


C_{3v}; 38

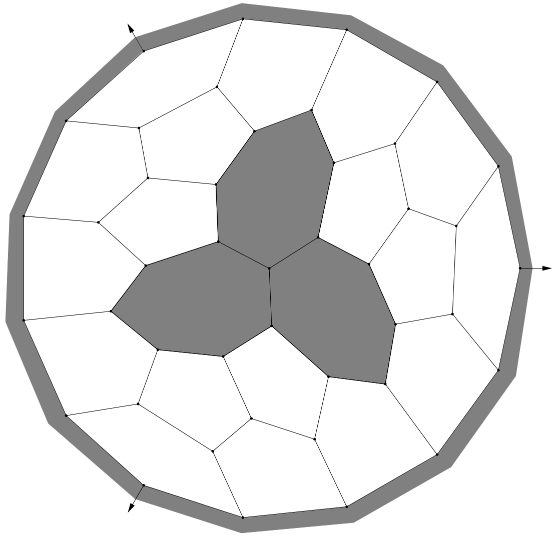


D_{5h}; 40

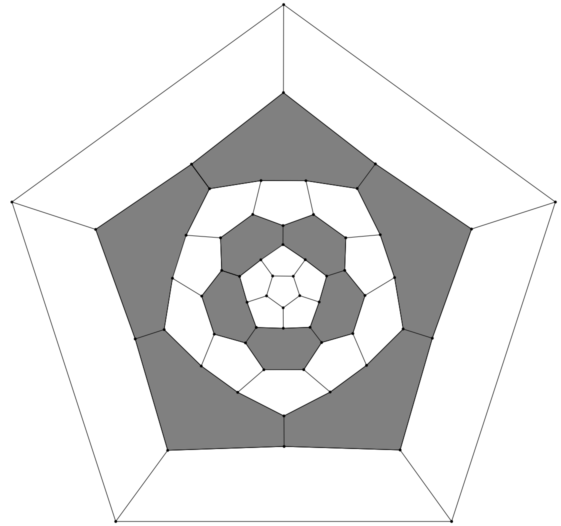
Two rings of 7-gons filled by 5-gons



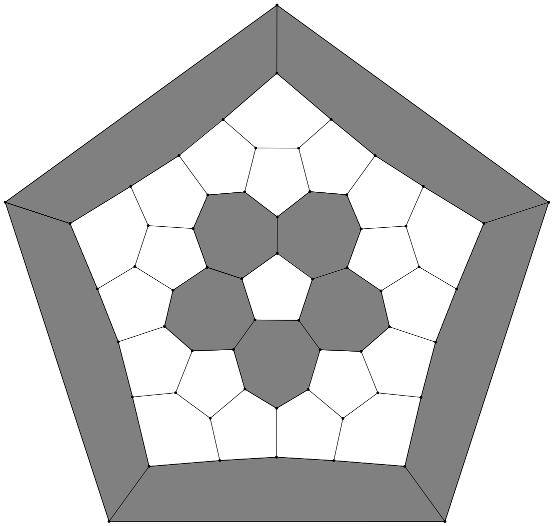
C_{2h}; 44



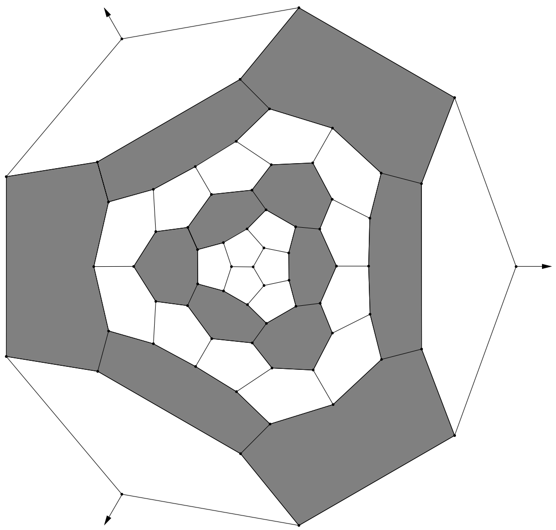
D_3; 44



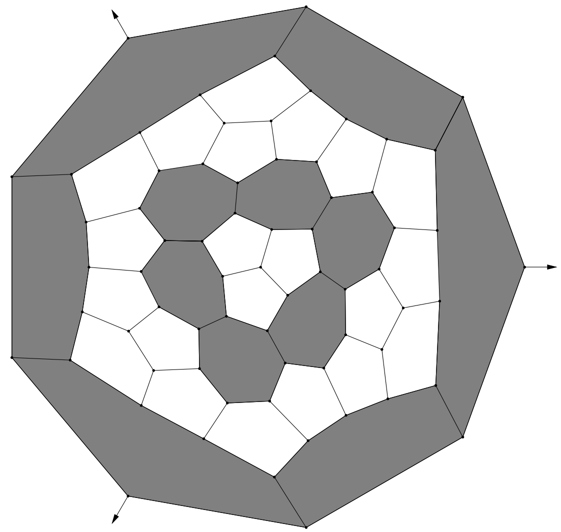
D_{5d}; 60



D_{5h}; 60

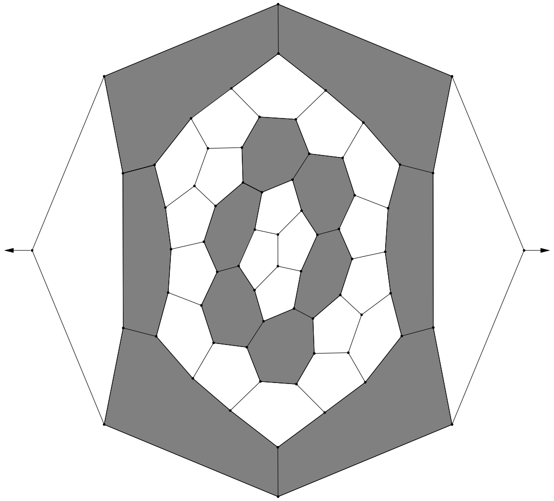


D_{3d}; 68

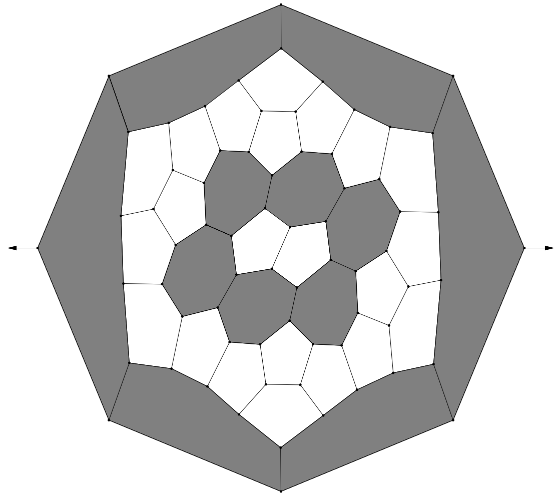


D_3; 68

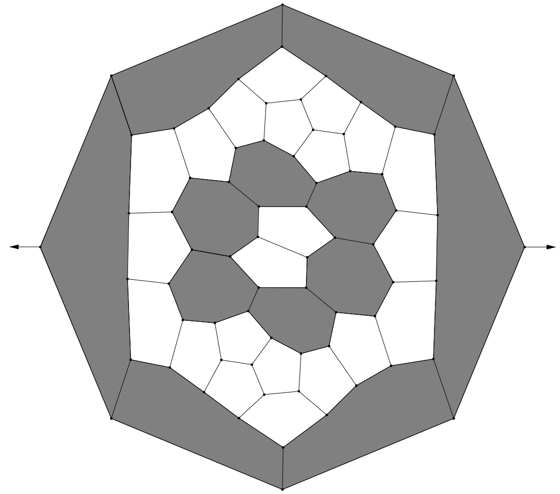
Two rings of 7-gons filled by 5-gons



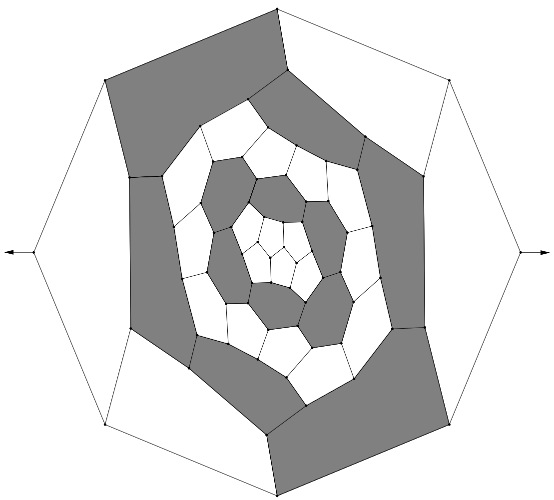
D_2; 68



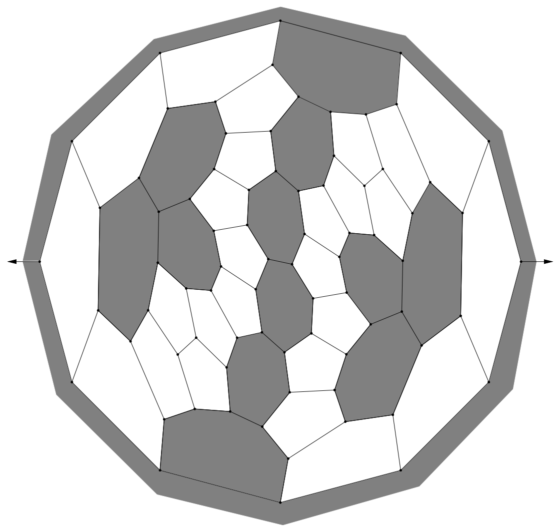
D_2; 68



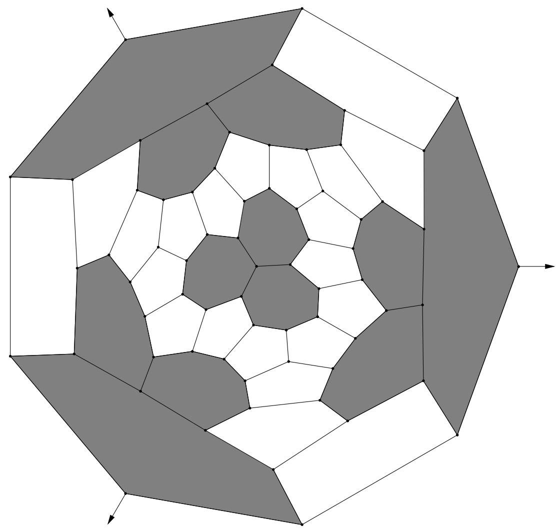
D_2; 68



D_2; 68

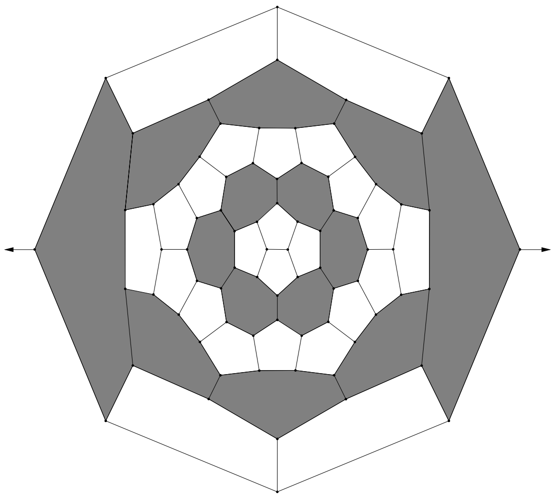


C_{2h}; 76

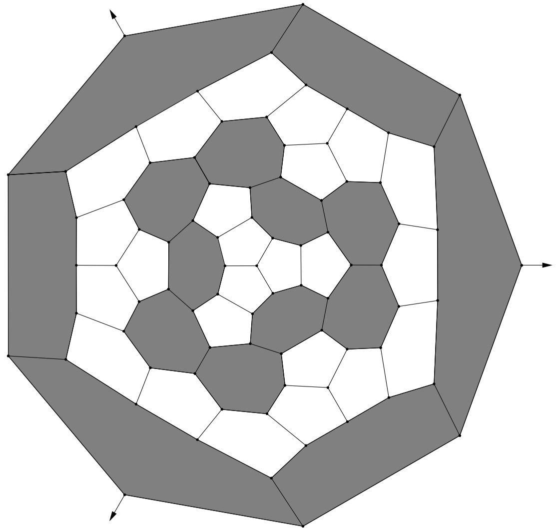


T; 68

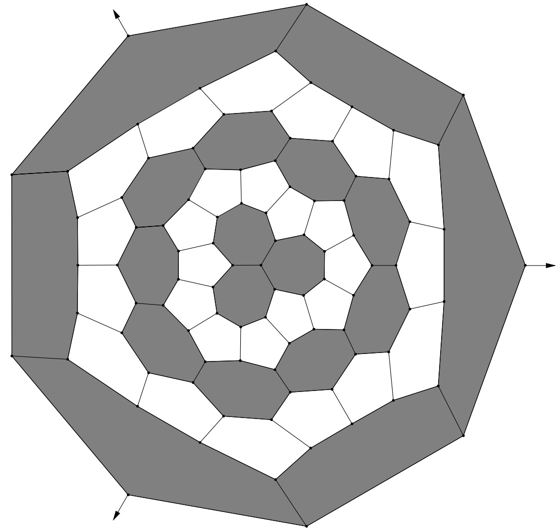
Remaining graphs $M_{...}(5,7)$ (azulenoids)



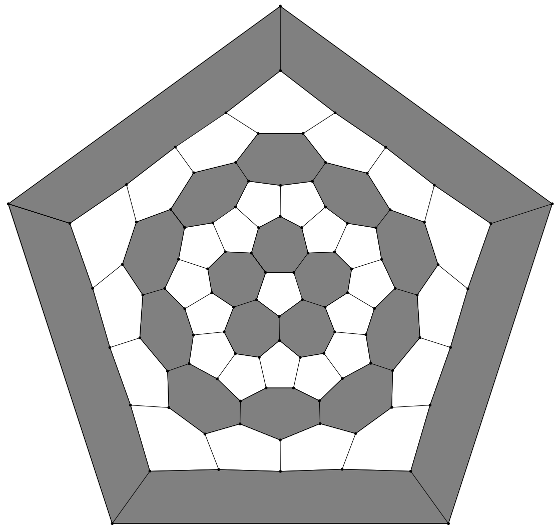
C_{2v}; 76



C_{3v}; 80



C_{3v}; 92

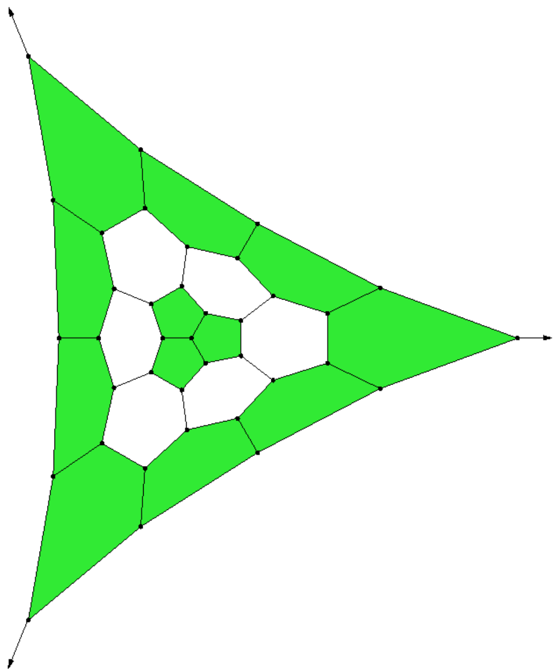


D_{5d}; 100

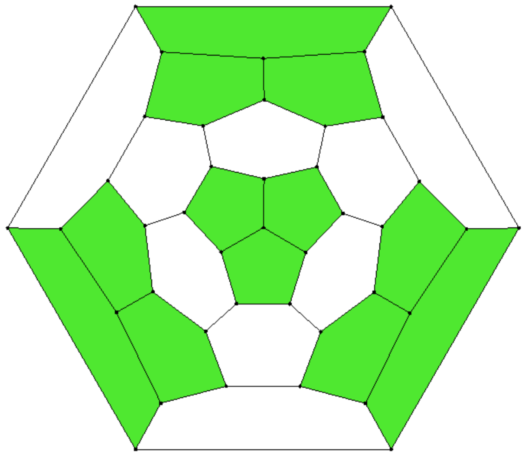
The case (p, q)=$(6, 5)$ (fullerenes)

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

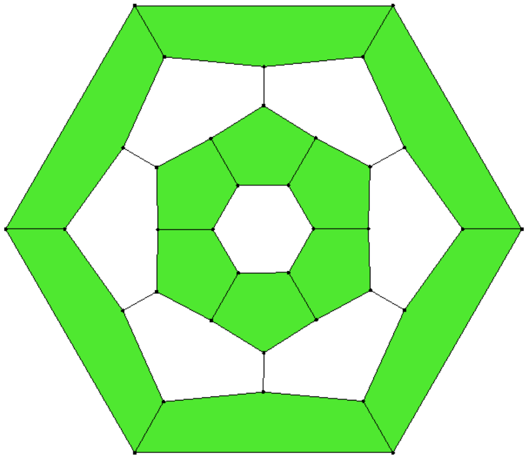
- four maps with exactly one ring of 5-gons,
- the maps:



special map



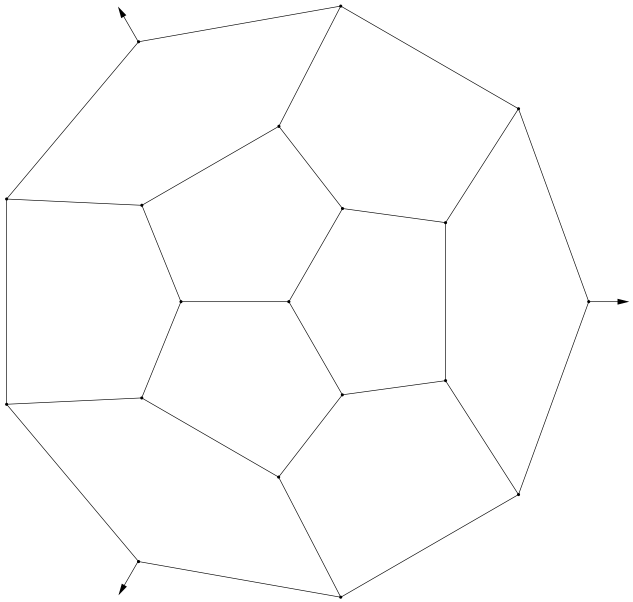
infinite family: 4 triples of pentagons

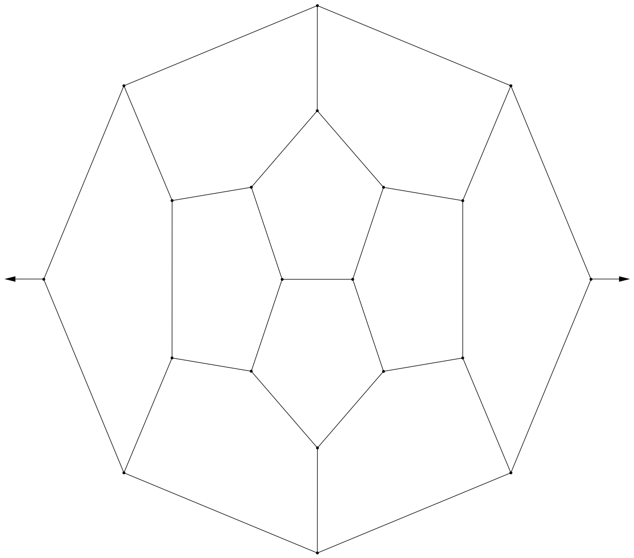


infinite family: $t \geq 1$ concentric 6-rings of hexagons

Infinite families

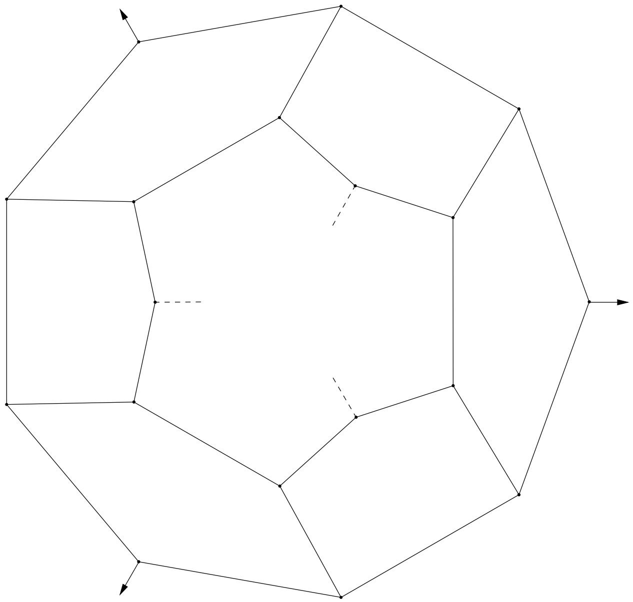
For any $t \geq 0$, there exists a map $M_{3,\ldots,3}(5,8)$ (with t 3-rings of 8-gons) and a map $M_{2,\ldots,2}(5,10)$ (with t 2-rings of 10-gons)

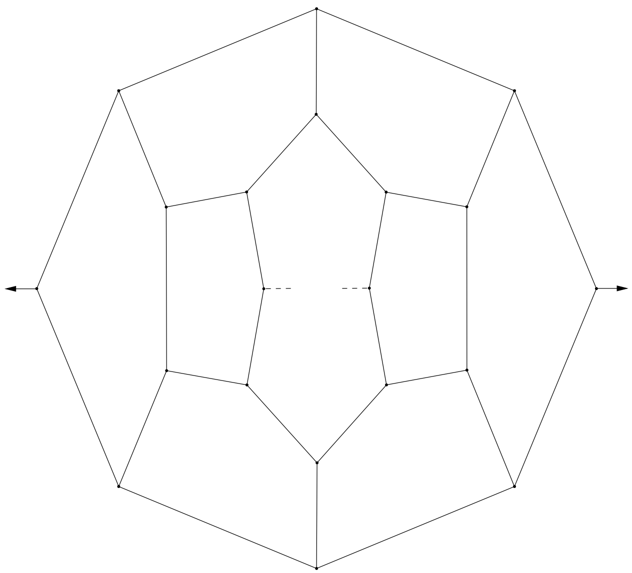




Infinite families

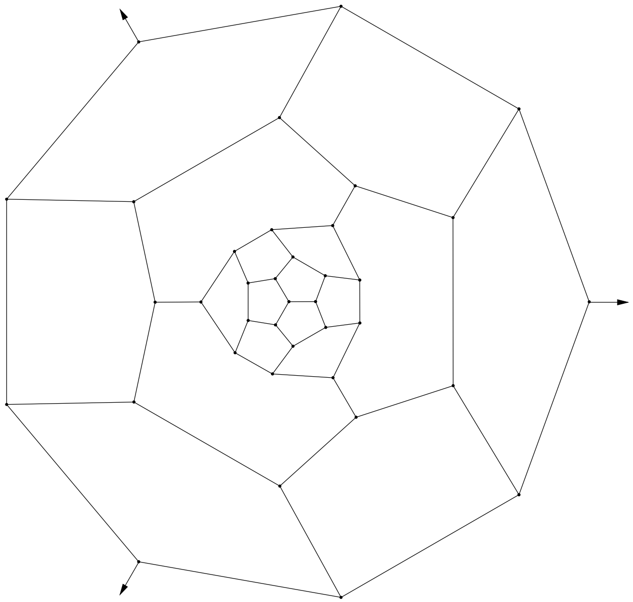
For any $t \geq 0$, there exists a map $M_{3,\ldots,3}(5,8)$ (with t 3-rings of 8-gons) and a map $M_{2,\ldots,2}(5,10)$ (with t 2-rings of 10-gons)

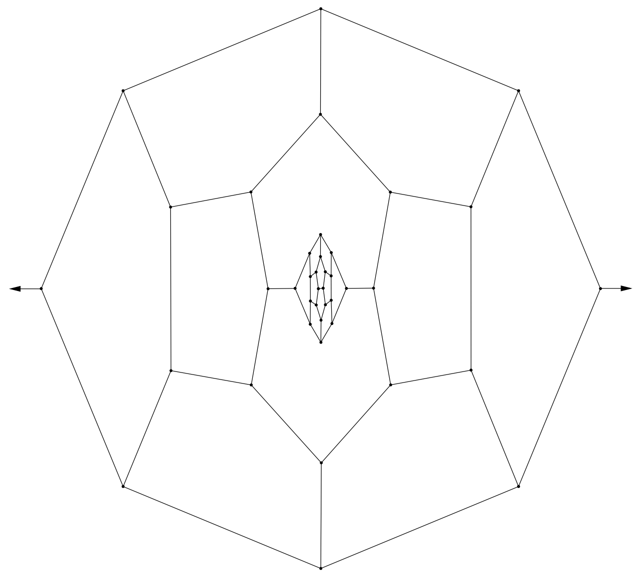




Infinite families

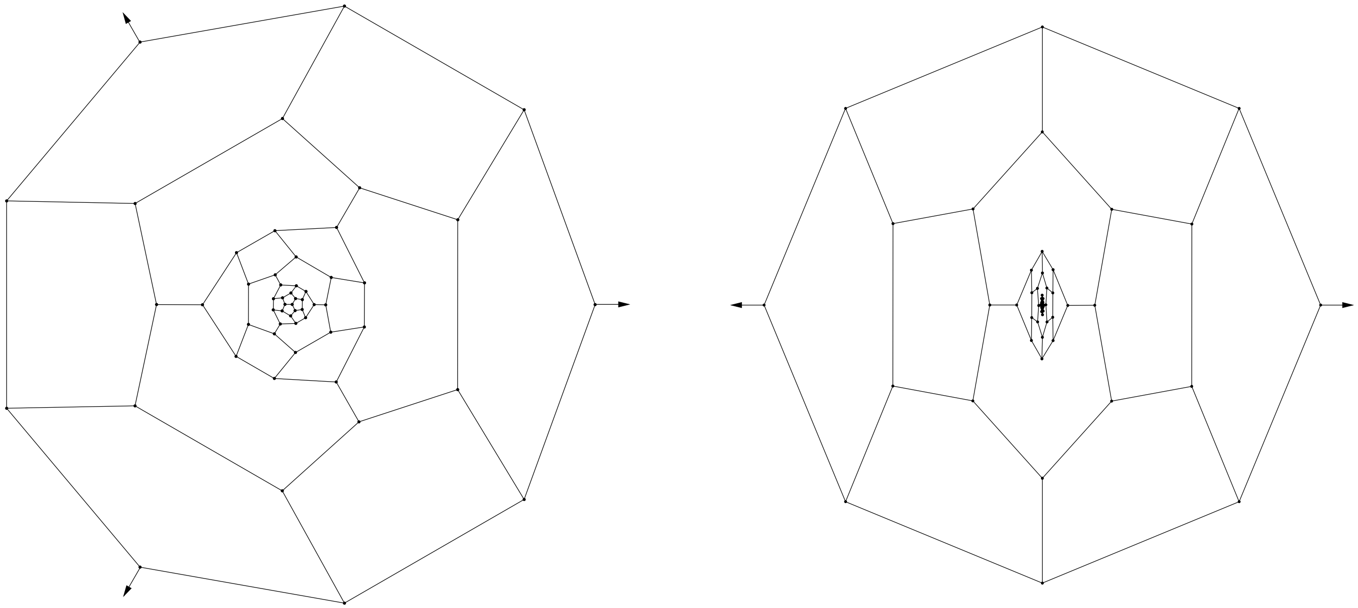
For any $t \geq 0$, there exists a map $M_{3,\ldots,3}(5,8)$ (with t 3-rings of 8-gons) and a map $M_{2,\ldots,2}(5,10)$ (with t 2-rings of 10-gons)





Infinite families

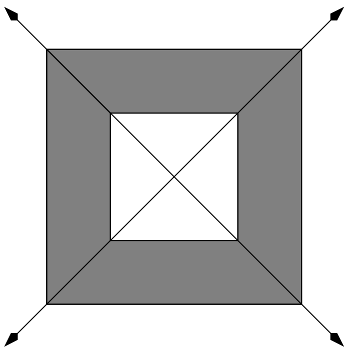
For any $t \geq 0$, there exists a map $M_{3,\dots,3}(5,8)$ (with t 3-rings of 8-gons) and a map $M_{2,\dots,2}(5,10)$ (with t 2-rings of 10-gons)



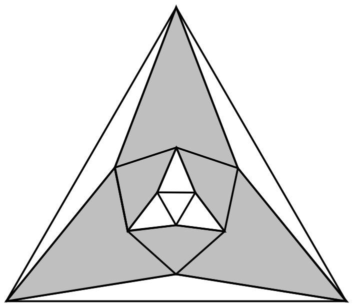
k-valent maps

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.

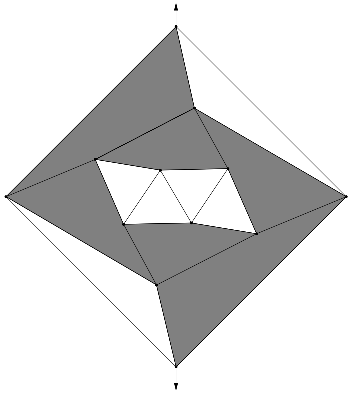
- The only $M_n^4(p,3)$ is p-gonal antiprism.
- All $M_n^4(3,4)$ are:



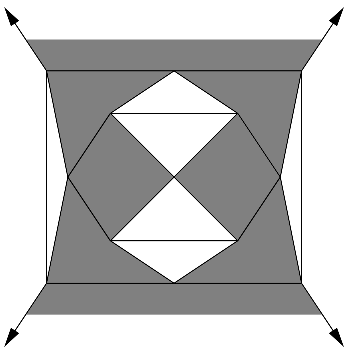
D_{4h}; 10



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}.