Automated Reasoning in Discrete Geometry: Discovery, Verification, and Symmetry

Marijn J.H. Heule





ModRef 2025 in Glasgow

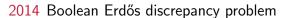
August 11, 2025

sat4math.com

50 Years of Successes in Computer-Aided Mathematics

1976 Four-Color Theorem

1998 Kepler Conjecture



2016 Boolean Pythagorean triples problem

2018 Schur Number Five

2019 Keller's Conjecture

2021 Kaplansky's Unit Conjecture

2022 Packing Number of Square Grid

2023 Empty Hexagon in Every 30 Points



50 Years of Successes in Computer-Aided Mathematics

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2014 Boolean Erdős discrepancy problem (using a SAT solver)

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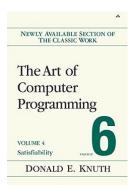
Breakthrough in SAT Solving in the Last 30 Years

Satisfiability (SAT) problem: Can a Boolean formula be satisfied?

mid '90s: formulas solvable with thousands of variables and clauses now: formulas solvable with millions of variables and clauses



Edmund Clarke: "a key technology of the 21st century" [Biere, Heule, vanMaaren, Walsh '09/'21]



Donald Knuth: "evidently a killer app, because it is key to the solution of so many other problems" [Knuth '15]

Introduction: Abstraction

Not all constraints are easy to encode into propositional logic

- ► Abstraction and refinement
- ► Underapproximation
- ► Satisfiability modulo theories

Solution: Only encode a subset of the problem

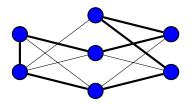
- Skip the constraints that are hard to encode
- If the subset is UNSAT, the full problem is UNSAT
- ► If an assignment that satisfies the subset also satisfies the full problem, then SAT
- Otherwise extend the subset (aka refinement)

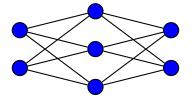
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Hamiltonian Cycles: Two Constraints

Hamiltonian Cycle Problem (HCP):

Does there exist a cycle that visits all vertices exactly once?

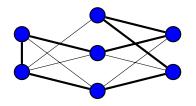


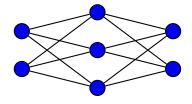


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Hamiltonian Cycles: Two Constraints

Hamiltonian Cycle Problem (HCP): Does there exist a cycle that visits all vertices exactly once?





Two constraints:

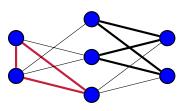
- Exactly two edges per vertex: easy cardinality constraints
- ▶ Exactly one cycle: hard to be compact and arc-consistent
 - ▶ One option is to ignore the constraint: incremental SAT.
 - ▶ Various encodings use $O(|V|^3)$. Too large for many graphs.
 - ► Effective encodings are quasi-linear in the number of edges.

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Hamiltonian Cycles: Refinement

Only encode: Exactly two edges per vertex

- ▶ Problem: Solutions can consist of multiple cycles
- ▶ How to implement refinement for a multi-cycle solution?

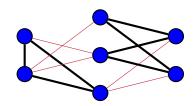


Block at least one subcycle

- ► E.g., block the smallest cycle
- Only a small number of cycles need to be blocked in practice

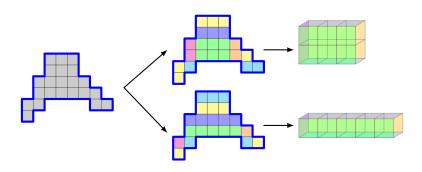
Constrain the cut edges

- At least 2 cut edges required
- Subcycles are an effective heuristic to pick the cut



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Common Unfolding Multiple Boxes



(Un)folding boxes along unit lines of polyominoes only

- ► Earlier works (non-SAT): Area ~ 90
- ► Earlier works (SAT full encoding): Area ~ 40
- ▶ Our encoding (SAT abstraction): Area ~ 180

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Common Unfoliding using Local Constraints [CADE'25]

- 1. Encode the existence of unfoldings as SAT formulas
- 2. Use efficient (local) under-approximations for encodings
- 3. UNSAT \rightarrow no unfoldings exist
- 4. SAT \rightarrow check satisfying assignments

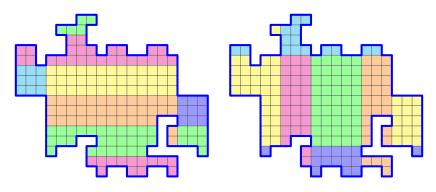


Figure: Common unfolding of $3\times3\times13$ and $3\times5\times9$

Introduction

Discrete Geometry

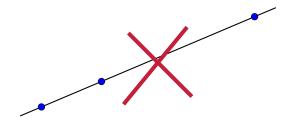
Orientation Variables and Symmetry

Empty Hexagon Number

Everywhere Unbalanced

Points in General Position

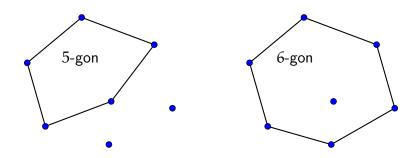
A finite point set S in the plane is in general position if no three points in S are on a line.



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Erdős-Szekeres Numbers

A k-gon (in S) is the vertex set of a convex k-gon



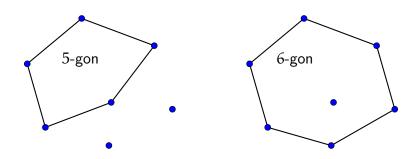
Theorem (Erdős & Szekeres 1935)

 $\forall k \in \mathbb{N}, \exists$ a smallest integer g(k) such that every set of g(k) points in general position contains a k-gon.

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Erdős-Szekeres Numbers

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Theorem (Erdős & Szekeres 1935)

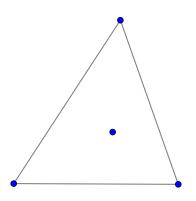
 $\forall k \in \mathbb{N}, \exists$ a smallest integer g(k) such that every set of g(k) points in general position contains a k-gon.

Is SAT solving suitable to answer such questions? Yes!

Bounds for Small k

Clearly, it takes exactly three points in general position to have a 3-gon (triangle)

Some sets of 4 points do not for a 4-gon:

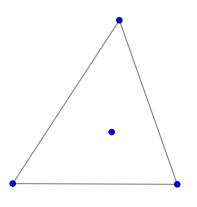


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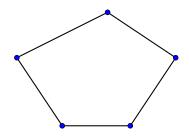
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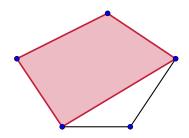
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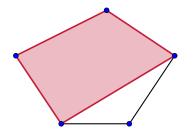
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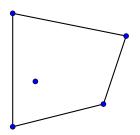


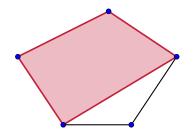
How many points imply a 4-gon?

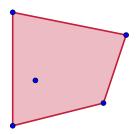


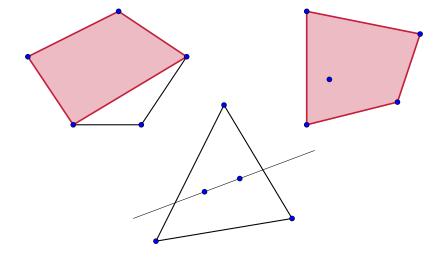




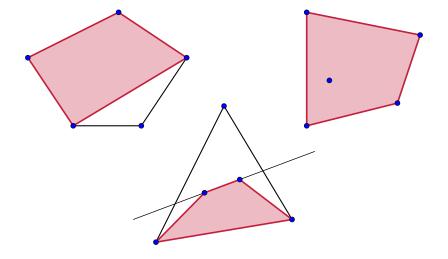




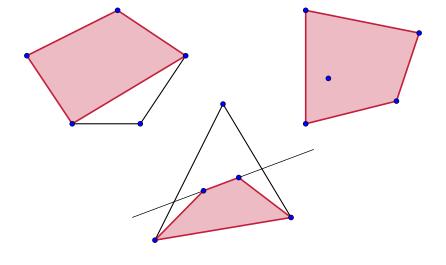




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Discrete Geometry 13 / 36

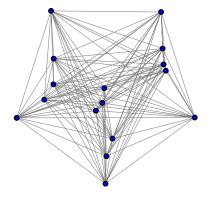


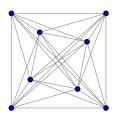
Happy ending problem

Bound Results for 5-Gon and 6-Gon

$$g(5) = 9$$

► [Kalbfleisch & Stanton '70]



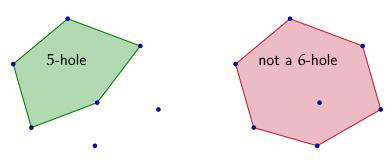


$$g(6) = 17$$

- ► Computer-assisted proof, 1500 CPU hours [SzekeresPeters '06]
- ➤ One CPU hour using a SAT solver [Scheucher '18]
- Only 10 seconds using new encoding

k-Holes

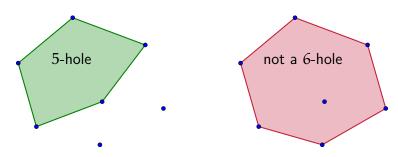
A k-hole (in S) is a k-gon containing no other points of S.



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k-Holes

A k-hole (in S) is a k-gon containing no other points of S.



Let h(k) denote the smallest number of points that contain a k-hole.

Erdős, 1970's: For k fixed, does every sufficiently large point set contain k-holes?

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k-Holes Overview

A k-hole (in S) is a k-gon containing no other points of S.

Erdős, 1970's: For k fixed, does every sufficiently large point set contain k-holes?

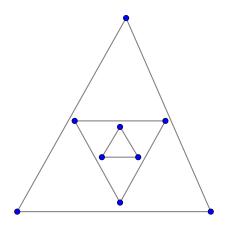
- ▶ 3 points $\Rightarrow \exists$ 3-hole
- ▶ 5 points $\Rightarrow \exists$ 4-hole
- ▶ 10 points $\Rightarrow \exists$ 5-hole [Harborth '78]
- ► Arbitrarily large point sets with no 7-hole [Horton '83]

Main open question: what about 6-hole?

- ▶ Lower bound of 30 [Overmars '02]
- Sufficiently large point sets contain a 6-hole [Gerken '08 and Nicolás '07, independently]

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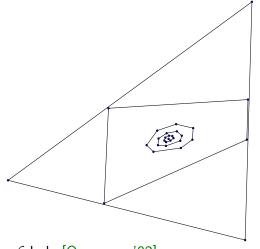
Lowerbound for 5-Hole: $h(5) \ge 10$



All 5-gons in these 9 points have an inner point: h(5) = 10

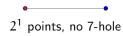
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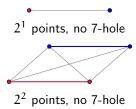
Lowerbound for 6-Hole: $h(6) \ge 30$

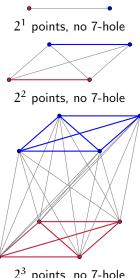


29 points, no 6-hole [Overmars '02]

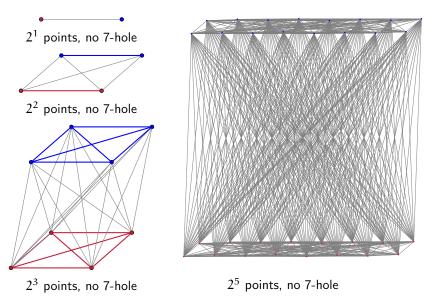
- ► Found using simulated annealing... is now easy using SAT
- ► This contains 7-gons. Each 9-gon contains a 6-hole







2³ points, no 7-hole



Discrete Geometry

Introduction

Discrete Geometry

Orientation Variables and Symmetry

Empty Hexagon Number

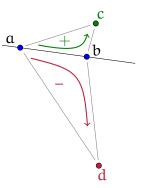
Everywhere Unbalanced

Orientation Variables [Knuth '92]

No explicit coordinates of points

Instead for every triple $\alpha < b < c$, one orientation variable O_{abc} to denote whether point c is above the line αb

Triple orientations are enough to express k-gons and k-holes

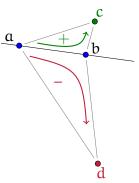


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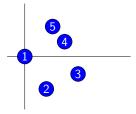
WLOG points are sorted from left to right

Not all assignments are realizable

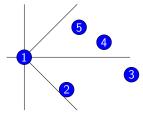
- ► Realizability is hard [Mnëv '88]
- ▶ Additional clauses eliminate many unrealizable assignments

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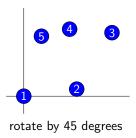
Symmetry Breaking: Sorted & Rotated Around Point 1



place leftmost point at origin

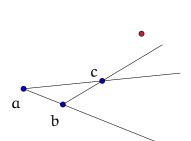


stretch points to the right to be within y = x and y = -x

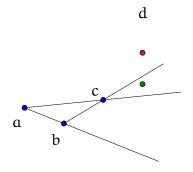


projective transformation $(x,y) \mapsto (y/(x+\epsilon),1/(x+\epsilon))$

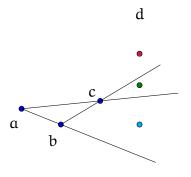
d



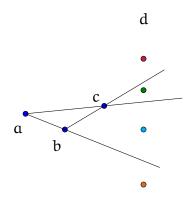
O_{abc}	O_{abd}	O_{acd}	O _{bcd}
+	+	+	+



O_{abc}	O_{abd}	O_{acd}	O_{bcd}
+	+	+	+
+	+	+	_

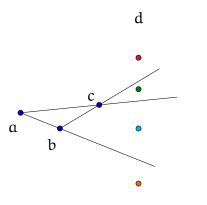


O_{abc}	O_{abd}	O_{acd}	O_{bcd}
+	+	+	+
+	+	+	_
+	+	_	_
+	+	_	_



Oabc	O_{abd}	O_{acd}	O_{bcd}
+	+	+	+
+	+	+	_
+	+	_	_
+	_	_	_

Under the assumption that points are sorted from left to right



$O_{\mathfrak{a}\mathfrak{b}\mathfrak{c}}$	$O_{abd} \\$	$O_{\alpha cd} \\$	O_{bcd}
+	+	+	+
+	+	+	_
+	+	_	_
+	_	_	_
_	_	_	_
_	_	_	+
_	_	+	+
_	+	+	+

Block multiple sign changes with $\Theta(n^4)$ (ternary) clauses

- $\blacktriangleright \ (\overline{O_{abc}} \lor O_{abd} \lor \overline{O_{acd}}) \land (O_{abc} \lor \overline{O_{abd}} \lor O_{acd})$
- $lackbox{(}\overline{O_{abc}}\lor O_{acd}\lor \overline{O_{bcd}})\land (O_{abc}\lor \overline{O_{acd}}\lor O_{bcd})$

Encoding Rotational Symmetry

Symmetric unavoidable polygons?

- ► No three points in a line
- ► Erdős-Szekeres 1935
- ▶ Avoid k-gon: at most 2^{k-2} points
- ► Happy Ending Problem
- ► Image from Wikipedia

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Encoding Rotational Symmetry

Symmetric unavoidable polygons?

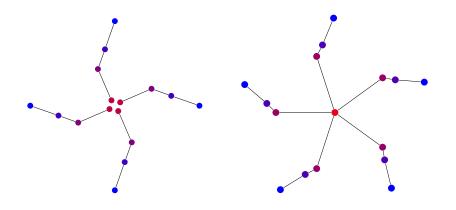
- ► No three points in a line
- ► Erdős-Szekeres 1935
- ▶ Avoid k-gon: at most 2^{k-2} points
- ► Happy Ending Problem
- ► Image from Wikipedia

Searching for k-rotational configurations is tricky:

- Points are no longer sorted from left to right
- More complicated axiom clauses
- Let $\pi(p)$ be the point after rotating p by $\frac{360}{k}$ degrees
- ▶ Variables O_{abc} and $O_{\pi(a)\pi(b)\pi(c)}$ are equivalent

Discrete Geometry

Two New, Symmetric Point Sets without Hexagons



Realized by the Localizer tool

▶ https://github.com/bsubercaseaux/localizer

Introduction

Discrete Geometry

Orientation Variables and Symmetry

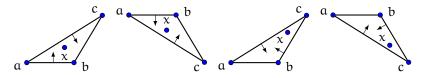
Empty Hexagon Number

Everywhere Unbalanced

Inside Variables

We introduce inside variables $I_{x;abc}$ which are true if and only if point x is in the triangle abc with a < x < b or b < x < c.

Four possible cases:

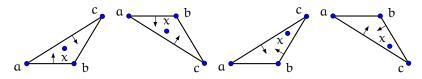


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Inside Variables

We introduce inside variables $I_{x;abc}$ which are true if and only if point x is in the triangle abc with a < x < b or b < x < c.

Four possible cases:



The left two cases with a < x < b:

$$I_{x;abc} \leftrightarrow \left(\left(O_{abc} \rightarrow (\overline{O_{axb}} \wedge O_{axc}) \right) \wedge \left(\overline{O_{abc}} \rightarrow (O_{axb} \wedge \overline{O_{axc}}) \right) \right)$$

The right two cases with b < x < c:

$$I_{x;abc} \leftrightarrow \left(\left(O_{abc} \rightarrow (O_{axc} \wedge \overline{O_{bxc}}) \right) \wedge \left(\overline{O_{abc}} \rightarrow (\overline{O_{axc}} \wedge O_{bxc}) \right) \right)$$

Hole Variables

We introduce hole variables H_{abc} which are true if and only if no points occur with the triangle abc with a < b < c.

$$\begin{array}{c} H_{abc} \vee \bigvee_{a < x < c} I_{x;abc} \\ \\ \bigwedge_{a < x < c} \overline{H_{abc}} \vee \overline{I_{x;abc}} \end{array} \qquad (\mathrm{redundant}) \end{array}$$

Hole Variables

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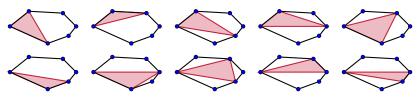
Simple 6-hole encoding:

$$\bigvee\nolimits_{\alpha,b,c\in X}\overline{H_{\alpha bc}} \quad \ \forall \ X\subset S \ \text{with} \ |X|=6$$

Given 6 points, how many empty triangles with these points guarantee an empty hexagon (possibly among other points)?

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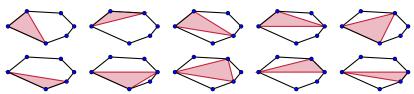
If the points may not be in convex position: 10



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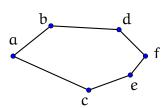
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If the points are in convex position:

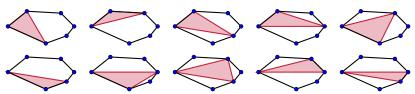
- Requires assignment to four orientation variables
- Includes info which points are above/below the line α to f



Discrete Geometry

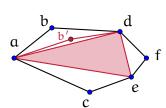
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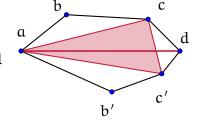
k-Hole Encoding Using $O(n^4)$ Clauses

Shorter clauses, thus more propagation, but still $O(n^6)$

Example

Introduce $O(n^3)$ auxiliary variables:

- $\begin{array}{c} \blacktriangleright \ A_{acd} \colon a \text{ 4-gon above the line } ad \\ \hline O_{abc} \land \overline{O_{bcd}} \to A_{acd} \\ \end{array}$
- ▶ $B_{ac'd}$: a 4-gon below the line ad $O_{ab'c'} \land O_{b'c'd} \rightarrow B_{ac'd}$
- Combine them to block 6-holes



$$\overline{A_{acd}} \vee \overline{B_{ac'd}} \vee \overline{H_{acc'}}$$

This reduces the size of the encoding to $O(n^4)$ clauses

Discrete Geometry

Comparison to Existing Work

Szekeres and Peters (2006) solved g(6) = 17 in 63 CPU days

- ► Roughly 40 CPU hours on today's hardware
- ▶ https://www.cpubenchmark.net/year-on-year.html

SAT solving, using the same abstraction, is much faster

- ▶ The independent SAT approaches by Marić and Scheucher required a few CPU hours
- lacktriangle Their encodings consist of $O(n^k)$ clauses

Our $O(n^4)$ encoding for k-gons and k-holes is even faster

- ▶ g(6) = 17 can be solved in 10 CPU seconds
- ▶ About 4 orders of magnitude faster than the original proof

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Verification

The optimization steps are validated or part of the proof

Concurrent solving and proof checking for the first time

- ▶ The solver pipes the proof to a verified checker
- ► This avoids storing/writing/reading huge files
- Verified checker can easily catch up with the solver

CMU students have formalized and verified all parts in Lean

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Introduction

Discrete Geometry

Orientation Variables and Symmetry

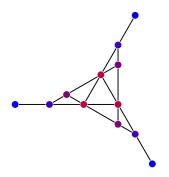
Empty Hexagon Number

Everywhere Unbalanced

Everywhere-Unbalanced Point Sets

Everywhere-unbalanced point sets:

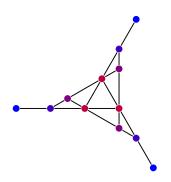
- ► For each line through 2+ points, unbalanced points by at least k
- ightharpoonup k = 1 is trivial (a triangle)
- ightharpoonup k = 2 with 12 points by Noga Alon
- Conjectured for every finite k
- Open: smallest odd configuration



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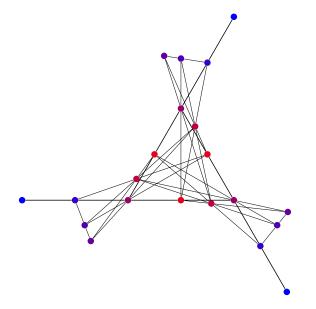


Encoding into SAT:

- ▶ Per triple: X_{abc} (c above ab) and Y_{abc} (c below ab)
- Constraints that enforce unbalancedness
- ► Also realizability constraints

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New, Optimal Result: 21 Points and 2-Unbalanced



Conclusions

Theorem

$$h(6) = 30$$

SAT appears to be the most effective technology to solve a range of problems in computational geometry

Many interesting open problems:

- ▶ Minimum number of 4-gons / 5-gons / 6-gons
- ▶ Determine whether g(7) = 33
- Unbalanced configurations (points can be collinear)

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