

Satisfiability: Theory, Practice, and Beyond

Simons Institute for the Theory of Computing

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Isomorph-Free Generation of Combinatorial Objects with SAT Modulo Symmetries

Stefan Szeider
TU Wien, Vienna, Austria



joint work with Katalin Fazekas, Markus Kirchweger, Tomas Peitl, and Manfred Scheucher

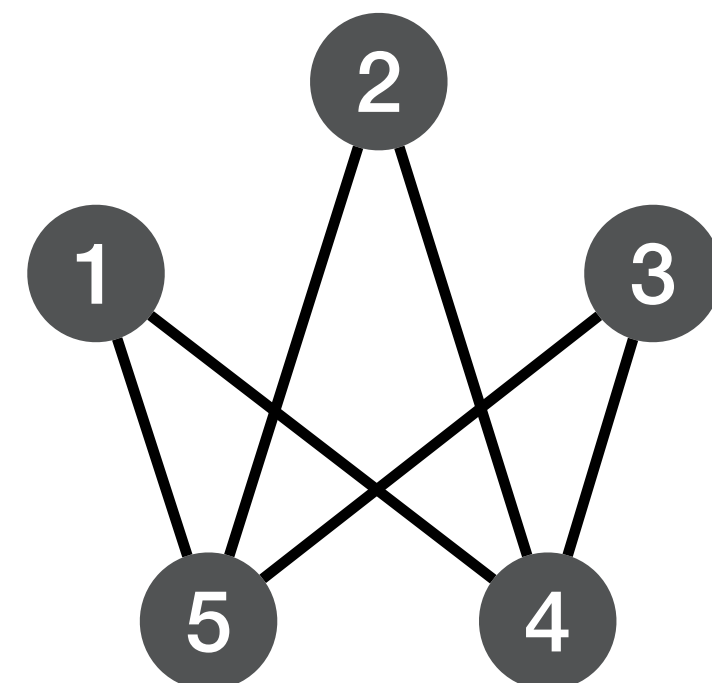


Generation of Combinatorial Objects

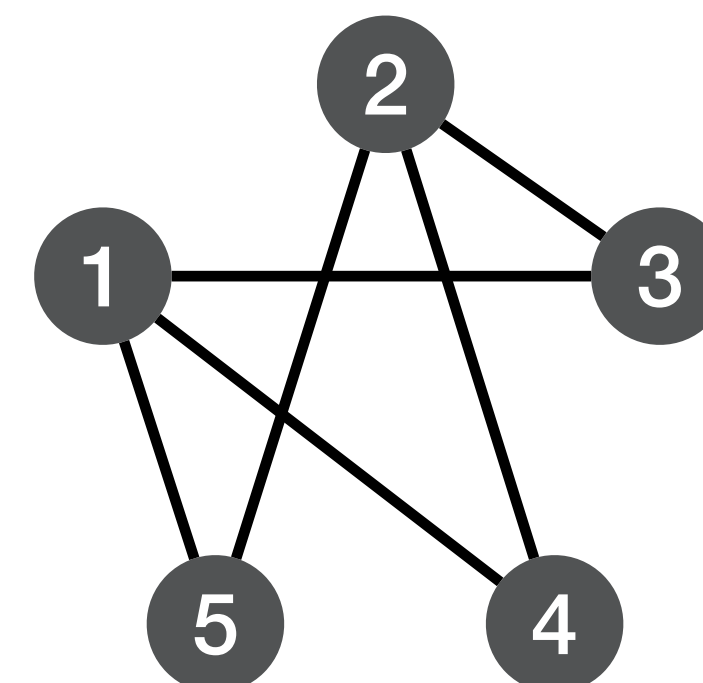
- Many problems in Discrete Mathematics ask for the (non-)existence of combinatorial objects with some property X .
- **Combinatorial objects:** graphs, hypergraphs, matroids, etc.
- **Enumeration problems:** Enumerate all objects of size n with property X ?
- **Extremal problems:** Graphs with smallest/largest number of edges and n vertices with property X ?
- **Counterexamples to Conjectures:** Show that there is no object with property X of size up to n .

Isomorph-Free Generation

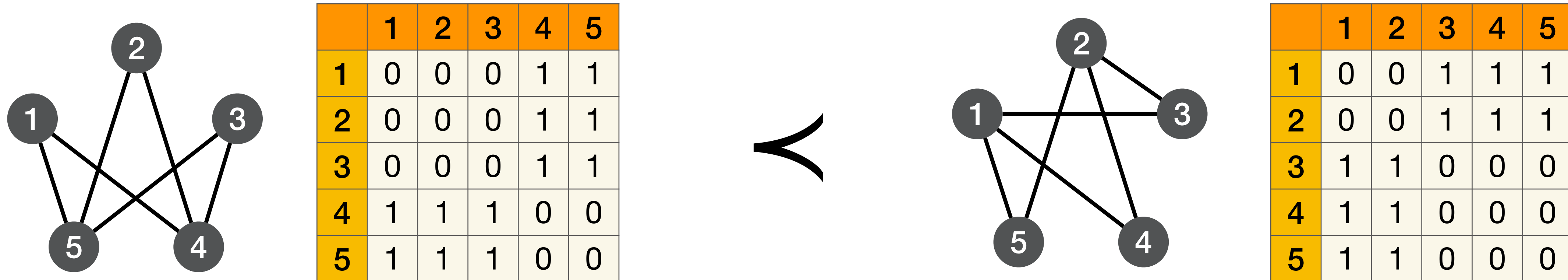
- **Isomorph-free generation:** Number of objects explode quickly, hence we want to avoid generating several isomorphic copies of the same object
- **Canonization:** map each object G to a unique representative $\alpha(G)$ of its isomorphism class
- **Canonical Objects:** Only generate objects G with $\alpha(G) = G$



1 \mapsto 5
2 \mapsto 4
3 \mapsto 3
4 \mapsto 1
5 \mapsto 2



Canonization by lexicographic ordering



- consider the adjacency matrix as a long string obtained by concatenating its rows
- order graphs lexicographically by this string
- $\alpha(G) = G$ if G is minimal in its isomorphism class

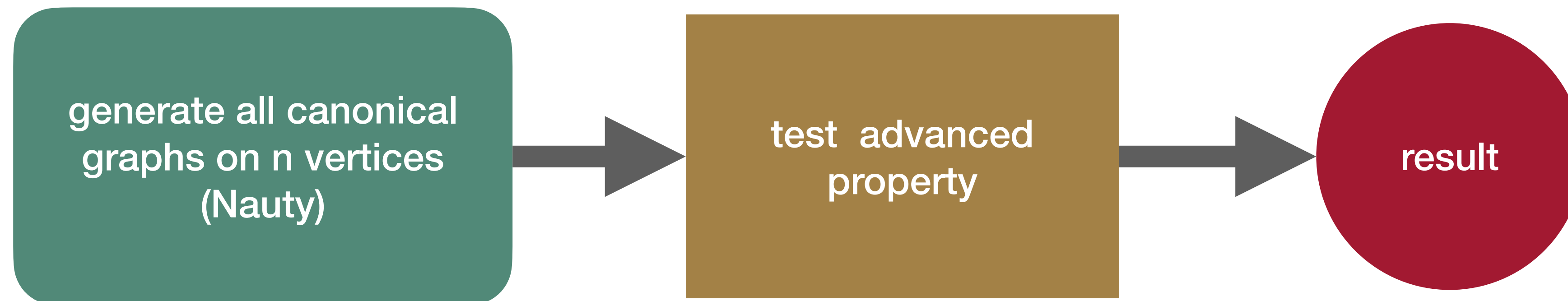
Example: connected graphs

n	<i>connected graphs</i> A001187	<i>canonical connected graphs</i> A001349
5	728	21
6	26704	112
7	1866256	853
8	251548592	11117
9	251548592	261080
10	≈ 66 billion	11716571
11	≈ 35 quadrillion (10^{15})	≈ 1 million
12	≈ 73 quintillion (10^{18})	≈ 16 billion

OEIS: The On-Line
Encyclopedia of Integer
Sequences lists > 36000
sequences oeis.org

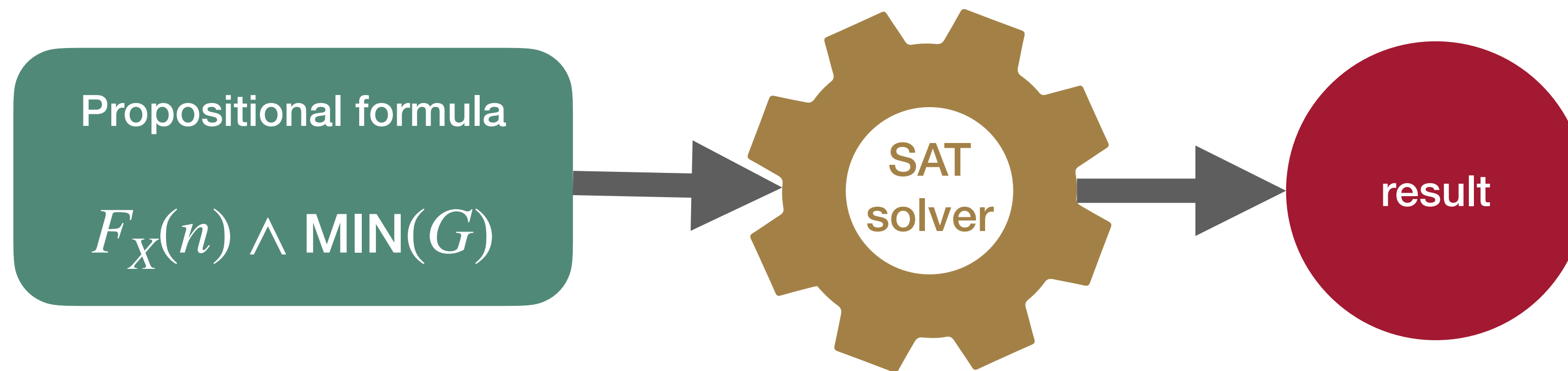
Generate & Test

- **Nauty:** popular tool for isomorph-free generation of graphs.
Based on *canonical construction path method* [McKay 1998]
- **Basic properties:** Good for enumerating graphs with very basic properties like degree restrictions
- **Advanced properties:** handled with generate and test, hence limited to $n \leq 11$ (or slightly larger if degrees are bounded)



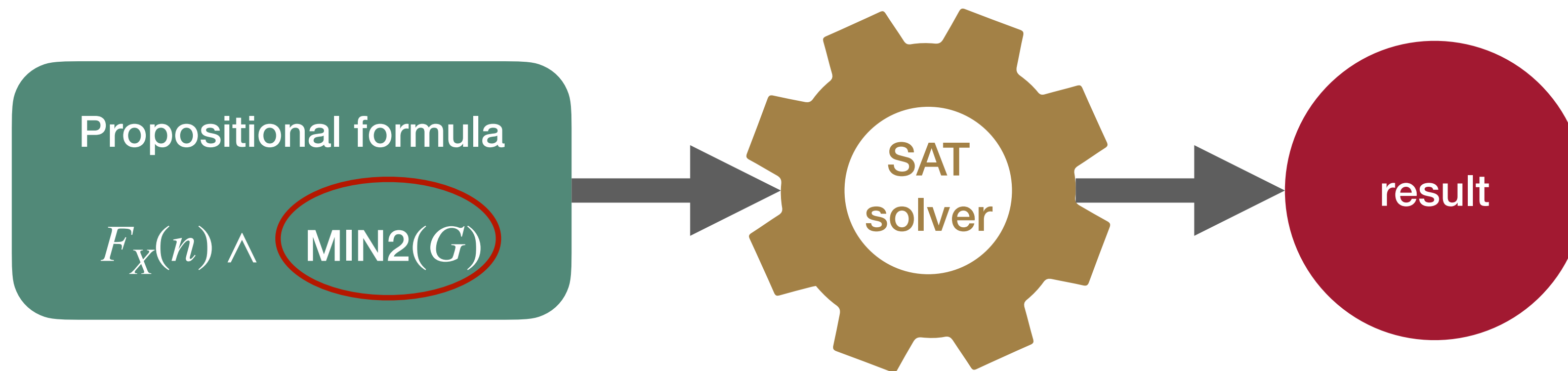
Static SAT approach

- **Idea:** use SAT to combine generate and test in one process
- **Property:** Express “ G is a graph with n vertices and property X ” in a propositional formula $F_X(n)$
- **Object variables:** for each pair i, j of vertices add a variable $e_{i,j}$ which is true iff the edge is present in the graph
- **Auxiliary variables:** used to express the desired property X



Problem: $\text{MIN}(G)$ no polynomial-size encoding known

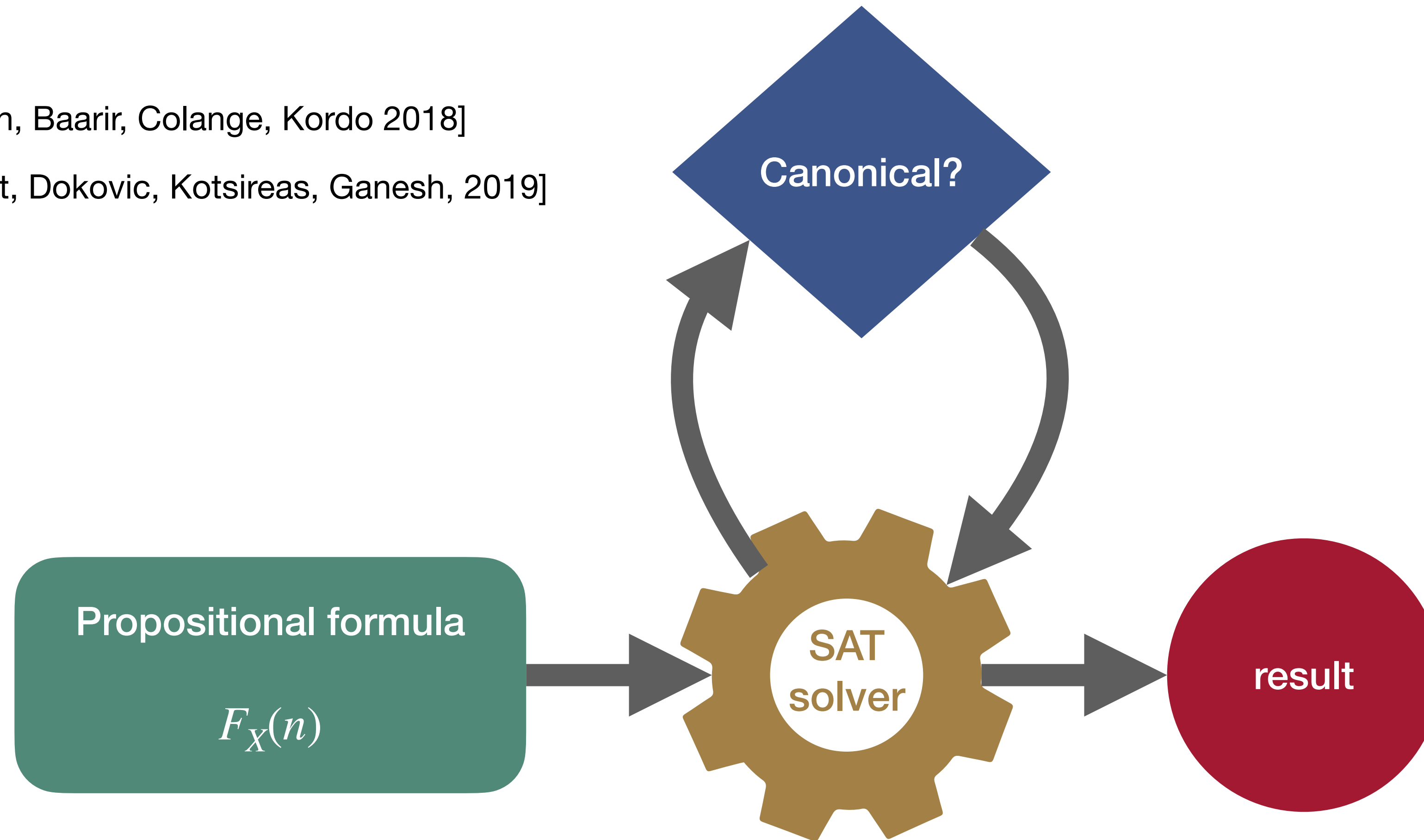
Static SAT approach



- **Incomplete Static Symmetry Breaking:**
 $\text{MIN2}(G)$ = “if we swap any two vertices the resulting graph isn’t lexicographically smaller”
- [Codish, Miller, Prosser, Stuckey, 2019]
- Good results, although only a small fraction of isomorphic copies is filtered.
- Can we do better?

Dynamic SAT approach

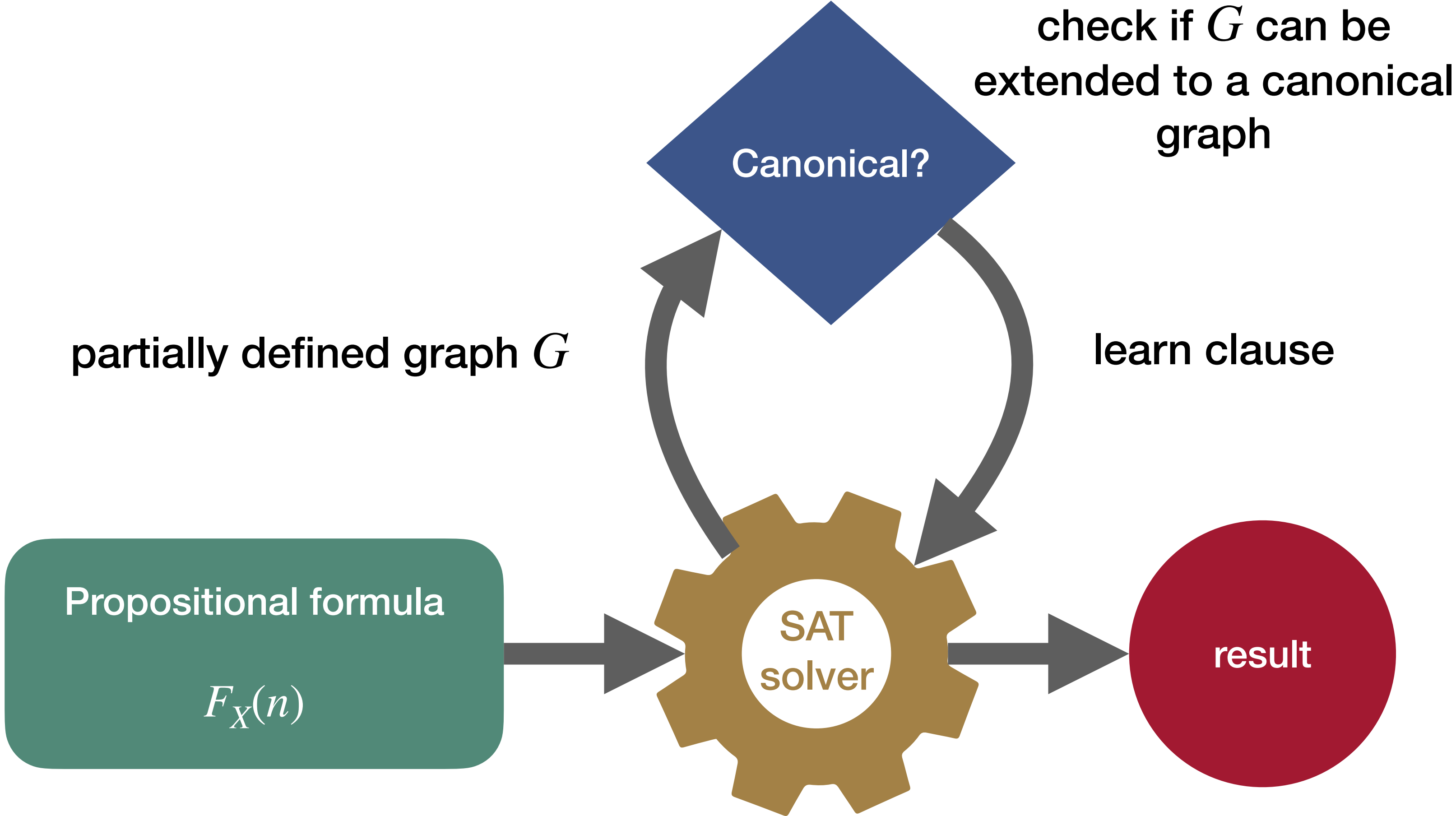
- CDCLSym [Metin, Baarir, Colange, Kordo 2018]
- SAT+CAS [Bright, Dokovic, Kotsireas, Ganesh, 2019]
- and others



SMS: SAT Modulo Symmetries

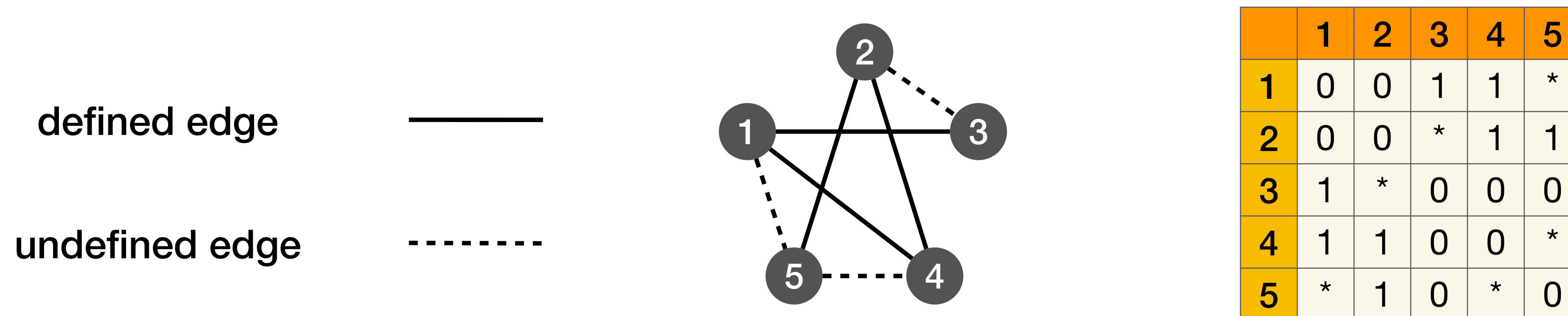
Dynamic symmetry breaking by checking the
lexicographic minimality of **partially defined graphs**
[Kirchweger and Sz. 2021]

Dynamic Symmetry Breaking with SMS



Partially Defined Graphs

- A partially defined graph is a graph where for some of its edges it is undecided whether they are present or not



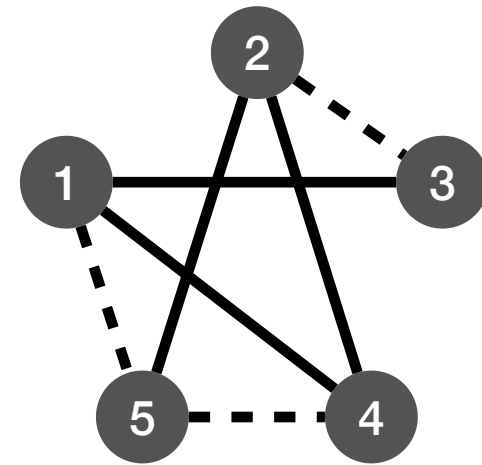
- G is specified by a partition of $E(G)$ into $D(G)$ and $U(G)$.
(the **d**efined edges and the **u**ndefined edges)

Natural partial order

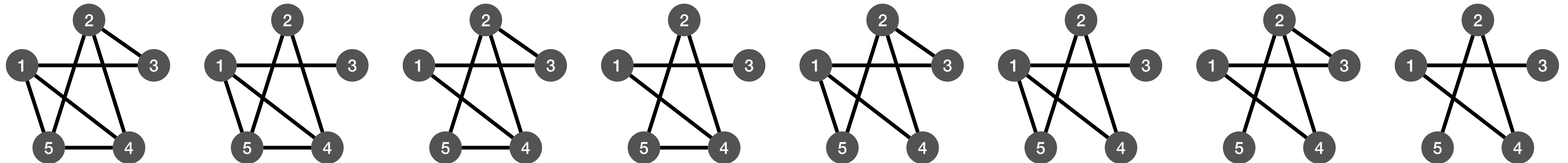
- The partially defined graphs over vertex set $\{1, \dots, n\}$ are partially ordered by $G_1 \sqsubseteq G_2$ if $D(G_1) \subseteq D(G_2)$ and $U(G_2) \subseteq U(G_1)$.
- The minimal element is the graph with all edges undefined.
- The maximal elements are all fully defined graphs over $\{1, \dots, n\}$.
- $\mathcal{X}(G) =$ all fully defined graphs H with $G \sqsubseteq H$

Extensions to fully defined graphs

partially defined graph G



$\mathcal{X}(G)$: set of all fully defined graphs G can be extended to



Canonicity of partially defined graphs

- **Ideal solution:** reject the current branch if G is **non-canonical** in the sense that none of $H \in \mathcal{X}(G)$ is canonical.
- I.e., if for all $H \in \mathcal{X}(G)$ there is a permutation π such that $\pi(H) < H$.
- Extremely difficult to check: need to consider an exponential number of graphs in $\mathcal{X}(G)$, each of them requiring exponential time in the worst case to find the permutation.
- Even if we have determined that G is not canonical, how can we verify this succinctly within a proof.
- Solution: weaker form of canonicity for partially defined graphs

Certified non-canonicity

- SMS uses the following weaker form of canonizity:
- We reject the current branch if G is **certified non-canonical**,
- i.e., if there is a permutation π such that $\pi(H) < H$ for all $H \in X(G)$.
- We can use the permutation π as a certificate that can be later verified and checked by an independent method.
- If G is fully defined, it is non-canonical iff it is certified non-canonical.
- Thus we have a **full symmetry breaking** since sooner or later all symmetries will be detected.

Minimizing learned clauses

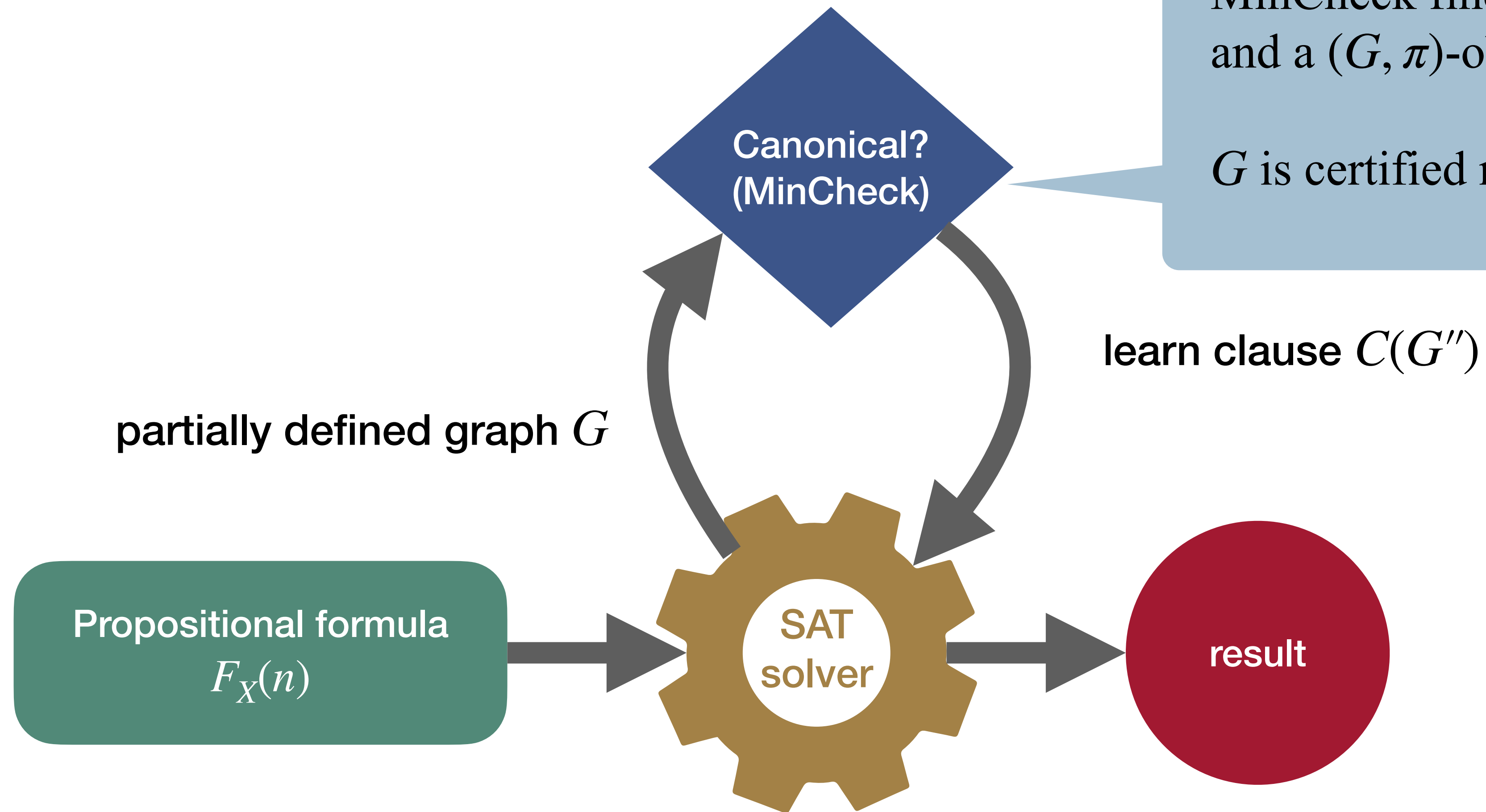
- If we have determined that G is certified non-minimal, we can learn a clause

$$C(G) = \bigvee_{ij \text{ is defined edge}} \neg e_{i,j} \vee \bigvee_{ij \text{ is non-edge}} e_{i,j}$$

which forbids G and all $G' \supseteq G$

- We can do even better: Compute a \subseteq -smallest graph $H \subseteq G$ such that π is a certificate for its non-canonizity. Then learn the clause $C(H)$.
- We call H a (G, π) -**obstruction**.

Completeness



Theorem:

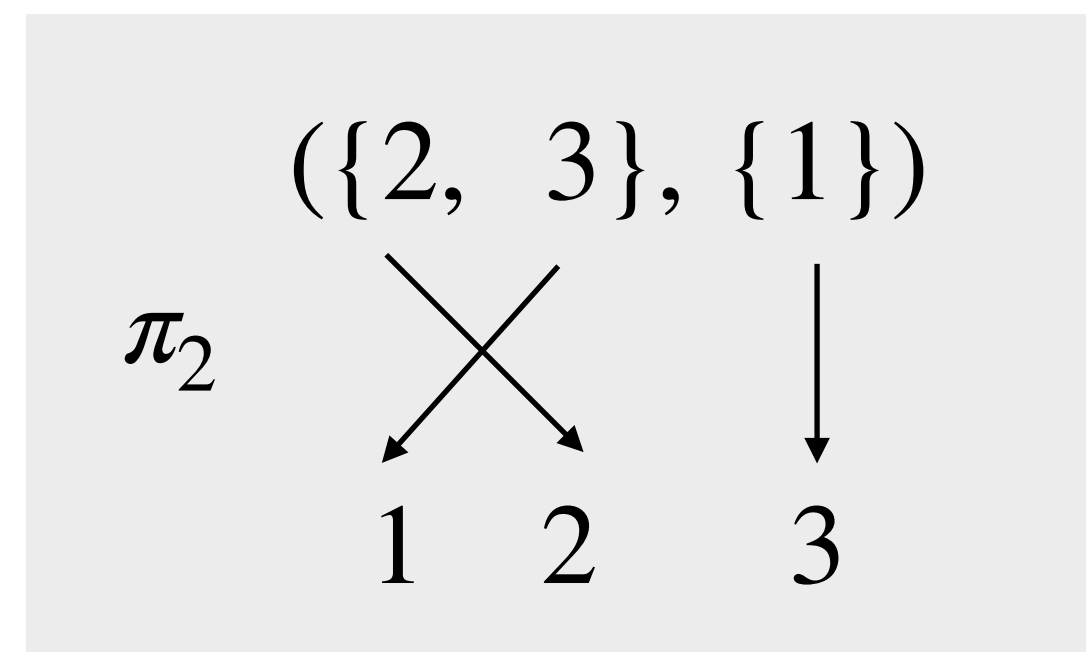
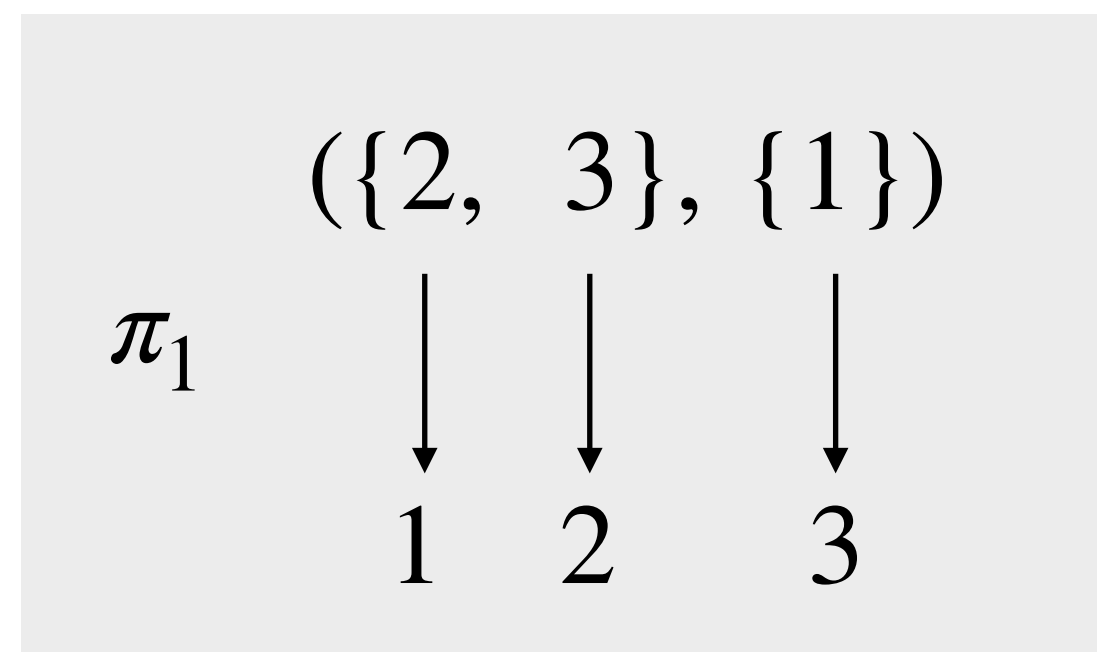
MinCheck finds a certificate π
and a (G, π) -obstruction H

\Leftrightarrow

G is certified non-canonical

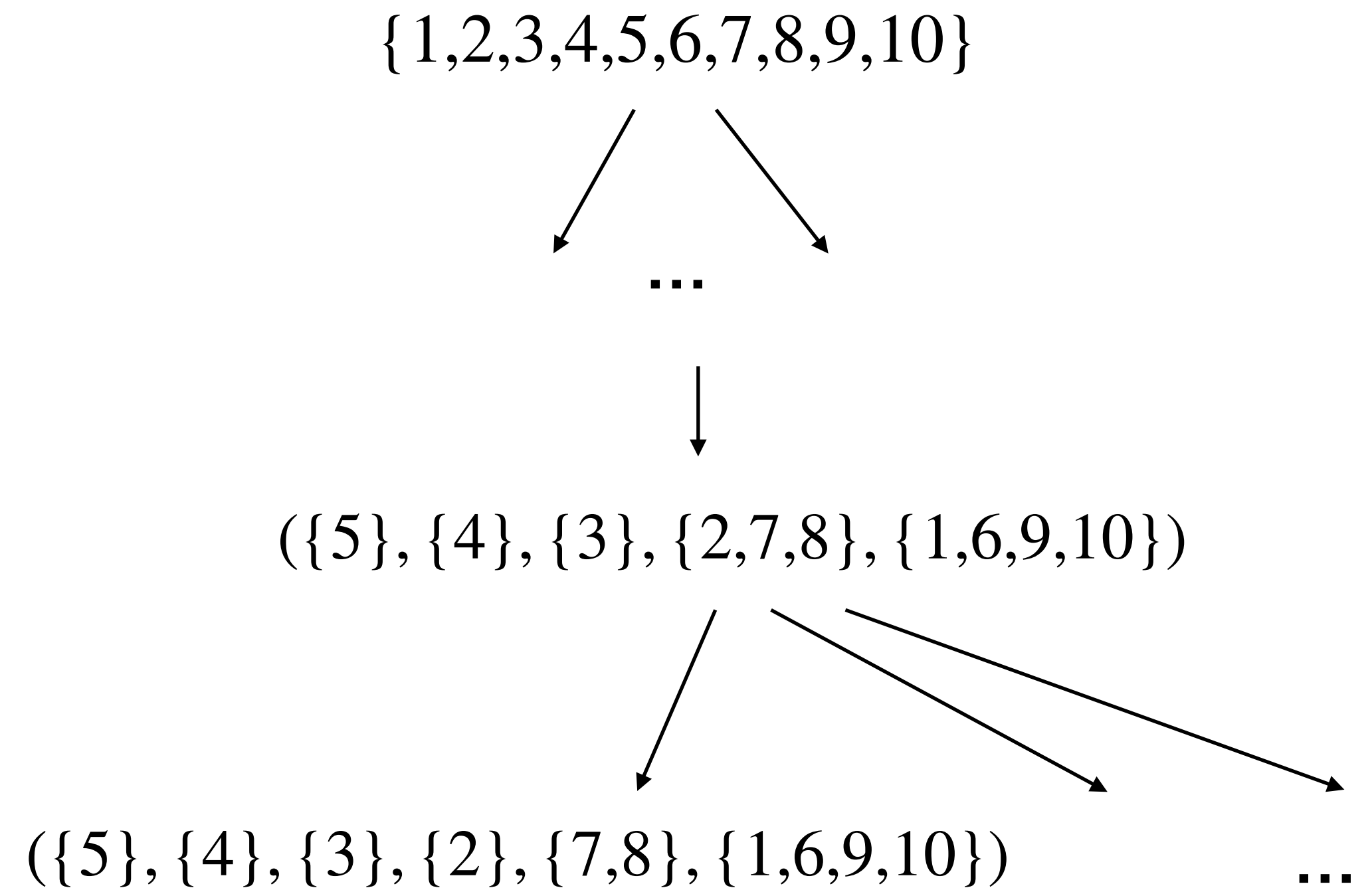
Ordered Partitions

- MinCheck operates on **ordered partitions** of the vertex set, a partition whose equivalence classes are totally ordered
- An ordered partition (V_1, \dots, V_r) represents all permutations π with the property that $u \in V_i, v \in V_j$ for $i < j$ implies $\pi(u) < \pi(v)$.



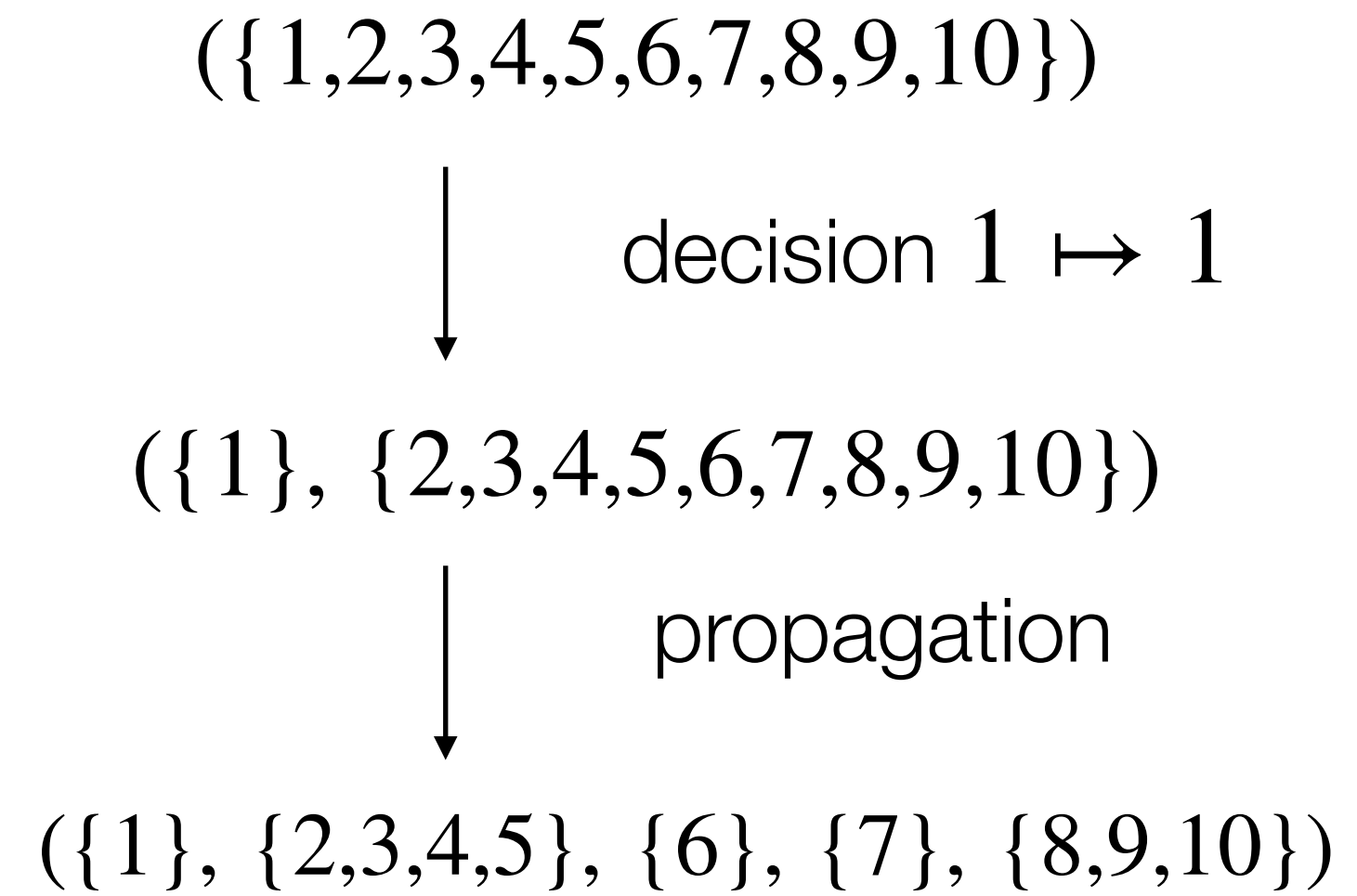
Iterative Ordered Partition Refinement

- We start with $P = (V)$, and refine it iteratively from left to right, trying all possibilities of splitting a V_i into a singleton and the rest.
- After each decision, we **propagate**: refine all other equivalence classes without losing potential certificates



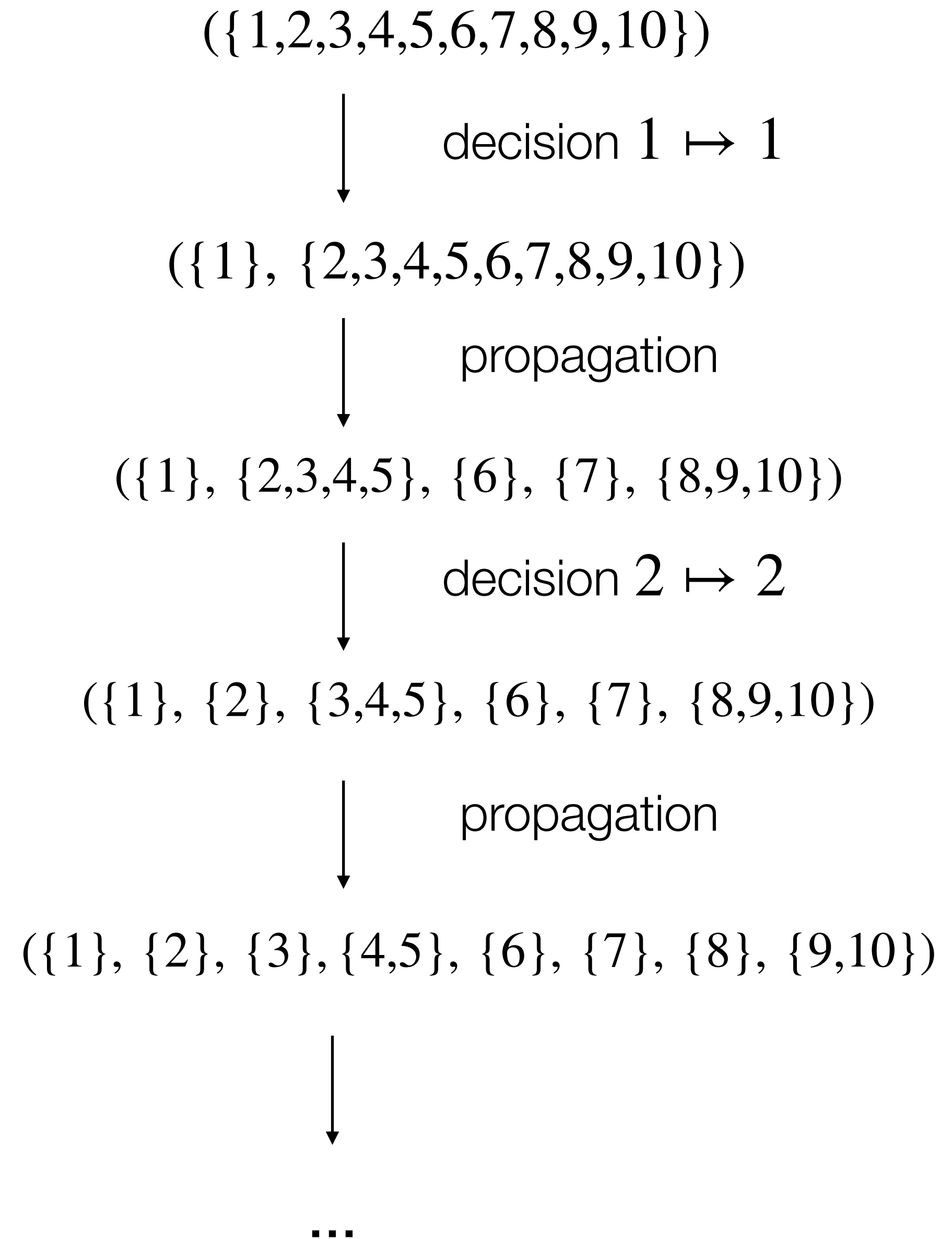
Propagation

	1	2	3	4	5	6	7	8	9	10
1	0	0	0	0	0	*	*	1	1	1
2	0	0	0	1	1	1	0	0	1	1
3	0	0	0	*	1	*	*	*	*	*
4	0	1	*	0	0	*	*	*	*	*
5	0	1	1	0	0	0	*	*	*	*
6	*	1	*	*	0	0	*	*	*	*
7	*	0	*	*	*	*	0	*	*	*
8	1	0	*	*	*	*	*	0	*	*
9	1	1	*	*	*	*	*	*	0	*
10	1	1	*	*	*	*	*	*	*	0



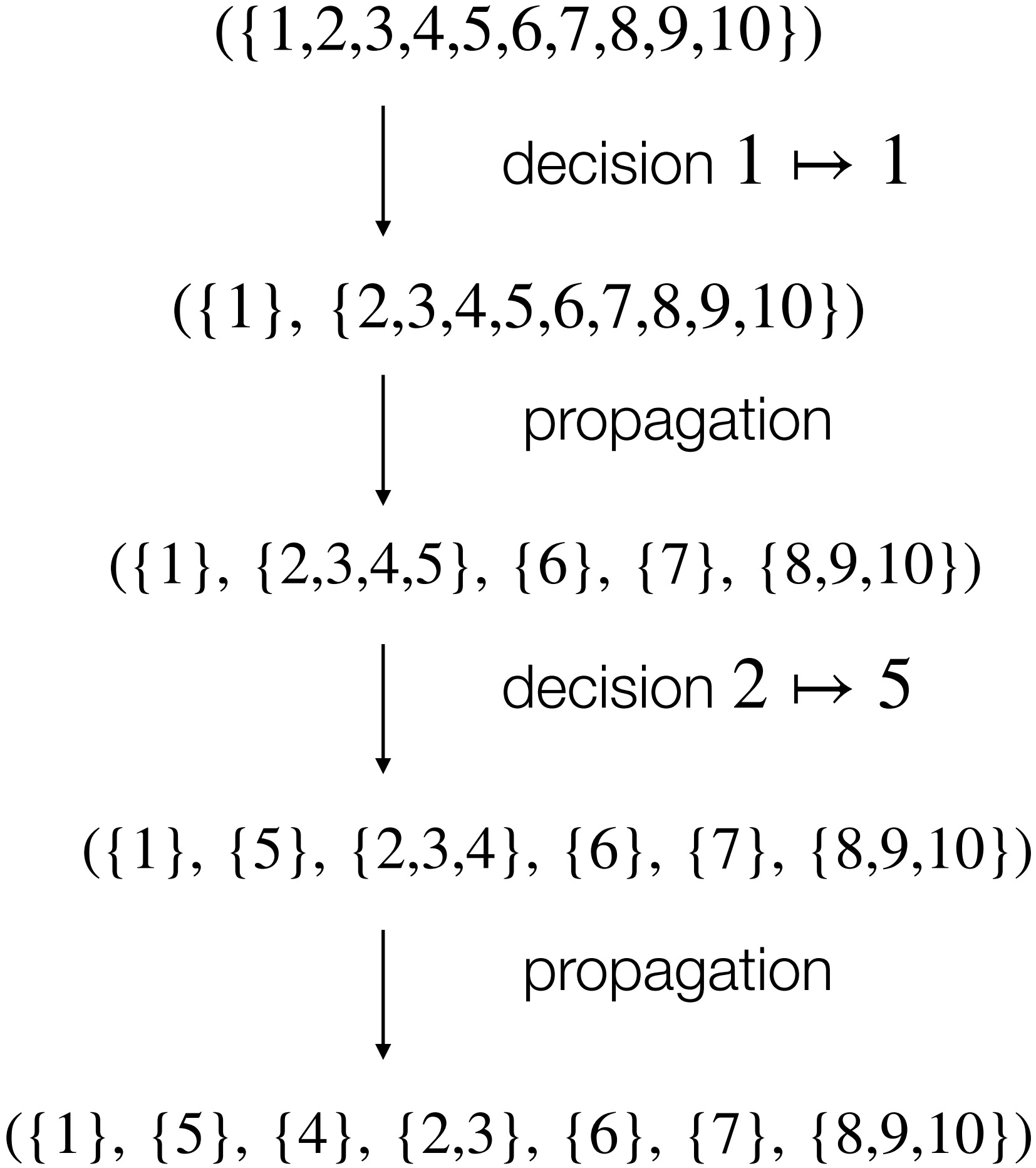
Propagation

	1	2	3	4	5	6	7	8	9	10
1	0	0	0	0	0	*	*	1	1	1
2	0	0	0	1	1	1	0	0	1	1
3	0	0	0	*	1	*	*	*	*	*
4	0	1	*	0	0	*	*	*	*	*
5	0	1	1	0	0	0	*	*	*	*
6	*	1	*	*	0	0	*	*	*	*
7	*	0	*	*	*	*	0	*	*	*
8	1	0	*	*	*	*	*	0	*	*
9	1	1	*	*	*	*	*	*	0	*
10	1	1	*	*	*	*	*	*	*	0



Propagation

	1	2	3	4	5	6	7	8	9	10
1	0	0	0	0	0	*	*	1	1	1
2	0	0	0	1	1	1	0	0	1	1
3	0	0	0	*	1	*	*	*	*	*
4	0	1	*	0	0	*	*	*	*	*
5	0	1	1	0	0	0	*	*	*	*
6	*	1	*	*	0	0	*	*	*	*
7	*	0	*	*	*	*	0	*	*	*
8	1	0	*	*	*	*	*	0	*	*
9	1	1	*	*	*	*	*	*	0	*
10	1	1	*	*	*	*	*	*	*	0



certifying permutation found!

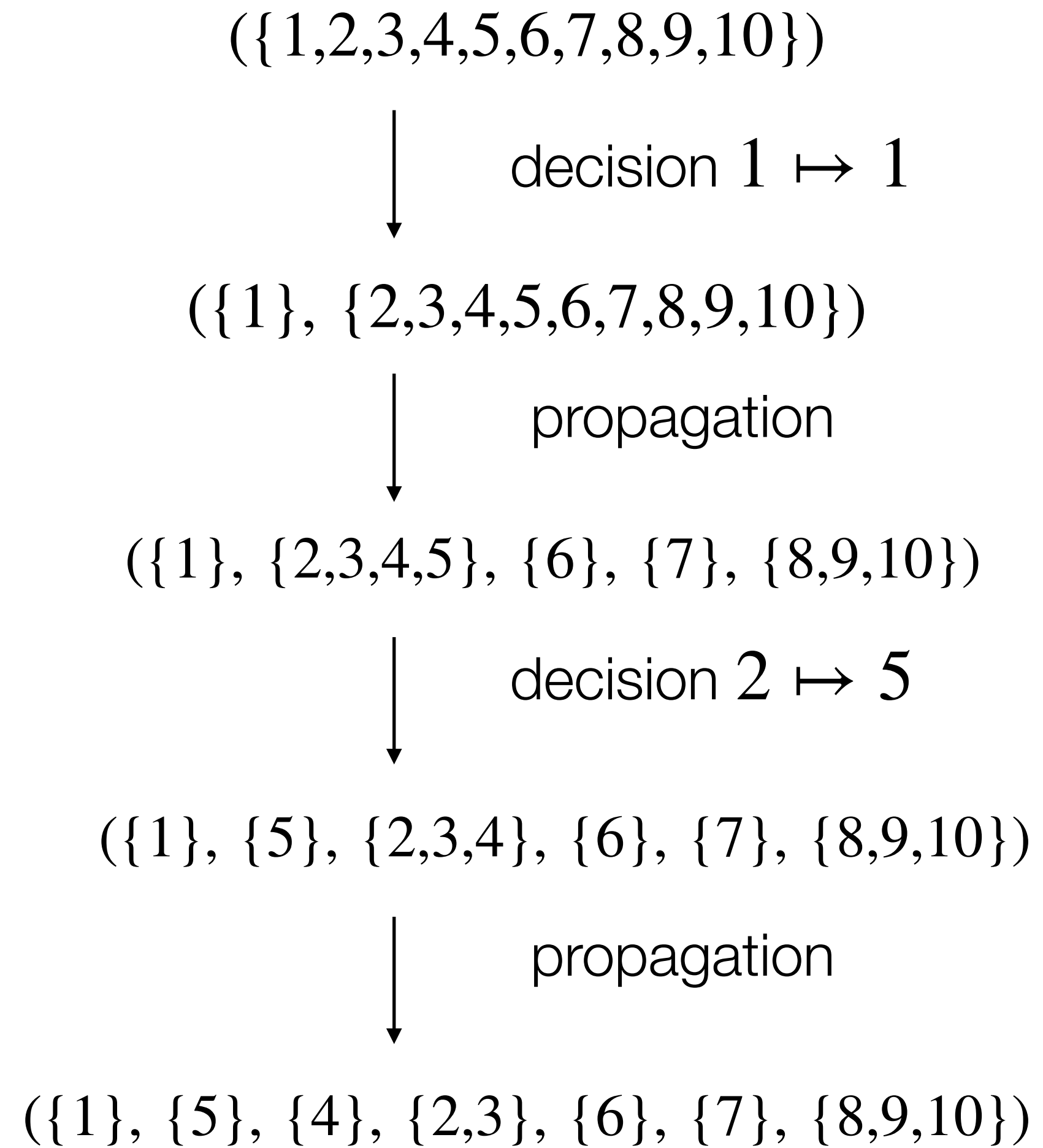
Propagation

G

	1	2	3	4	5	6	7	8	9	10
1	0	0	0	0	0	*	*	1	1	1
2	0	0	0	1	1	1	0	0	1	1
3	0	0	0	*	1	*	*	*	*	*
4	0	1	*	0	0	*	*	*	*	*
5	0	1	1	0	0	0	*	*	*	*

$\pi(G)$

	1	5	4	2	3	6	7	8	9	10
1	0	0	0	0	0	*	*	1	1	1
5	0	0	0	1	1	0	*	*	*	*
3	0	1	*	0	0	*	*	*	*	*
4	0	0	0	1	*	*	*	*	*	*
2	0	1	1	0	0	1	0	0	1	1



pick any π that is compatible with the current ordered partition

Obstruction

	1	2	3	4	5	6	7	8	9	10
1	0	0	0	0	0	*	*	1	1	1
2	0	0	0	1	1	1	0	0	1	1
3	0	0	0	*	1	*	*	*	*	*
4	0	1	*	0	0	*	*	*	*	*
5	0	1	1	0	0	0	*	*	*	*
6	*	1	*	*	0	0	*	*	*	*
7	*	0	*	*	*	*	0	*	*	*
8	1	0	*	*	*	*	*	0	*	*
9	1	1	*	*	*	*	*	*	0	*
10	1	1	*	*	*	*	*	*	*	0

Edges and non-edges of the obstruction graph:

- Include all edges/non edges that come before the indicator pair that are not stable under π .
- Include the indicator pair (2,6) and its image $(\pi(2), \pi(6)) = (5,6)$.

As a clause:

$$e_{1,2} \vee e_{1,3} \vee e_{1,4} \vee e_{1,5} \vee e_{2,3} \vee \neg e_{2,4} \vee \neg e_{2,6} \vee e_{5,6}$$

Performance of MinCheck

- In the worst case, MinCheck needs to consider all $n!$ permutations.
- In practice, the worst case is rarely attained, propagation excludes many cases.
- If MinCheck uses a significant amount of the solving time:
 - call MinCheck only every k 'th time a decision on an edge variable has been made
 - call MinCheck only up to ℓ recursive calls
- Isomorph-freeness still guaranteed by either running unrestricted MinCheck at the end or check set of solutions for isomorphic copies with separate tool

Implementation

- MinCheck implemented in C++
- variants for graphs, directed graphs, matroids, hypergraphs
- hosting solver: originally clasp (CDCL ASP solver)
- since recently CaDiCal (modern CDCL SAT solver with inprocessing)
- CaDiCal with IPASIR-UP interface [Fazekas et al. SAT 2023]
- For instances with many clauses, this gives an order-of-magnitude speedup
- Python wrapper for easy use, supports many graph properties from the command line

Ressources

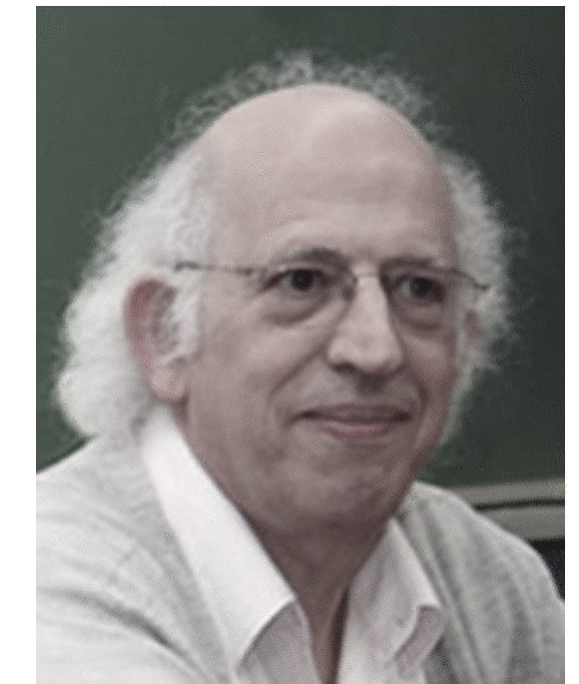
Tool <https://github.com/markirch/sat-modulo-symmetries/>

Documentation <https://sat-modulo-symmetries.readthedocs.io/>

Applications

Diameter-2-critical graphs: background

- the **diameter** of a graph is the longest distance between any two of its vertices.
- A graph is **diameter- d -critical** if its diameter is d but deleting any edge decreases the diameter.
- The study of extremal properties of graphs of given diameter goes back to the 1960s [Erdős and Rényi], much work has been done on diameter- d -critical graphs.
- **Simon-Murty Conjecture 1979:** a diameter-2-critical graph with n vertices has at most $\lfloor n^2/4 \rfloor$ edges, with equality holds exactly for the complete bipartite graph $K_{\lfloor n/2 \rfloor, \lceil n/2 \rceil}$.



Imre Simon



U.S.R. Murty

Diameter-2-critical graphs: encoding

- We use SMS to enumerate diameter-2-critical graphs up to $n = 13$ and verify the Simon-Murty Conjecture up to $n = 19$
- Previous results only up to $n = 10$ with generate-and-test method based on Nauty [Radosavljević and Živković 2020]
- We use auxiliary variables $c_{i,j,k} \leftrightarrow e_{i,k} \wedge e_{j,k}$ to indicate that i, j have a common neighbor k
- With these variables it is easy to express that (i) the diameter is 2 and that (ii) deleting any edge gives a diameter > 2
- We use a **frequency** parameter, calling MinCheck only every k 'th time a decision on an object variable has been made ($k = 20$)

Diameter-2-critical graphs: results

n	#-graphs	SMS		Static	
		#-sol	time	#-sol	time
3	1	1	0.00(23%)	1	0.00
4	2	2	0.00(22%)	2	0.00
5	3	3	0.00(23%)	4	0.00
6	5	5	0.00(32%)	11	0.00
7	10	10	0.01(37%)	32	0.01
8	30	30	0.05(47%)	163	0.04
9	103	103	0.17(39%)	1024	0.30
10	519	519	0.73(26%)	9836	3.58
11	3746	3748	4.48(18%)	135010	77.00
12	40866	40876	47.71(14%)	t.o.	t.o.
13	688120	688143	1184.47(8%)	t.o.	t.o.

limit for generate and test
[Radosavljević and Živković 2020]

- Enumeration of diam-2-critical graphs and verifying the Simon-Murty conjecture. (X%) gives time for MinCheck

Diameter-2-critical graphs: results

n	total time	max-time	#-comb
14	16 minutes	9 sec	406
15	2.2 hours	20 sec	1729
16	7.9 hours	35 sec	3480
17	19.9 hours	74 sec	5620
18	3.4 days	132 sec	12974
19	23.7 days	312 sec	50054

- For verifying the Simon-Murty Conjecture, we can utilize results that restrict the vertex degrees [Fan 1987, Haynes, Henning, Merwe, Yeo 2014], which allows us to scale the search even further.
- If we fix the degree of vertices, we can start MinCheck with an ordered partition where vertices of the same degree form equivalence classes.
- max-time: time for a single combination. #-comb: number of combinations

Proofs with SMS

- With SMS we can certify the correctness of results by means of DRAT proofs.
- Adding the clauses generated by MinCheck to the original encoding, we can produce a DRAT proof by any CDCL solver that supports DRAT.
- The added clauses can also be verified independently when certificate permutation is logged.
- This gives an additional application domain for SMS: providing further confidence in known results obtained by other methods.
- For enumeration tasks, we add clauses excluding all the previously found solutions. This way, we can certify the completeness of the enumeration.

Ramsey Sets: background

- For positive integers x and y , the **Ramsey set** $\mathcal{R}(x, y, n)$ is the set of all n -vertex graphs up to isomorphism not containing an independent set of size x nor a clique of size y .
- The **Ramsey number** $R(x, y)$ is the smallest integer such that $\mathcal{R}(x, y, R(x, y)) = \emptyset$.
- Encoding the Ramsey property is straightforward (go over all subsets of vertices of size x and require that the set induces an edge; go over all subsets of vertices of size y and require that the set induces a non-edge)



Frank P. Ramsey
(1903-1930)

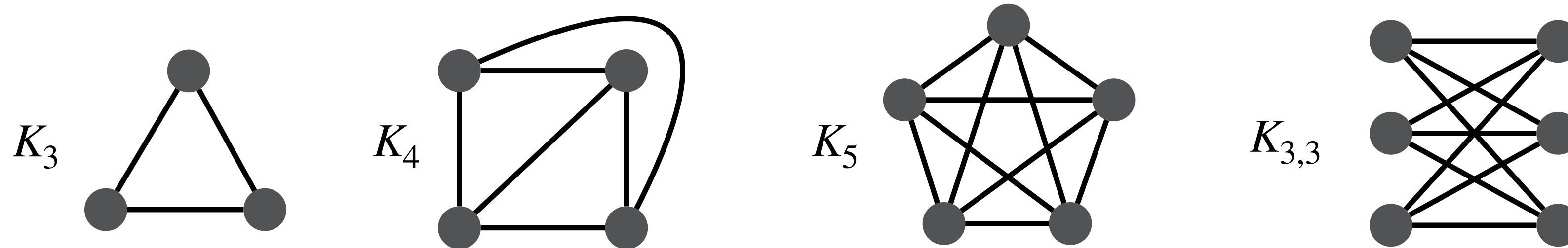
Ramsey Sets: results

- $R(3,5) = 14$, $R(4,4) = 18$
- First proofs for the numbers

n	$\mathcal{R}(3, 5, n)$		$\mathcal{R}(4, 4, n)$	
	#-sol	time	#-sol	time
1	1	0.00	1	0.00
2	2	0.00	2	0.00
3	3	0.00	4	0.00
4	7	0.00	9	0.00
5	13	0.00	24	0.00
6	32	0.00	84	0.01
7	71	0.01	362	0.03
8	179	0.03	2079	0.16
9	290	0.05	14701	1.25
10	313	0.05	103706	11.99
11	105	0.05	546356	80.92
12	12	0.03	1449166	531.44
13	1	0.02	1184231	227.95
14			130816	28.70
15			640	0.66
16			2	0.15
17			1	0.14
total	1029	0.24	3432184	883.41

Generating Planar Graphs with SMS

- A graph is **planar** if it can be drawn on the plane such that edges are represented by continuous curves that do not intersect in the interior.

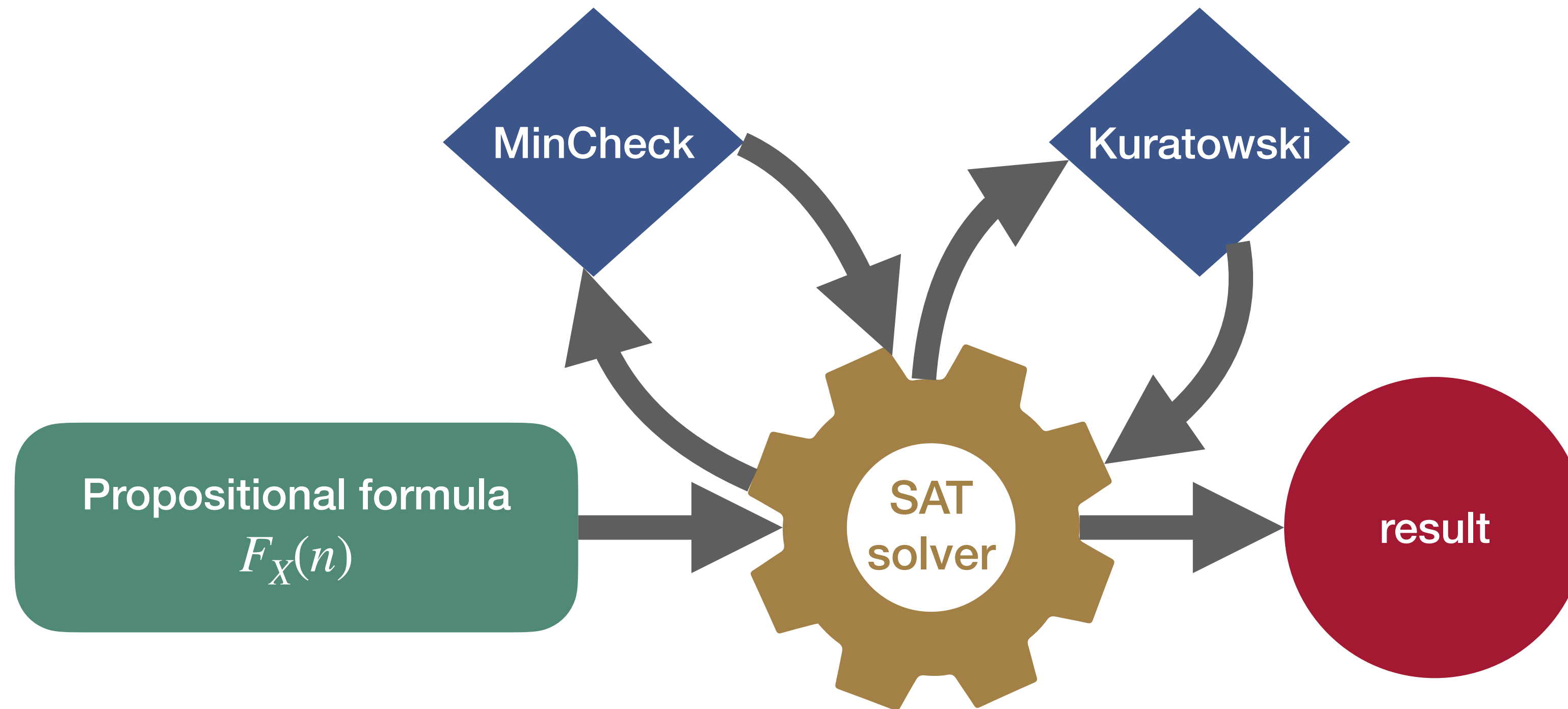


- The best known planarity criterium is **Kuratowski's Theorem**. It is a **negative criterium**: a graph is planar iff it does not contain a subdivision of $K_{3,3}$ or K_5 as subgraph. We implemented this with a **propagator**.
- Similar to they **co-certificate learning (CCL)**, used for finding lower bounds for the size of Kochen-Specker Systems [Kirchweger, Peitl, S. IJCAI 2023]
- One can encode planarity in CNF with a polynomial number of clauses. We tried two positive planarity criteria for that **Schnyder Orders** and **Universal Sets**.



Kazimierz Kuratowski
(1896-1980)

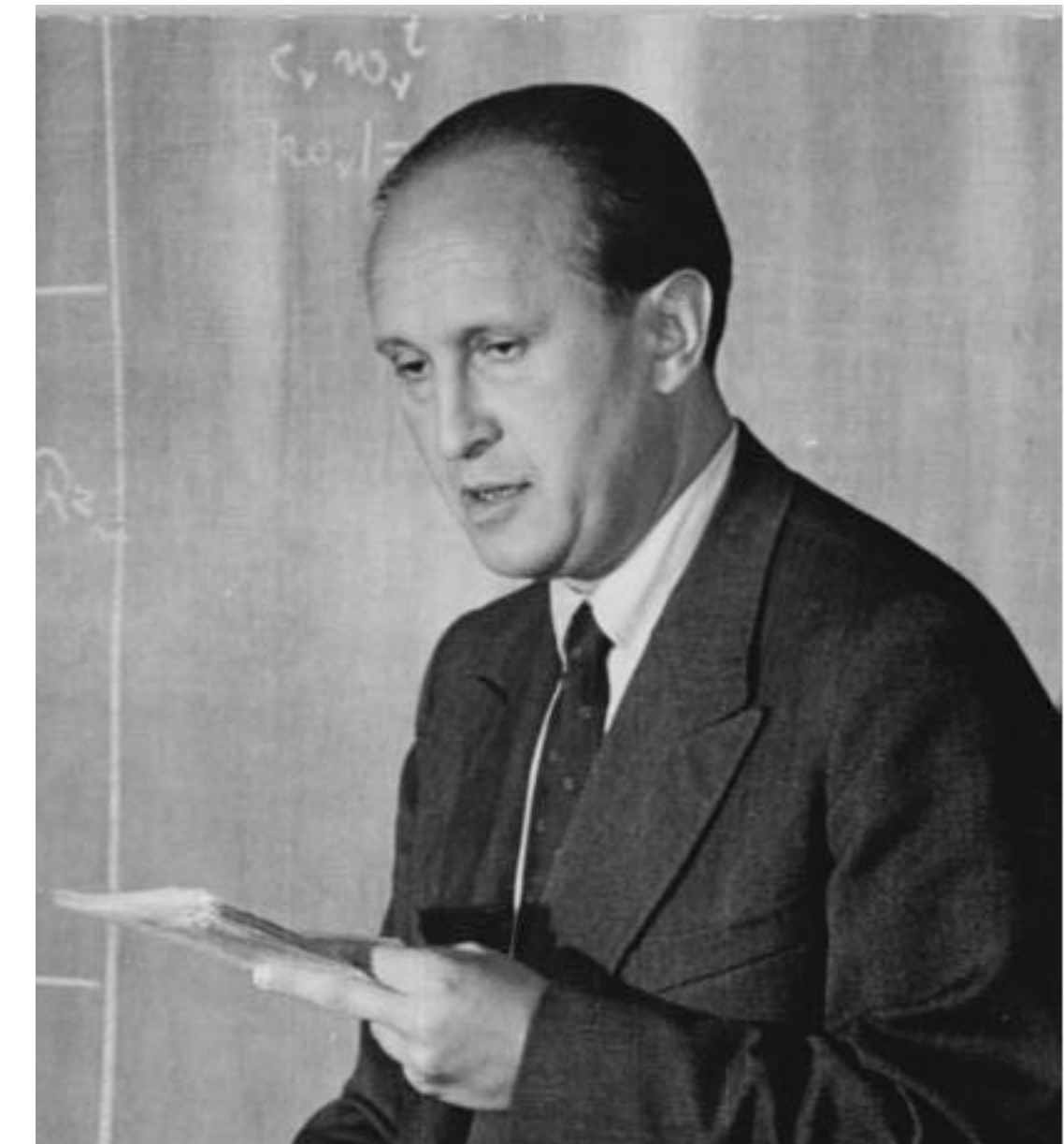
Lazy planarity encoding based on Kuratowski



- Planarity testing algorithm that produces $K_{3,3}$, K_5 subdivisions [Boyer and Myrvold 2004]
- Run it on the fully defined graph obtained from the partially defined graph by considering all undefined edges as non-edges
- Clearly outperforms the eager encodings.
- Provides a competitive alternative to **plantri** [Brinkmann and McKay 2007]

Planar Turán Numbers: background

- **Turán numbers:** $ex(n, H)$ maximum number of edges in an n -vertex graph that excludes a subgraph H . Turán's Theorem [1941] covers the case where H is a clique.
- **Planar Turán numbers:** $ex_P(n, H)$ = maximal number of edges in an n -vertex **planar** graph that excludes H .
- Has been studied for $H = C_4$, $H = C_5$ [Dowden 2016]
- Encoding: simply go over all sets of $k = 4, 5$ vertices and add a clause that requires the vertices do not generate a cycle



Pál Turán
(1910-1976)

Planar Turán Numbers: results $k = 4$

n	$\text{ex}_P(n, C_4)$	SAT		UNSAT	
		Kura	Ord	Kura	Ord
4	4	0.00	0.00	0.00	0.00
5	6	0.00	0.00	0.00	0.00
6	7	0.00	0.00	0.00	0.01
7	9	0.01	0.01	0.01	0.02
8	11	0.01	0.02	0.02	0.03
9	13	0.03	0.04	0.05	0.05
10	16	0.04	0.07	0.07	0.06
11	18	0.16	0.44	0.16	0.23
12	20	0.27	0.98	0.56	2.29
13	22	0.23	0.14	1.96	15.27
14	24	0.20	0.44	6.46	340.11
15	27	1.00	0.85	21.39	294.07
16	29	5.87	24.90	172.90	31142.08
17	31	5.19	83.59	3479.65	t.o.
18	33	14.69	14.85	59862.72	t.o.

Planar Turán Numbers: results $k = 5$

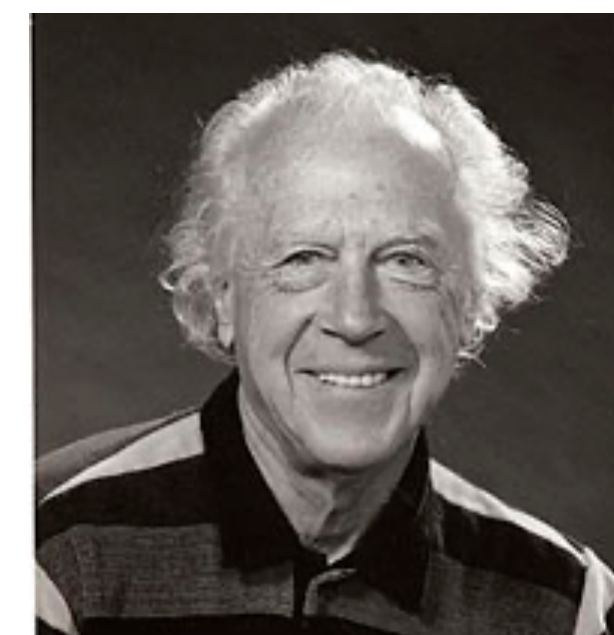
n	$ex_P(n, C_5)$	SAT		UNSAT	
		Kura	Ord	Kura	Ord
5	7	0.00	0.01	0.00	0.00
6	9	0.00	0.01	0.01	0.01
7	12	0.01	0.02	0.02	0.01
8	13	0.02	0.07	0.05	0.11
9	15	0.03	0.06	0.07	0.38
10	18	0.10	0.29	0.23	1.67
11	19	0.12	0.30	0.57	4.89
12	22	1.83	1.72	1.99	33.08
13	24	0.48	1.61	11.45	271.18
14	27	3.18	7.63	35.24	1174.85
15	29	2.24	10.82	277.78	15459.24
16	31	4.71	59.09	3172.27	235353.58
17	34	207.49	890.98	29023.55	t.o.
18	36	1851.84	1249.38	t.o.	t.o.

Earth-Moon problem: background

- **Four-Color Theorem:** The most famous computer assisted mathematical proof [Appel, Haken 1977]. Every planar graph is 4-colorable.
- **Ringel's Earth-Moon problem 1959:** How many colors are sufficient for a **biplanar** graph (edges can be partitioned into two planar graphs): every country has a colony on the moon. Each country gets the same color as its colony.
- The Earth-Moon problem is “hard as two or three four-color theorems” [Hutchinson 2016]

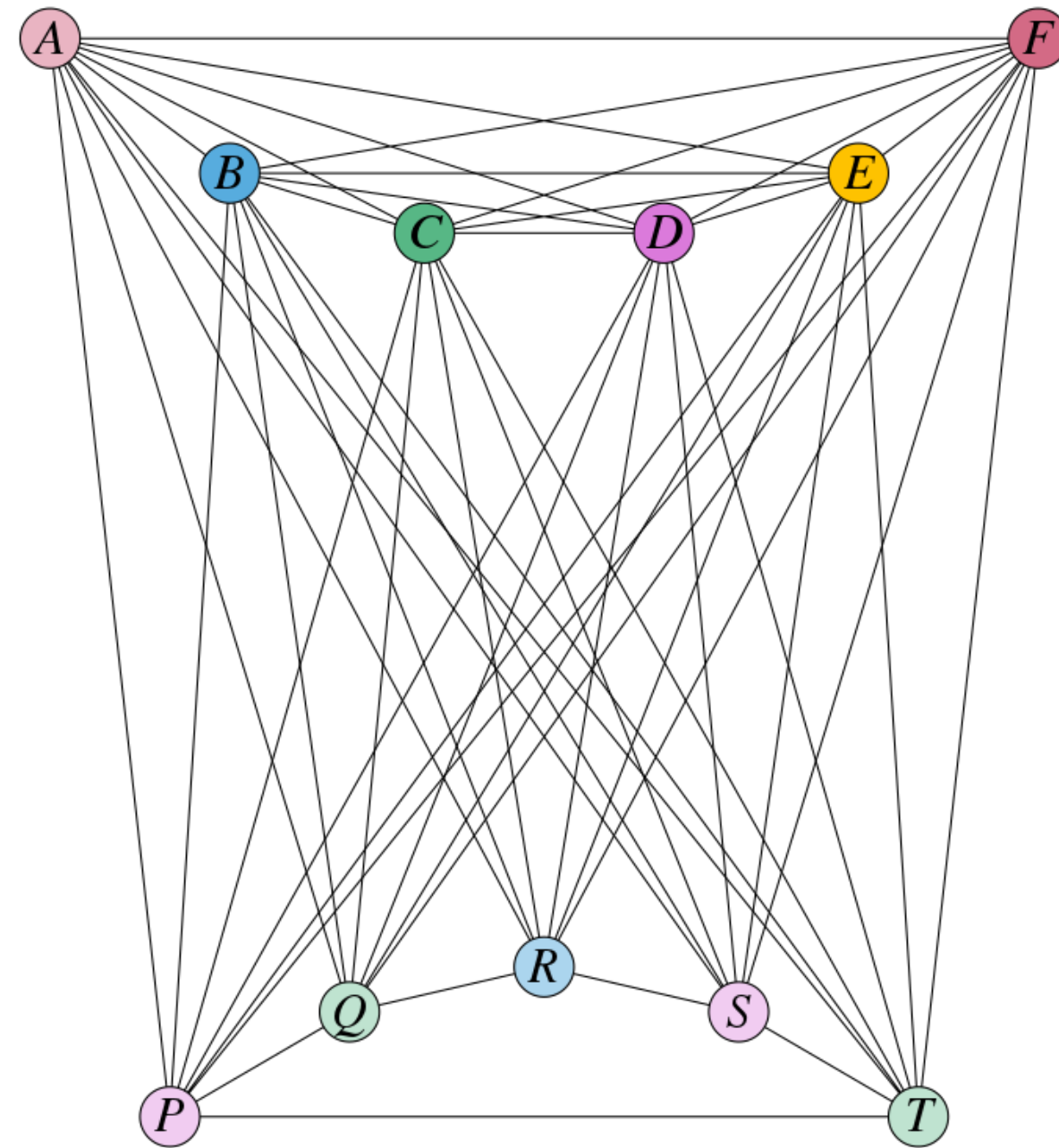


Kenneth Appel
Wolfgang Haken

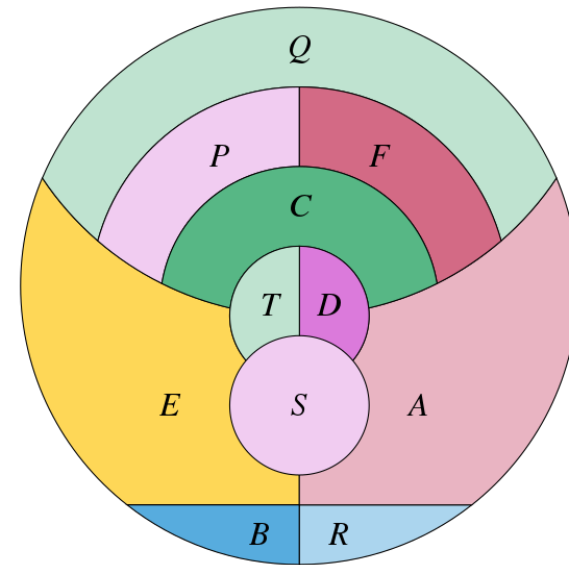


Gerhard Ringel

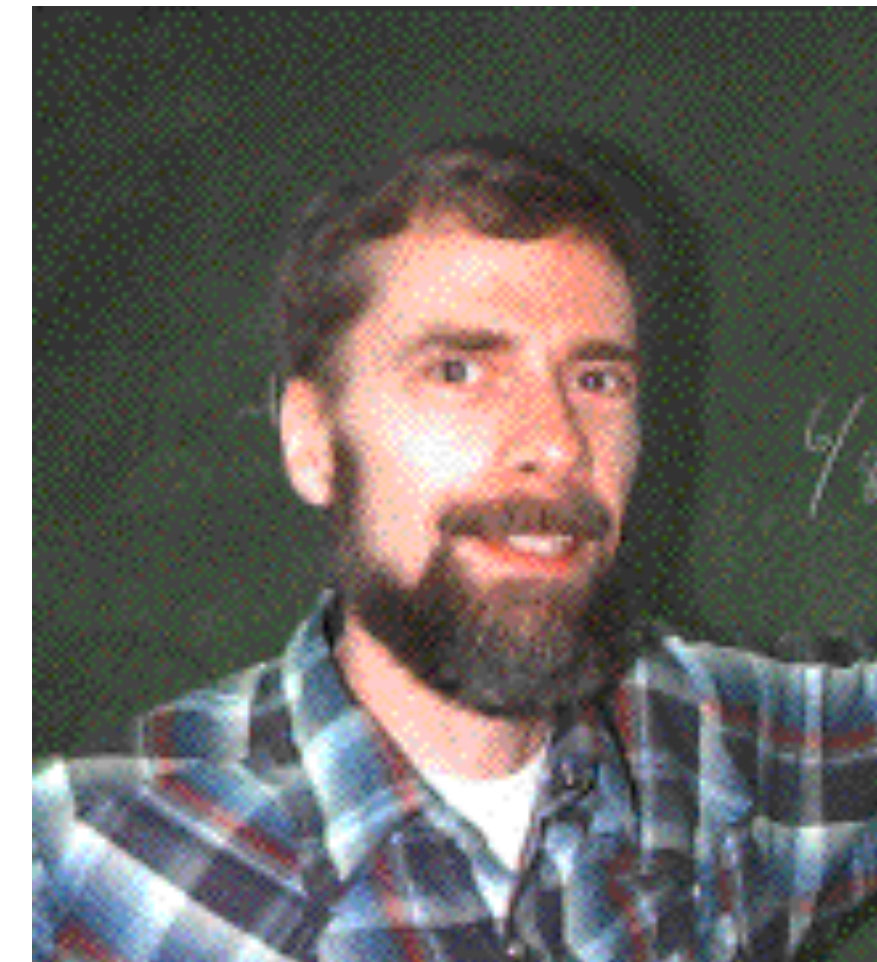
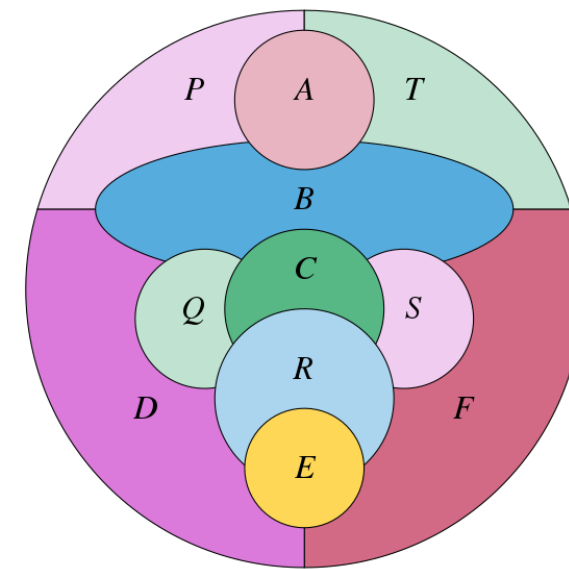
Sulanke's Graph



Moon



Earth

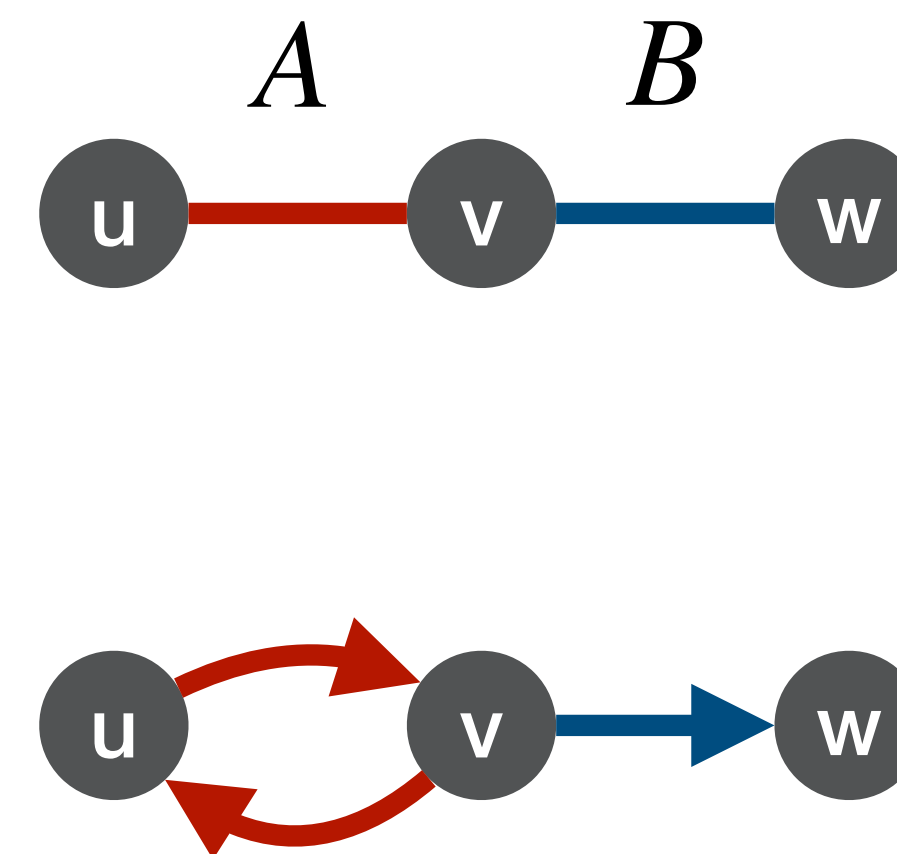


Thom Sulanke

- **Known:** answer lies between 9 and 12
9 is due to Sulanke [1973], 12 follows by Euler's formula.
Biplanar graph with 11 vertices that needs 9 colors, found 1973 by Sulanke.

Earth-Moon problem: encoding

- We encode the bipartition of the edge set $E = A \uplus B$ as a directed graph
- Developed a MinCheck variant for directed graphs
- Planarity of graphs A and B checked with Kuratowski's criterium
- non k -colorability checked by coloring clauses (consider all possible partitions of V into k color classes)
- feasible since n is small



Earth-Moon problem: results

n	# colors:	8	9	10	11	12	13
8		K_8					
9			K_9				
10			new	K_{10}			
11			Sulanke	new	K_{11}		
12				new	new	K_{12}	
13				new	new	new	K_{13}
14				open	open	open	

- Theorem: All biplanar graphs on $n \leq 13$ vertices are 9-colorable.

SMS for Hypergraphs

- **Hypergraphs:** reuse graph MinCheck by starting with a special ordered partition.
- Verified the *Erdős-Faber-Lovász Conjecture* [1072] for $n \leq 12$ and several cases of $13 \leq n \leq 18$.



Erdős



Faber



Lovász

	e_1	e_2	e_3	e_4
v_0	1	1	0	0
v_1	1	0	1	0
v_2	1	0	0	1
v_3	0	1	1	1

incidence matrix

	v_0	v_1	v_2	v_3	e_1	e_2	e_3	e_4
v_0	0	0	0	0	1	1	0	0
v_1	0	0	0	0	1	0	1	0
v_2	0	0	0	0	1	0	0	1
v_3	0	0	0	0	0	1	1	1
e_1	1	1	1	0	0	0	0	0
e_2	1	0	0	1	0	0	0	0
e_3	0	1	0	1	0	0	0	0
e_4	0	0	1	1	0	0	0	0

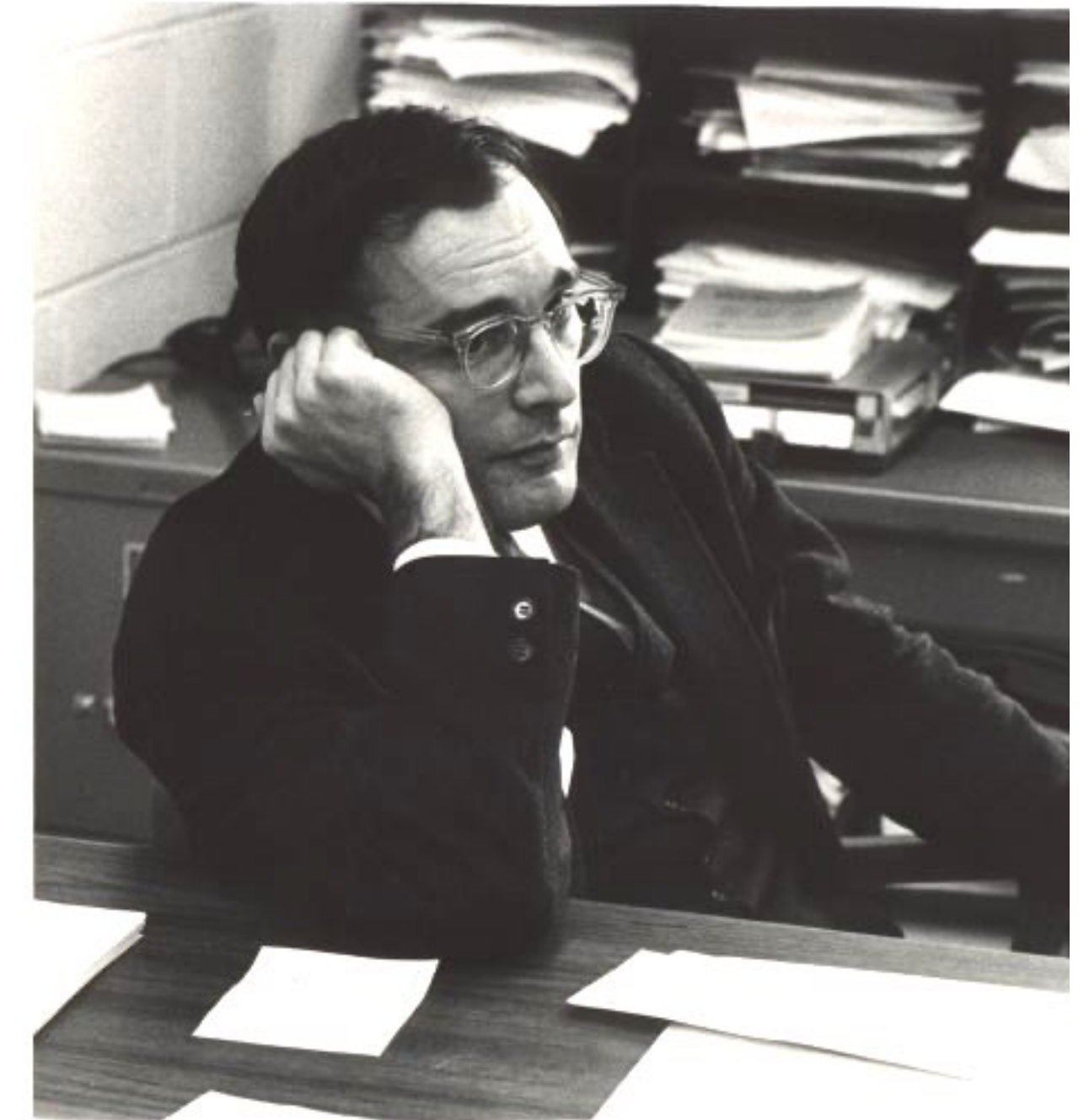
adjacency matrix of incidence graph

start with ordered partition
 $(\{v_0, v_1, v_2, v_3\}, \{e_1, e_2, e_3, e_4\})$

SMS for Matroids

- **Matroids:** we have developed a new variant of MinCheck for matroids of bounded rank.
- With SMS we could verify *Rota's Basis Conjecture* [1994] for matroids of rank 4 and matroids of rank 5 and girth 4.

[Kirchweger, Scheucher, Sz. 2022]



Gian Carlo Rota
(1932-1999)

Summary

- SMS provides a powerful framework for isomorph-free generation of combinatorial objects
- At its heart is an efficient algorithm that checks for certified non-canonicity of partially defined objects through an iterative refinement of ordered partitions
- Utilizes the power of modern CDCL SAT solver through the IPASIR-UP interface
- Generates DRAT proofs for independent verification
- Several applications: graphs (directed, undirected, planar), hypergraphs, and matroids of bounded rank.
- Better Minimality Check? CSP approach?
- Combine SMS with static symmetry breaking?
- SMS for QBF?

Thanks!

Tool <https://github.com/markirch/sat-modulo-symmetries/>

Documentation <https://sat-modulo-symmetries.readthedocs.io/>