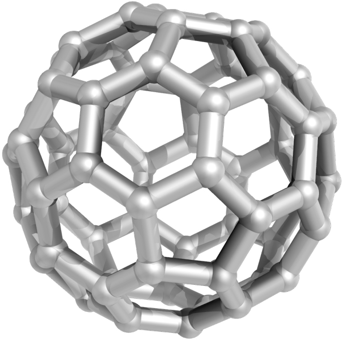
Université Grenoble Alpes

# Combinatorial aspects of fullerenes and quadrangulations of surfaces

Matěj Stehlík

# Fullerene molecules



- Fullerenes are spherically shaped molecules built entirely from carbon atoms.
- Each carbon atom has bonds to exactly three other carbon atoms.
- The carbon atoms form rings of either five atoms (pentagons) or six atoms (hexagons).
- Osawa predicted the existence of fullerene molecules in 1970.
- First fullerene molecule ($C_{60}$) produced in small quantities by Curl, Kroto and Smalley in 1985.

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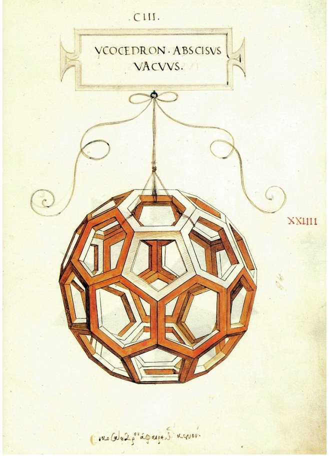
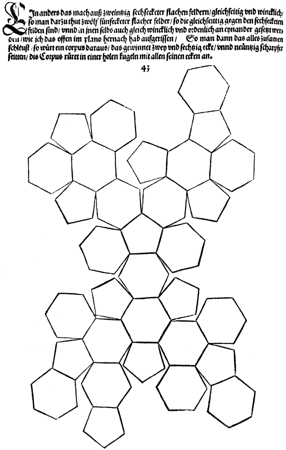
# Named after Buckminster Fuller (1895–1983)

# Fullerenes were known to Leonardo and Dürer



Ein anders das mach auß zweintzig sechsecketer flachen feldern/ gleichseitig vnd wincklich/ so man darzu thut zwölf fünfecketer flacher felder/ so die gleichseittig gegen den sechsecketen felden sind/ vnnd in jnen selbs auch gleich wincklich vnd ordenlich an eynander gesetzt werden/ wie jch das offen im plano hernach hab aufgerissen/ So man dann das alles zusamen schleust/ so würt ein corpus daraus/ das gewinnet zwey vnd sechtzig ecke/ vnnd neüntzig scharpfer seitten/ dis Corpus rüret in einer holen kugeln mit allen seinen ecken an.

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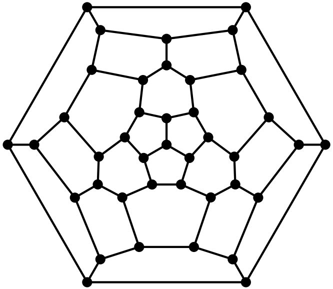
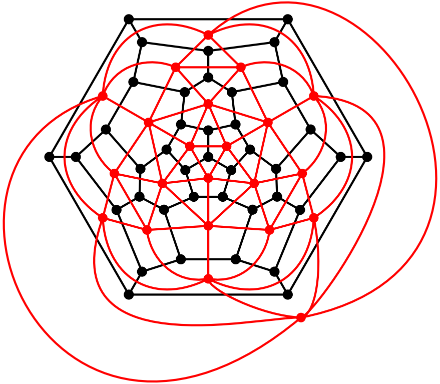
# Fullerene graphs and their duals



A *fullerene graph* is:

- plane
- cubic
- bridgeless
- all faces have size 5 or 6.

# Fullerene graphs and their duals



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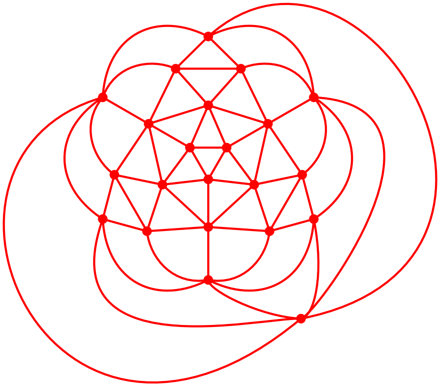


A *fullerene graph* is:

- plane
- cubic
- bridgeless
- all faces have size 5 or 6.

Its dual is:

- plane
- triangulation
- no loops or multiple edges
- all vertices have degree 5 or 6.

# Why study of fullerene graphs?

## Central question

Do the mathematical properties of the graph predict the chemical properties of the molecule?

- Fullerene graphs corresponding to chemically stable fullerene molecules seem to satisfy certain properties.
- For instance, the pentagonal faces do not touch ('isolated pentagon rule').

## Odd cycle transversals of fullerenes

- Stable fullerenes also seem to be 'far from bipartite'.
- Let $\tau_{\text{odd}}(G)$ be the minimum number of edges whose removal results in a bipartite graph.

**Theorem (Došlić and Vukičević 2007)**

If $G$ is a fullerene graph on $n = 60k^2$ vertices with the full icosahedral automorphism group, then $\tau_{\text{odd}}(G) = 12k = \sqrt{12n/5}$.

**Conjecture (Došlić and Vukičević 2007)**

If $G$ is a fullerene graph on $n$ vertices, then $\tau_{\text{odd}}(G) \leqslant \sqrt{12n/5}$.

## Odd cycle transversals in fullerenes

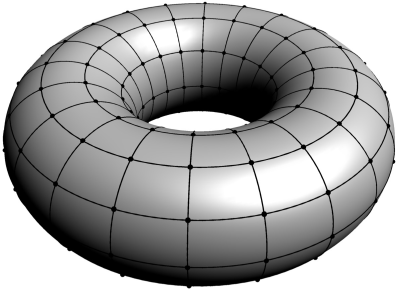
### Theorem (Faria, Klein and MS 2012)

If $G$ is a fullerene graph on $n$ vertices, then $\tau_{\text{odd}}(G) \leqslant \sqrt{12n/5}$. Equality holds iff $n = 60k^2$ and $G$ has the full icosahedral automorphism group.

- Extended to 3-connected cubic plane graph with all faces of size at most 6 (Nicodemos and MS 2018).
- These graphs (and their dual triangulations) correspond to surfaces of genus 0 of non-negative curvature.
- $\tau_{\text{odd}}$ can be linear in $n$ if we allow faces of size 7 (negative curvature).

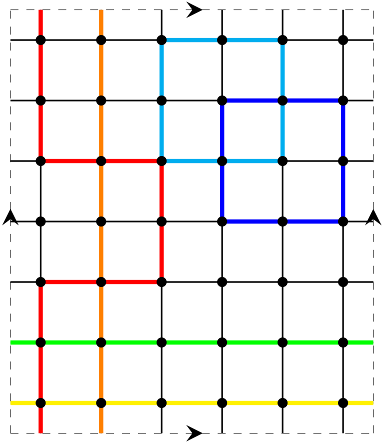
# Even-faced graphs and quadrangulations

- An even-faced graph in a surface $S$: embedding of a graph in $S$ such that every face is bounded by an even number of edges.
- A quadrangulation of a surface $S$: embedding of a graph in $S$ such that every face is bounded by 4 edges.



# Parity of cycles in even-faced graphs

- Consider a graph $G$ embedded in a surface $S$.
- Two cycles are homologous if their symmetric difference is the boundary of a set of faces.



## Observation

The length of homologous cycles in an even-faced graph has the same parity.

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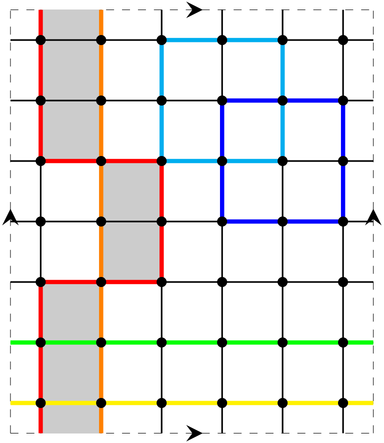

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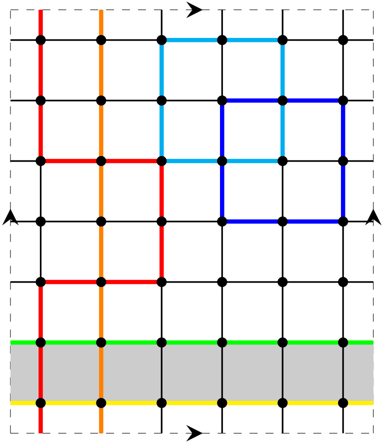

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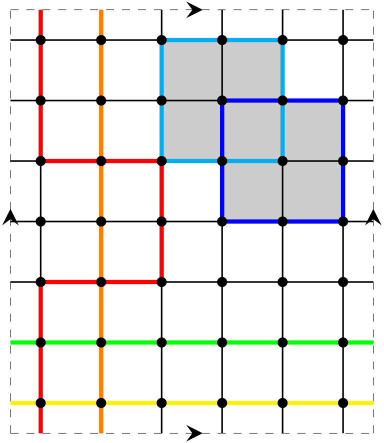


# Even-faced graphs in the projective plane

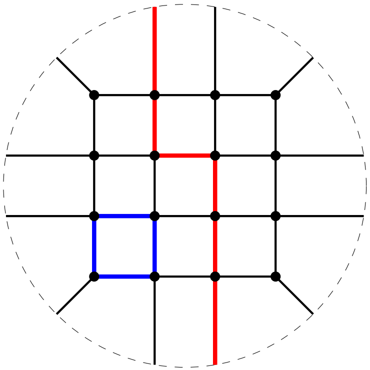
## Lemma

Projective plane $\mathbb{R}P^2$ has two homology classes:

- contractible cycles;
- non-contractible cycles.

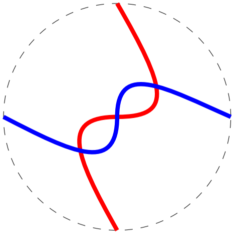
## Corollary

An even-faced graph in $\mathbb{R}P^2$ is non-bipartite if and only it has a non-contractible odd cycle.



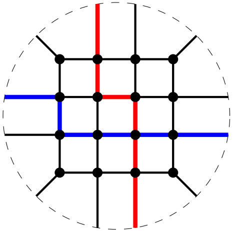
## Graphs with pairwise intersecting odd cycles

### Lemma
Two non-contractible simple closed curves in $\mathbb{R}\mathrm{P}^2$ intersect an odd number of times.



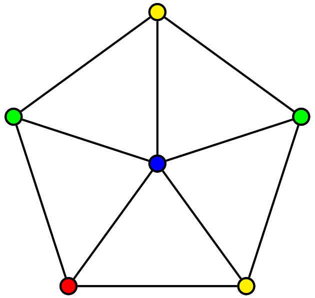
### Corollary
The odd cycles in an even-faced graph in $\mathbb{R}\mathrm{P}^2$ are pairwise intersecting.

### Theorem (Lovász)
The odd cycles in an internally 4-connected graph $G$ are pairwise intersecting iff $G$ has an even-faced embedding in $\mathbb{R}\mathrm{P}^2$ or $G$ belongs to a few exceptional classes.



## Graph colouring and the chromatic number

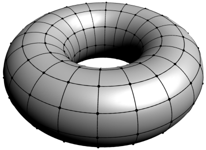
- Colouring of $G$: assignment of colours to the vertices of $G$ such that adjacent vertices receive different colours.
- Smallest number of colours: chromatic number $\chi(G)$.
- If $\chi(G) \leqslant 2$, we say $G$ is bipartite.
- Equivalent to $G$ having no odd cycles.
- If $\chi(G - e) < \chi(G)$ for any edge $e$, $G$ is critical.
- If $\chi(G - v) < \chi(G)$ for any vertex $v$, $G$ is vertex-critical.



# Colouring quadrangulations

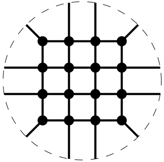
Theorem (Hutchinson 1995)

If $G$ is an even-faced graph in an orientable surface and all non-contractible cycles are sufficiently long, then $\chi(G) \leqslant 3$.



Theorem (Youngs 1996)

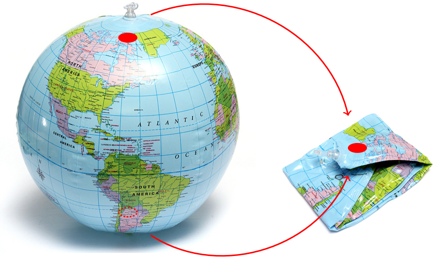
If $G$ is a quadrangulation of $\mathbb{R}\mathrm{P}^2$, then $\chi(G) = 2$ or $\chi(G) = 4$.



Question (Youngs 1996)

Can Youngs's theorem be extended to higher dimension?

# A (very) useful tool from algebraic topology



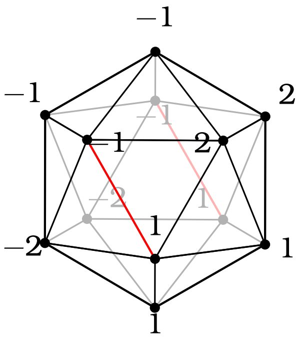

## Borsuk–Ulam Theorem (Borsuk 1933)

For every continuous mapping $f : S^n \to \mathbb{R}^n$ there exists a point $x \in S^n$ with $f(x) = f(-x)$.

## Equivalent formulation

There is no continuous map $f : S^n \to S^{n-1}$ that is equivariant, i.e., $f(-x) = -f(x)$ for all $x \in S^n$.

# A discrete version of Borsuk–Ulam

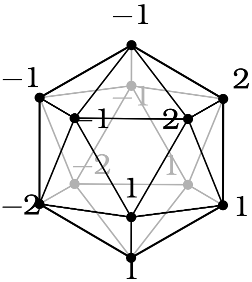



## Tucker's lemma (Tucker 1946)

- Let $K$ be a centrally symmetric triangulation of $S^n$.
- Let $\lambda : V(K) \to \{\pm 1, \ldots, \pm n\}$ be a labelling such that $\lambda(-v) = -\lambda(v)$ for all $v \in V(K)$.
- Then there exists an edge $\{u, v\}$ s.t. $\lambda(u) + \lambda(v) = 0$.

## Equivalence of Tucker and Borsuk–Ulam

- Tucker follows from Borsuk–Ulam by considering $\lambda$ as a simplicial map from $K$ to the boundary complex of the $n$-dimensional cross-polytope, and extending it to a continuous map.

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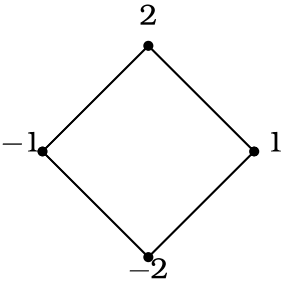
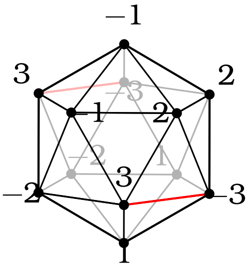



- Borsuk–Ulam follows from Tucker by taking sufficiently fine triangulations of $S^n$ and using compactness.

# Another discrete version of Borsuk–Ulam

## (A corollary of) Fan's lemma

- Let $K$ be a centrally symmetric triangulation of $S^n$.
- Let $\lambda : V(K) \to \{\pm 1, \dots, \pm(n+1)\}$ be a labelling such that $\lambda(-v) = -\lambda(v)$ for all $v \in V(K)$, and every $n$-simplex has vertices of both signs.
- Then there exists an edge $\{u, v\} \in K$ s.t. $\lambda(u) + \lambda(v) = 0$.

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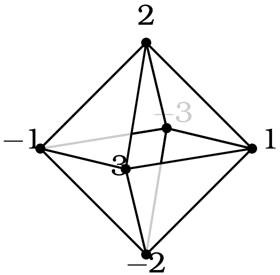


## An application of Fan's lemma

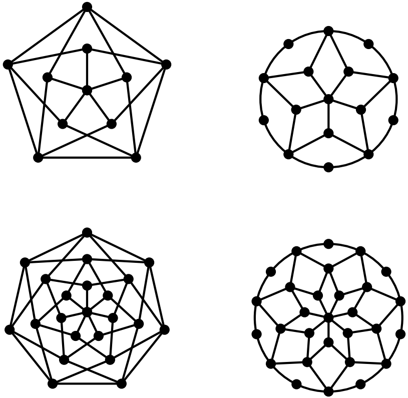
- Let $K$ be a centrally symmetric triangulation of $S^n$.
- Consider the graph consisting of the vertices and edges of $K$.
- Label the vertices $+$ or $-$ so that
  - antipodal vertices receive opposite labels;
  - every facet is incident to at least one $+$ and at least one $-$.
- Delete all edges between vertices of the same sign.
- Identify all pairs of antipodal vertices.
- The resulting graph is a (non-bipartite) quadrangulation of $\mathbb{R}P^n$.

**Theorem (Kaiser and MS 2015)**

Every quadrangulation of $\mathbb{R}P^n$ is at least $(n+2)$-chromatic, unless it is bipartite.

# Generalised Mycielski and projective quadrangulations

- The Mycielski construction: one of the earliest constructions of triangle-free graphs of arbitrarily high chromatic number
- Generalised in 1985 by Stiebitz.
- Generalised Mycielski graphs are non-bipartite projective quadrangulations.
- Their chromatic number can be deduced from the generalisation of Youngs's theorem.



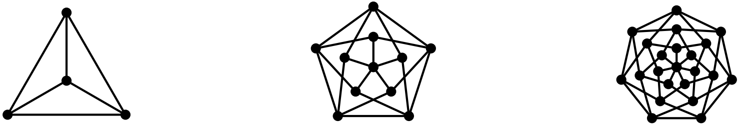
## A question of Erdős

- Graphs without short odd cycles are ‘locally bipartite’.
- How long can the shortest odd cycle be in a $k$-chromatic graph?

### Question (Erdős 1974)

Does every 4-chromatic $n$-vertex graph $G$ have an odd cycle of length $O(\sqrt{n})$?

- YES (Kierstead, Szemerédi and Trotter 1984)
- Generalised Mycielski graphs provide examples of 4-chromatic $n$-vertex graphs whose shortest odd cycles have length $\frac{1}{2}(1+\sqrt{8n-7})$.



## A refinement of Erdős's question

**Conjecture (Esperet, MS 2018)**

Every 4-chromatic $n$-vertex graph has an odd cycle of length at most $\frac{1}{2}(1+\sqrt{8n-7})$.

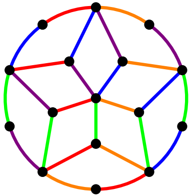
**Theorem (Esperet, MS 2018)**

The conjecture holds if all odd cycles are pairwise intersecting.

- The proof combines Lovász's characterisation of graphs with pairwise intersecting odd cycles and the following theorem.

**Theorem (Lins 1981)**

The minimum length of a non-contractible cycle in an even-faced graph in $\mathbb{R}P^2$ equals the maximum size of a packing of non-contractible co-cycles.



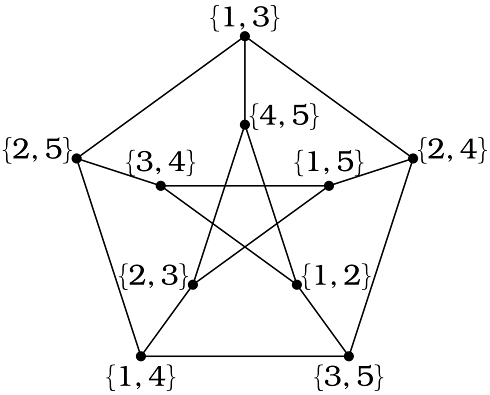
## **Kneser graph** $KG(n, k)$

$k \geqslant 1$

$n \geqslant 2k$

### Definition

- Vertices: all $k$-subsets of $\{1, \ldots, n\}$
- Edges between disjoint subsets




$KG(5, 2)$

### Conjecture (Kneser 1955)

$\chi(KG(n, k)) = n - 2k + 2$

- Proved by Lovász in 1977 using the Borsuk–Ulam theorem
- Schrijver sharpened the result in 1978

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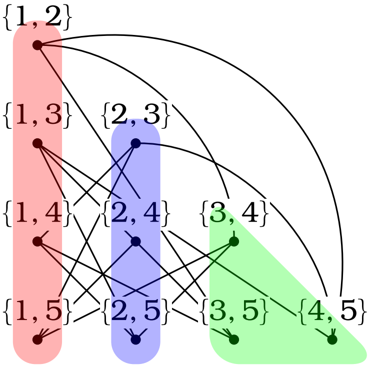
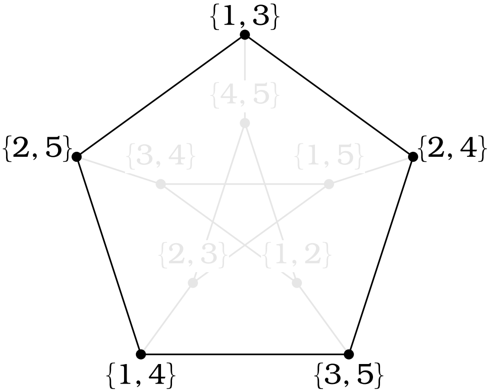



$KG(5, 2)$

## **Schrijver graph** $SG(n,k)$

- Subgraph of $KG(n,k)$ induced by $k$-subsets of $\{1,\ldots,n\}$ without consecutive elements modulo $n$




$SG(5,2)$

### Theorem (Schrijver 1978)

$\chi(SG(n,k)) = n - 2k + 2$ and $SG(n,k)$ is vertex-critical

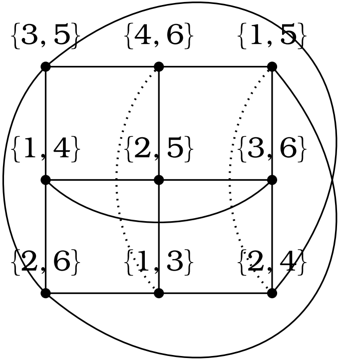
## Schrijver graphs and quadrangulations

**Theorem (Kaiser and MS 2015)**
There is a quadrangulation of $\mathbb{R}\mathrm{P}^{n-2k}$ homomorphic to $SG(n,k)$.

**Theorem (Kaiser and MS 2017)**
$SG(n,k)$ contains a spanning subgraph that is a quadrangulation of $\mathbb{R}\mathrm{P}^{n-2k}$.

**Theorem (Simonyi and Tardos 2019)**
$SG(2k+2,k)$ contains a spanning subgraph that is a quadrangulation of the Klein bottle.

# $SG(n,k)$ is not edge-critical in general




$SG(6,2)$

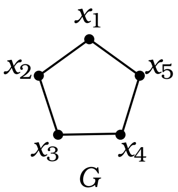
**Problem**

Give a simple definition of an $(n-2k+2)$-chromatic edge-critical subgraph of $SG(n,k)$.


- Case $k=2$ done (Kaiser and MS 2020).
- The graph is a non-bipartite quadrangulation of $\mathbb{R}P^{n-4}$.

# A connection between graph theory and commutative algebra

Graph $G$ $\leftrightarrow$ Square-free unmixed height 2 monomial ideal, called the cover ideal of $G$




$$I = \langle x_1, x_2\rangle \cap \langle x_2, x_3\rangle \cap \langle x_3, x_4\rangle \cap \langle x_4, x_5\rangle \cap \langle x_5, x_1\rangle$$
$$= \langle x_1x_2x_4, x_1x_3x_4, x_1x_3x_5, x_2x_3x_5, x_2x_4x_5\rangle$$

## Monomial ideals

- Let $R = k[x_1, \ldots, x_n]$ be a polynomial ring over a field $k$.
- An ideal in $R$ is monomial if it is generated by a set of monomials.
- A monomial ideal is square-free if it has a generating set of monomials where the exponent of each variable is at most $1$.
- Given an ideal $I$ of $R$, a prime ideal $P$ is associated to $I$ if there exists an element $m \in R$ such that $P = I : \langle m \rangle = \{r \in R \mid r\langle m \rangle \subseteq I\}$.
- The set of associated primes is denoted by $\mathrm{Ass}(I)$.

### Example

If $I$ is the cover ideal of the 5-cycle, then

$$\mathrm{Ass}(I) = \{\langle x_1, x_2 \rangle, \langle x_2, x_3 \rangle, \langle x_3, x_4 \rangle, \langle x_4, x_5 \rangle, \langle x_5, x_1 \rangle\}.$$

## The persistence conjecture

- Brodmann (1979) showed that $\mathrm{Ass}(I^s) = \mathrm{Ass}(I^{s+1})$ for all sufficiently large $s$.
- An ideal $I$ has the persistence property if $\mathrm{Ass}(I^s) \subseteq \mathrm{Ass}(I^{s+1})$ for all $s \geqslant 1$.

### Example

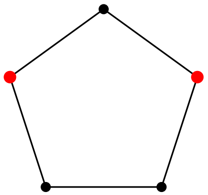
If $I$ is the cover ideal of the 5-cycle, then $\mathrm{Ass}(I^2) = I \cup \{\langle x_1, x_2, x_3, x_4, x_5 \rangle\}$, and $\mathrm{Ass}(I^s) = \mathrm{Ass}(I^{s+1})$ for all $s \geqslant 2$. So $I$ has the persistence property.

### Persistence conjecture

All square-free monomial ideals have the persistence property.

# A conjecture on critical graphs

- To replicate a vertex $w \in V(G)$, add a copy $w'$ of $w$ and make it adjacent to $w$ and all its neighbours.
- Let $G^W$ be the graph obtained from $G$ by replicating the vertices in $W$ (order is irrelevant).



Conjecture (Francisco, Hà and Van Tuyl 2010)

For any positive integer $k$ and any $k$-critical graph $G$, there is a set $W \subseteq V(G)$ such that $G^W$ is $(k+1)$-critical.

- Implies the persistence conjecture.

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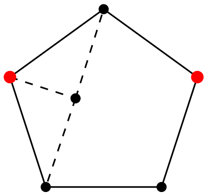

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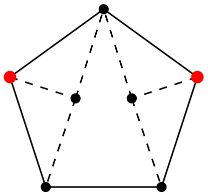


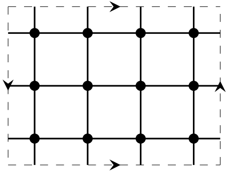
Conjecture (Francisco, Hà and Van Tuyl 2010)

For any positive integer $k$ and any $k$-critical graph $G$, there is a set $W \subseteq V(G)$ such that $G^W$ is $(k+1)$-critical.

- Implies the persistence conjecture.

## A counterexample

- For $n \geqslant 3$, let $H_n$ be the $3 \times n$ grid embedded in the Klein bottle.
- $\chi(H_n) = 4$ and $H_n$ is critical for all $n \geqslant 4$ (Gallai 1963).



$H_4$

**Theorem (Kaiser, MS and Škrekovski 2014)**

For any $n \geqslant 4$ and any $W \subseteq V(H_n)$, the graph $H_n^W$ is not 5-critical.

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The cover ideal of $H_4$ does not satisfy the persistence property.

- The cover ideal of $H_4$ also gives a negative answer to a question of Herzog and Hibi (2005) about the depth function of square-free monomial ideals.

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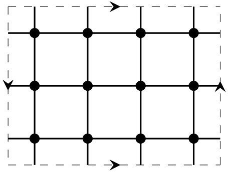

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**Merci !**