Automated Mathematical Discovery and Verification

Minimizing Pentagons in the Plane

Bernardo Subercaseaux, John Mackey, Marijn Heule, and Ruben Martins

Carnegie Mellon University





Automated Reasoning (CS) meets Math





Marijn Heule CMU CS

Ruben Martins CMU CS



Me CMU CS



John Mackey CMU Math



A mathematician's toolbox









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founded in 1964 by N. J. A. Sloane	
of Integer Sequences!)	Hints
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Cenchy Schwerz $\left(\sum_{i=1}^n u_i v_i
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ight) \left($ $\left({{\sum\limits_{i}^{n} {v_{i}^{2}} } }
ight)$



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page 1 <u>2 3 4 5 6 7 8 9 10</u> <u>45</u>
[*] n + 1. +20 805
, 25, 27, 29, 31, 33, 35, 37, 39, 41, 43, 45, 47, 49, 51, 75, 77, 79, 81, 83, 85, 87, 89, 91, 93, 95, 97, 99, 101, 9, 121, 123, 125, 127, 129, 131 (<u>list; graph; refs; listen;</u>

Cenchy Schwarz $\left(\sum_{i=1}^n u_i v_i
ight)^2 \leq \left(\sum_{i=1}^n u_i^2
ight) \left(\sum_{i=1}^n v_i^2
ight)$

Satisfiability $\in \mathcal{NP}$ $(x_1 \lor \neg x_2 \lor x_3) \land (x_1 \land (\neg x_1 \lor x_2) \land x_3)$

SAT Solvers?



 $(x_1 \lor x_4 \lor \overline{x_5}) \land (x_2 \lor \overline{x_3} \lor x_4) \land (\overline{x_1} \lor \overline{x_4}) \land (\overline{x_1} \lor \overline{x_2} \lor x_3)$

SAT Solvers

• Hyper-optimized programs for solving a single problem: **Boolean satisfiability**





$$(x_1 \lor x_4 \lor \overline{x_5}) \land (x_2 \lor \overline{x_3} \lor x_4) \land (\overline{x_1} \lor \overline{x_4}) \land (\overline{x_1} \lor \overline{x_2} \lor x_3)$$
$$x_1 = 0, \quad x_2 = 1, \quad x_3 = 1, \quad x_4 = 1, \quad x_5 = 0$$

SAT Solvers

• Hyper-optimized programs for solving a single problem: **Boolean satisfiability**





4

$$(\mathbf{x}_1 \lor \mathbf{x}_4 \lor \overline{\mathbf{x}_5}) \land (\mathbf{x}_2 \lor \overline{\mathbf{x}_3} \lor \mathbf{x}_4) \land (\overline{\mathbf{x}_1} \lor \overline{\mathbf{x}_4}) \land (\overline{\mathbf{x}_1} \lor \overline{\mathbf{x}_2} \lor \mathbf{x}_3)$$
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$$(\mathbf{x}_1 \lor \mathbf{x}_4 \lor \overline{\mathbf{x}_5}) \land (\mathbf{x}_2 \lor \overline{\mathbf{x}_3} \lor \mathbf{x}_4) \land (\overline{\mathbf{x}_1} \lor \overline{\mathbf{x}_4}) \land (\overline{\mathbf{x}_1} \lor \overline{\mathbf{x}_2} \lor \mathbf{x}_3)$$
$$x_1 = 0, \quad x_2 = 1, \quad x_3 = 1, \quad x_4 = 1, \quad x_5 = 0$$

• Because of NP-completeness, it can encode a variety of combinatorial problems!

SAT Solvers

• Hyper-optimized programs for solving a single problem: **Boolean satisfiability**













































































































```
def encode(clues):
```

```
Encode a sudoku puzzle as a SAT problem.
```

Parameters

clues : list of lists of ints 9x9 int matrix, non-zero values represent clues

Returns

model : eznf.Model

A SAT model representing the sudoku puzzle.

create vars for i in range(9): for j in range(9): for n in range(1, 10):

Z = modeler.Modeler() # modeler object from my library, always starts like this.

Z.add_var(f"x_{i, j, n}", description=f"Cell ({i}, {j}) gets number {n}")



exactly one number per cell for i in range(9): for j in range(9):

respect clues for i in range(9): for j in range(9): if clues[i][j] != 0: Z.constraint(f"x_{i, j, clues[i][j]}")

exactly-one constraints for n in range(1, 10): # rows for i in range(9): Z.exactly_one([f"x_{i, j, n}" for j in range(9)])

cols for j in range(9): Z.exactly_one([f"x_{i, j, n}" for i in range(9)])

sub_grids sub_grids = [[[] for sj in range(3)] for si in range(3)] for i in range(9): for j in range(9): sub_grids[i//3][j//3].append((i, j)) for si in range(3): for sj in range(3): Z.exactly_one([f"x_{*cell, n}" for cell in sub_grids[si][sj]])

Z.exactly_one([f"x_{i, j, n}" for n in range(1, 10)])



SAT Solvers in Math Some success stories:

- (2016) Boolean Pythagorean Triples
- (2018) Schur Number 5
- (2019) Keller's Conjecture
- (2023) Packing Chromatic Number of the Grid
- (2024) An Empty Hexagon in every 30 points



• (2014) Boolean Erdős Discrepancy Problem



SAT Solvers in Math Some success stories:

These all follow a common pattern:

Using SAT solvers to tackle a hard combinatorial problem that brute force computation (i.e., backtracking) would take forever on



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These all follow a common pattern:

Using SAT solvers to tackle a hard combinatorial problem that brute force computation (i.e., backtracking) would take forever on

• (2024) An Empt

Today we will talk about a different use:

SAT solvers can be used at different stages of mathematical research; to build examples, get ideas and ellicit conjectures.

y Hexagon in every 30 points



























N	$\mu_5(N)$
4	0
8	0





N	$\mu_5(N)$
4	0
8	0
9	





N	$\mu_5(N)$
4	0
8	0
9	1





N	$\mu_5(N)$
4	0
8	0
9	1
15	





N	$\mu_5(N)$
4	0
8	0
9	1
15	77





How many points without 3 on a line guarantee a **convex quadrilateral**?









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Answer: 5, Klein, "Happy Ending Theorem"





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Case 3: 3 points in Convex Hull





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Insight: we can reason by cases in terms of which points are above or below lines formed by other points!





Combinatorial Structure: Triple Orientations





Combinatorial Structure: Triple Orientations



$\sigma(a, b, c) = \text{true}$ $\begin{bmatrix} a_x & b_x & c_x \\ a_y & b_y & c_y \end{bmatrix} > 0$





Szekeres and Peters: 8 cases for convex pentagons







Szekeres and Peters: 8 cases for a convex pentagon Encoding Example: ea $\neg \sigma(a, b, d) \land \neg \sigma(b, d, e) \land \sigma(a, c, e)$





Szekeres and Peters: 8 cases for a convex pentagon Encoding Example: $\neg \sigma(a, b, d) \land \neg \sigma(b, d, e) \land \sigma(a, c, e)$ ea

So to forbid that pentagon in one clause we do

 $\sigma(a, b, d) \lor \sigma(b, d, e) \lor \neg \sigma(a, c, e)$





We just said:



$\neg \sigma(a, b, d) \land \neg \sigma(b, d, e) \land \sigma(a, c, e)$





We just said:



Question: is the converse **----** also true?

$\neg \sigma(a, b, d) \land \neg \sigma(b, d, e) \land \sigma(a, c, e)$





We just said:



Question: is the converse **----** also true?

Not necessarily! We don't know if a σ -assignment corresponds to an actual pointset !

$\neg \sigma(a, b, d) \land \neg \sigma(b, d, e) \land \sigma(a, c, e)$





SAT algorithm that minimize falsified clauses by flipping variables. No guarantees!

Stochastic Local Search





We add, for each ordered five tuple (a, b, c, d, e), the 8 clauses that forbid the (mutually exclusive) different ways those points could form a convex pentagon

Stochastic Local Search

SAT algorithm that minimize falsified clauses by flipping variables. No guarantees!





We add, for each ordered five tuple (a, b, c, d, e), the 8 clauses that forbid the (mutually exclusive)

Number of falsified clauses \approx Number of convex pentagons*

Stochastic Local Search

SAT algorithm that minimize falsified clauses by flipping variables. No guarantees!

different ways those points could form a convex pentagon



Stochastic Local Search Results

Ν	Best	Time
9	1	0.00 s
10	2	0.00 s
11	7	0.00 s
12	12	0.00 s
13	27	0.01 s
14	42	0.01 s
15	77	0.01 s
16	112	0.02 s

Note: these are not necessarily optimal

Ν	Best	Time
23	1254	12 s
24	1584	472 s
25	2079	64 s
26	2574	5269 s
27	3289	1556 s
28	4004	1792 s
29	5005	467 s
30	6007	18244 s



We would like to know:

$$c_5 = \lim_{N \to \infty} \frac{\mu_5(N)}{\binom{N}{5}}$$



We would like to know:

$$c_{5} = \lim_{N \to \infty} \frac{\mu_{5}(N)}{\binom{N}{5}}$$
$$\hat{c}_{5}(N) = \frac{\mu_{5}(N)}{\binom{N}{5}}$$





Best	$\hat{c}_5(N)$
1	0.007936
2	0.007936
7	0.015151
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```
In[67]:= (*Define the points*)
      points = {\{10, 2\}, \{12, 12\}, \{14, 42\}, \{16, 112\}, \{18, 252\}, \{20, 504\}, \{22, 924\},
          {24, 1584}};
       (*Compute the interpolating polynomial of degree 5*)
      poly = InterpolatingPolynomial[points, n];
       (*Simplify the polynomial to make it easier to read*)
      simplifiedPoly = Simplify[poly];
       (*Display the simplified polynomial*)
      simplifiedPoly
      n(384 - 400 n + 140 n^2 - 20 n^3 + n^4)
Out[70]=
                      1920
                      n (384 – 400 n + 140 n<sup>2</sup>
In[71]:= FullSimplify
                                     1920
       (-8+n) \times (-6+n) \times (-4+n) \times (-2+n) n
Out[71]=
                        1920
```



Out[71]=
$$\frac{(-8 + n) \times (-6 + n)}{\ln[72] = \text{Binomial}[n, 5]}$$

Out[72]= $\frac{1}{120} \times (-4 + n) \times (n)$

 $n) \times (-4 + n) \times (-2 + n) n$ 1920

$(-3 + n) \times (-2 + n) \times (-1 + n) n$



Out[71]=
$$\frac{(-8+n) \times (-6+n) \times (-4+n) \times (-2+n) n}{1920}$$

In[72]:= Binomial[n, 5]

n

5

Out[72]=
$$\frac{1}{120} \times (-4 + n) \times (-3 + n) \times (-2 + n) \times (-1 + n) n$$

$$= \frac{n \cdot (n-1) \cdot (n-2) \cdot (n-3) \cdot (n-4)}{120}$$

$$= \frac{2n \cdot (2n-2) \cdot (2n-4) \cdot (2n-6) \cdot (2n-8)}{120 \cdot 32}$$

$$= \frac{2n \cdot (2n-2) \cdot (2n-4) \cdot (2n-6) \cdot (2n-8)}{\mu(2n)}$$

$$\frac{n \cdot (n-1) \cdot (n-2) \cdot (n-3) \cdot (n-4)}{120}$$

$$\frac{2n \cdot (2n-2) \cdot (2n-4) \cdot (2n-6) \cdot (2n-8)}{120 \cdot 32}$$

$$\frac{2n \cdot (2n-2) \cdot (2n-4) \cdot (2n-6) \cdot (2n-8)}{\mu(2n)} - \mu(2n)$$

$$\frac{n \cdot (n-1) \cdot (n-2) \cdot (n-3) \cdot (n-4)}{120}$$

$$\frac{2n \cdot (2n-2) \cdot (2n-4) \cdot (2n-6) \cdot (2n-8)}{120 \cdot 32}$$

$$2n \cdot (2n-2) \cdot (2n-4) \cdot (2n-6) \cdot (2n-8) - \widehat{\mu(2n)}$$

 $2 \cdot 1920$



2

$$I = \frac{(-8+n) \times (-6+n) \times (-4+n) \times (-2+n) n}{1920}$$

$$2I = Binomial[n, 5]$$

$$2I = \frac{1}{120} \times (-4+n) \times (-3+n) \times (-2+n) \times (-1+n)$$

$$I = \frac{n \cdot (n-1) \cdot (n-2) \cdot (n-3) \cdot (n-4)}{120}$$

$$= \frac{2n \cdot (2n-2) \cdot (2n-4) \cdot (2n-6) \cdot (2n-8)}{120 \cdot 32}$$

$$= \frac{2n \cdot (2n-2) \cdot (2n-4) \cdot (2n-6) \cdot (2n-8)}{2 \cdot 1920} = \frac{\widehat{\mu(2n)}}{2}$$

Out[71]=
$$\frac{(-8+n) \times (-6+n) \times (-4+n) \times (-2+n) n}{1920}$$

In[72]= Binomial[n, 5]
Out[72]=
$$\frac{1}{120} \times (-4+n) \times (-3+n) \times (-2+n) \times (-1+n) \times (-1+n)$$

$$\begin{aligned} \text{ut[71]} &= \frac{(-8+n) \times (-6+n) \times (-4+n) \times (-2+n) \text{ n}}{1920} \\ \text{n[72]:= Binomial[n, 5]} \\ \text{ut[72]= } \frac{1}{120} \times (-4+n) \times (-3+n) \times (-2+n) \times (-1+n) \\ \text{ut[72]= } \frac{1}{120} \times (-4+n) \times (-3+n) \times (-2+n) \times (-1+n) \\ \text{Issuer} \\ \text{Idea!} \end{aligned}$$

$$= \frac{n \cdot (n-1) \cdot (n-2) \cdot (n-3) \cdot (n-4)}{120} \\ = \frac{2n \cdot (2n-2) \cdot (2n-4) \cdot (2n-6) \cdot (2n-8)}{120 \cdot 32} \\ = \frac{2n \cdot (2n-2) \cdot (2n-4) \cdot (2n-6) \cdot (2n-8)}{2 \cdot 1920} = \frac{\widehat{\mu(2n)}}{2} \end{aligned}$$

$$\frac{(-8+n) \times (-6+n) \times (-4+n) \times (-2+n) n}{1920}$$
= Binomial[n, 5]
= $\frac{1}{120} \times (-4+n) \times (-3+n) \times (-2+n) \times (-1+1) \times (-4+n) \times (-4+n) \times (-3+n) \times (-2+n) \times (-1+1) \times (-4+n) \times (-3+n) \times (-2+n) \times (-1+1) \times (-4+n) \times (-2+n) \times (-4+n) \times (-4+n) \times (-2+n) \times (-4+n) \times (-4$

$$\frac{(-8+n) \times (-6+n) \times (-4+n) \times (-2+n) n}{1920}$$

Binomial[n, 5]

$$\frac{1}{120} \times (-4+n) \times (-3+n) \times (-2+n) \times (-1+1) \times (-1+1) \times (-4+n) \times (-3+n) \times (-2+n) \times (-1+1) \times (-1+1) \times (-4+n) \times (-3+n) \times (-2+n) \times (-1+1) \times (-1+1) \times (-4+n) \times (-3+n) \times (-2+n) \times (-1+1) \times (-1+1) \times (-4+n) \times (-3+n) \times (-2+n) \times (-1+1) \times (-2+n) \times (-2+$$





How do these solutions look like?

We need to solve the **Realizability** problem ($\exists \mathbb{R}$ complete): Given a set of orientations, can they all be *realized* by a configuration of points in the plane

(Only available at the in-person talk, sorry)



How do these solutions look like?

We need to solve the **Realizability** problem ($\exists \mathbb{R}$ complete): Given a set of orientations, can they all be *realized* by a configuration of points in the plane

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How do these solutions look like?







Generalize them as constructions!

10







Generalize them as constructions!



Pinwheel



Parabolic



General Upper Bound





 $\mu_5(N) \le \binom{\lfloor n/2 \rfloor}{5} + \binom{\lceil n/2 \rceil}{5}$



General Upper Bound







 $\mu_5(N) \le \binom{\lfloor n/2 \rfloor}{5} + \binom{\lceil n/2 \rceil}{5}$



General Upper Bound



We conjecture this bound to be tight! (\$500)



$$\leq \binom{\lfloor n/2 \rfloor}{5} + \binom{\lceil n/2 \rceil}{5}$$







We need to be careful though!



$$i, 2 + rac{i^2}{n^2}
ight), orall i \in \left[\left\lfloor rac{n}{2}
ight
floor
ight] \quad ext{and} \quad p_i^\perp = \left(i, -2 - rac{i^2}{n^2}
ight), orall i \in \left[\left\lceil rac{n}{2}
ight
ceil
ight]$$



Remember something odd?

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9	1	0.007936
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Inspired Math Idea!



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Theorem: Odd-Even

If the conjecture holds for 2N+1,

Then it must hold for 2N+2





A major benefit of SAT (or its optimization variant MaxSAT) is the community emphasis on verification

MaxSAT Verification





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MaxSAT Verification

We generate independently-checkable proofs for the optimal bounds up to N = 15





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Therefore we verify the conjecture up to N = 16:

MaxSAT Verification

We generate independently-checkable proofs for the optimal bounds up to N = 15





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