When Algorithms Learn:
Discrete Optimization Meets Machine Learning

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Mathematical Modelling, Simulation and Optimization (Gas Networks)

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SFB TRR 154

ZUSE INSTITUTE BERLIN

Berlin Mathematics Research Center MATH+

What is this talk about?

Introduction

A personal, highly-biased, and incomplete take of what AI can do in Mathematics et al.

Why? AI methods increasingly shape how scientific discovery is performed, configured, and accelerated.

Today: Two (three-ish) recent use-cases / perspectives from my own work.

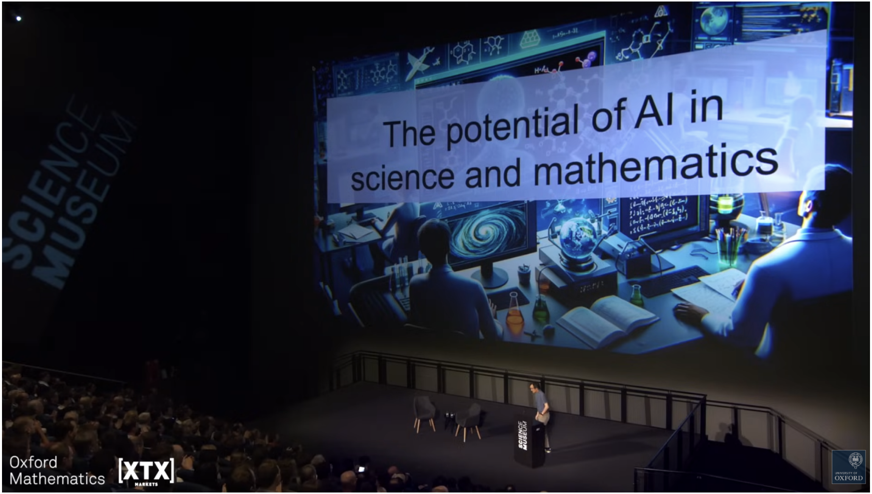
Outline

- A bit of high-level perspective
- Agentic AI Researcher framework
- Neural Colorings of the plane

(Hyperlinked) References are not exhaustive; check references contained therein.

What is this talk about?

AI and Mathematics et al



[The Potential for AI in Science and Mathematics - Terence Tao]

What is this talk about?

AI and Mathematics et al

Various levels of co-creation. [Haase and Pokutta, 2026]

- **Digital Pen**: basically like autocorrect, bibtex lookup, etc. “2000s”
- **AI Task Specialist**: ChatGPT, Claude, Gemini, etc. 2022 - 2025
- **AI Assistant**: Agents with integrated tools, verification, etc. 2025 -
- **AI Co-creator**: Fully integrated, autonomous, co-creator 2027(??) -

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Broadly. Two categories: (a) co-creation agent and (b) tool in larger system.

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Capabilities are impressive but unstable:

- SOTA models achieve post-PhD level scores on benchmarks, yet in day-to-day use make trivial (logical) errors.
- No hard verification of results and randomness across runs.
- Prompting and scaffolding are still a challenge.
- Availability of tools for verification etc crucial.

What is this talk about?

Mathematics with computers is not new

Various high-profile examples from the past.

- Four Color Theorem: massive computer-based case checking

  [Appel and Haken, 1977, Robertson et al., 1997]

- Kepler Conjecture / Hales’ Theorem: extensive computer verification

  [Hales et al., 2017]

- Classification of Finite Simple Groups: Formal verification with Lean/Coq
- Boolean Pythagorean Triples Problem: A spectacular 200TB SAT-solver proof.

  [Heule et al., 2016]

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Crucial role in computational mathematics / scientific computing

- Finite Elements
- Numerical Simulations
- Optimization
- Engineering
- ...

The Agentic Researcher

A Practical Guide to AI-Assisted Research
in Mathematics and Machine Learning

joint work with: Max Zimmer, Nico Pelleriti, Christophe Roux

preprint (2026)
https://arxiv.org/abs/2603.15914

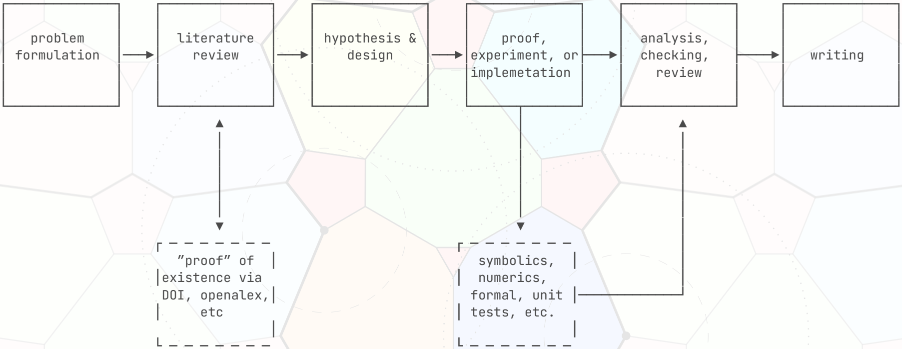
Partially supported by ExC MATH+ Project EF-LiOpt-3
Agent AI in Mathematics

[Zimmer et al., 2026, Pokutta, 2026]

AI in the Scientific Discovery Workflow

The agentic researcher framework

AI systems can be used at almost any stage of the scientific workflow.



(workflow simplified. for illustration only.)

Note. The researcher needs to be in charge and responsible(!!) throughout.

Building a practical tool

The agentic researcher framework

```
Let me now wait for the final check:

● Task Output bwzs8ty88
  1-hour mid-training status check
      Waiting for task (esc to give additional instructions)

* Gitifying… (8h 39m 19s · ↓ 39.3k tokens · thought for 20s)
└ Tip: Run /install-github-app to tag @claude right from your Github issues and PRs
──────────────────────────────────────────────────────────────────────────────────
Background tasks
10 active shells

› sleep 2700 &&echo "≡ Final completion check ≡" &&python3 << 'PYEOF'…   (running)
  sleep 3600 &&echo "≡ 1h mid-training ≡" &&python3 -c "…   (running)
  sleep 5400 &&echo "≡ Final completion check ≡" &&for exp in E023_no_nor…   (running)
  source ~/.bashrc &&CUDA_VISIBLE_DEVICES=6 uv run torchrun --standalone --npr…   (running)
  source ~/.bashrc &&CUDA_VISIBLE_DEVICES=5 uv run torchrun --standalone --npr…   (running)
  source ~/.bashrc &&CUDA_VISIBLE_DEVICES=4 uv run torchrun --standalone --npr…   (running)
  source ~/.bashrc &&CUDA_VISIBLE_DEVICES=3 uv run torchrun --standalone --npr…   (running)
  source ~/.bashrc &&CUDA_VISIBLE_DEVICES=2 uv run torchrun --standalone --npr…   (running)
  source ~/.bashrc &&CUDA_VISIBLE_DEVICES=1 uv run torchrun --standalone --npr…   (running)
```

Screenshot from a run of the framework.

- Born out of the MATH+ project *Agentic AI in Mathematics*.
- Refined over roughly 1.5 years of day-to-day research use.
- Sandboxed CLI agents with project instructions, tools, Git, LaTeX, and GPU-backed experiments.
- Puts a premium on verification: record everything, verify citations, and verify before claiming.

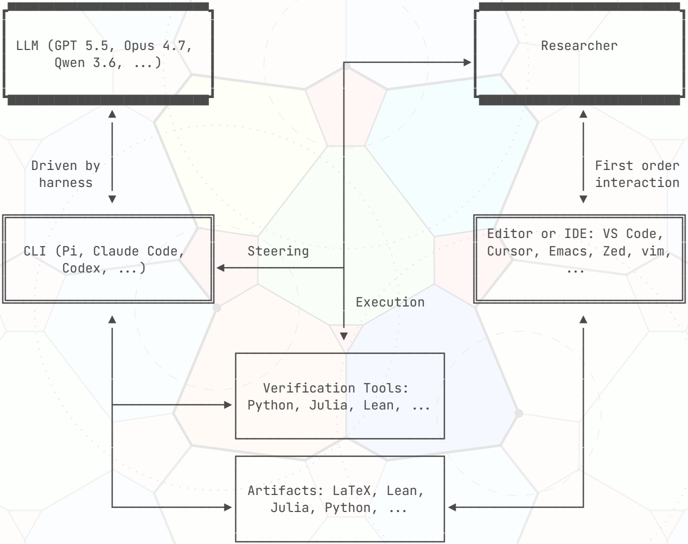
[blog post] [arXiv] [GitHub]

Does it works? Several real-world use-cases in paper

1. Convergence lower bounds for Frank-Wolfe on uniformly convex sets
2. Multi-Variable Dual Tightening for Boscia.jl for MINLPs
3. Weight Reconstruction in LLM pruning
4. ...

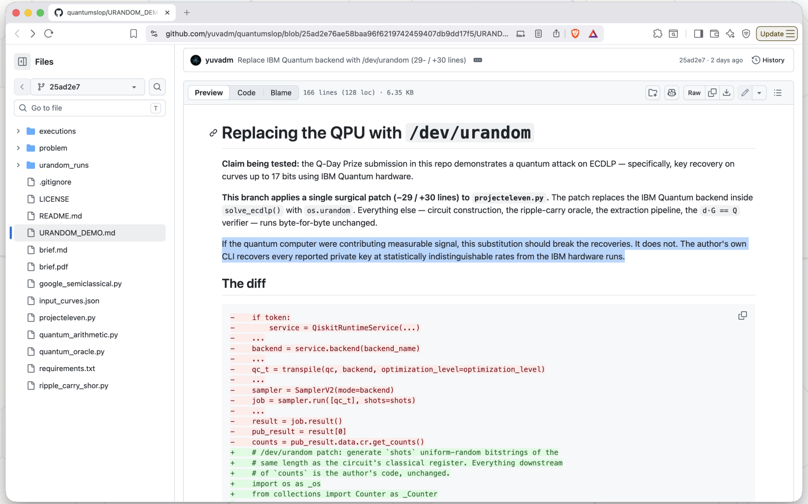
Interacting with the System

The agentic researcher framework



Why Verification is Crucial

The agentic researcher framework



Replacing the QPU with `/dev/urandom`

Claim being tested: the Q-Day Prize submission in this repo demonstrates a quantum attack on ECDLP — specifically, key recovery on curves up to 17 bits using IBM Quantum hardware.

This branch applies a single surgical patch (−29 / +30 lines) to `projecteleven.py`. The patch replaces the IBM Quantum backend inside `solve_ecdlp()` with `os.urandom`. Everything else — circuit construction, the ripple-carry oracle, the extraction pipeline, the `d·G == Q` verifier — runs byte-for-byte unchanged.

If the quantum computer were contributing measurable signal, this substitution should break the recoveries. It does not. The author's own CLI recovers every reported private key at statistically indistinguishable rates from the IBM hardware runs.

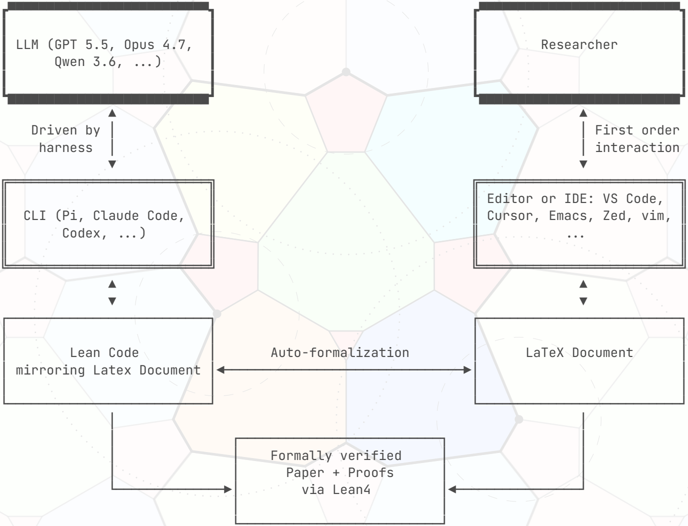
The diff

```
-    if token:
-        service = QiskitRuntimeService(...)
-    ...
-    backend = service.backend(backend_name)
-    ...
-    qc_t = transpile(qc, backend, optimization_level=optimization_level)
-    ...
-    sampler = SamplerV2(mode=backend)
-    job = sampler.run([qc_t], shots=shots)
-    ...
-    result = job.result()
-    pub_result = result[0]
-    counts = pub_result.data.cr.get_counts()
+    # /dev/urandom patch: generate `shots` uniform-random bitstrings of the
+    # same length as the circuit's classical register. Everything downstream
+    # of `counts` is the author's code, unchanged.
+    import os as _os
+    from collections import Counter as _Counter
```

[GitHub Repository]

End-2-End Formal Verification with Lean 4

The agentic researcher framework



When generation is cheap, verification is everything.

[Pokutta, 2026]

The Hadwiger-Nelson Problem

joint work with: Aldo Kiem, Konrad Mundinger,
Christoph Spiegel, Max Zimmer

ICML 2025 (oral)
https://arxiv.org/abs/2404.05509

Partially supported by ExC MATH+ Project EF-LiOpt-3

Agent AI in Mathematics

[Mundinger et al., 2025]

The Hadwiger-Nelson Problem

Problem (Nelson 1950, also: Gardner, Moser, Erdős, Harary, Tutte, ...)

What is the smallest number of colors sufficient for coloring the plane in such a way that no two points of the same color are at a unit distance apart?

Infinite graph with vertex set $\mathbb{E}^2$ and edges $\{x, y\}$ for any $x, y \in \mathbb{E}^2$ with $\|x - y\| = 1$

$\Rightarrow$ chromatic number of the plane $\chi(\mathbb{E}^2)$

Theorem

Assuming Axiom of Choice (AoC): [Bruijn and Erdos, 1951]

Any graph is k-colorable iff every finite subgraph of it is k-colorable.

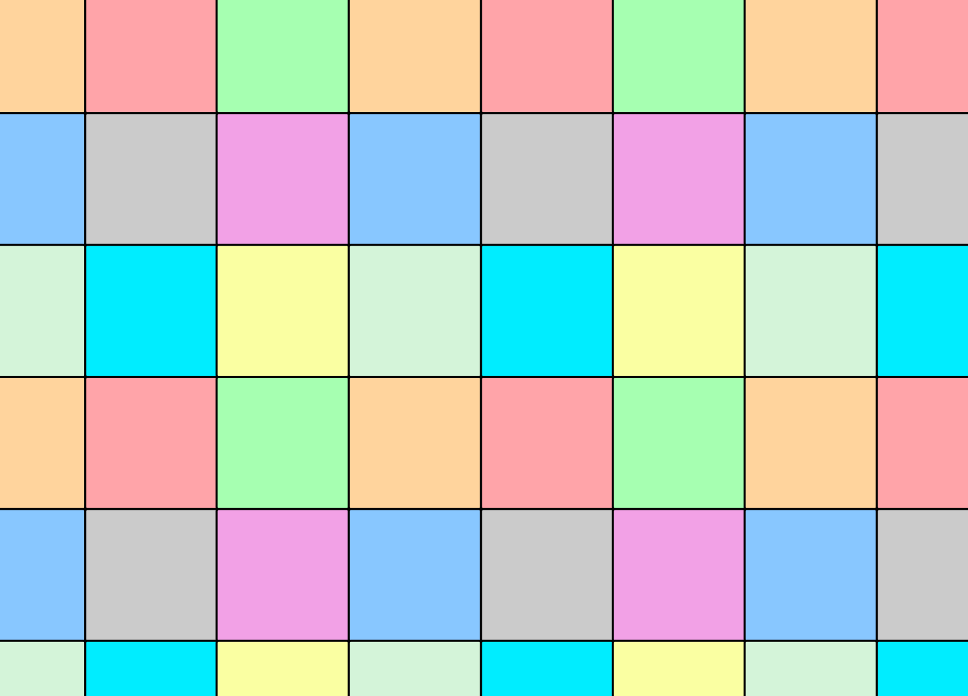
This problem has a long and complicated history... over 14 pages in [Soifer, 2024]

Upper bounds through colorings

The Hadwiger-Nelson Problem

Explicit colorings $g : \mathbb{E}^2 \to [c] := \{1, \ldots, c\}$, usually derived through tesselations using simple polytopal shapes, give

$$5 \leq \chi(\mathbb{E}^2) \leq \ldots$$



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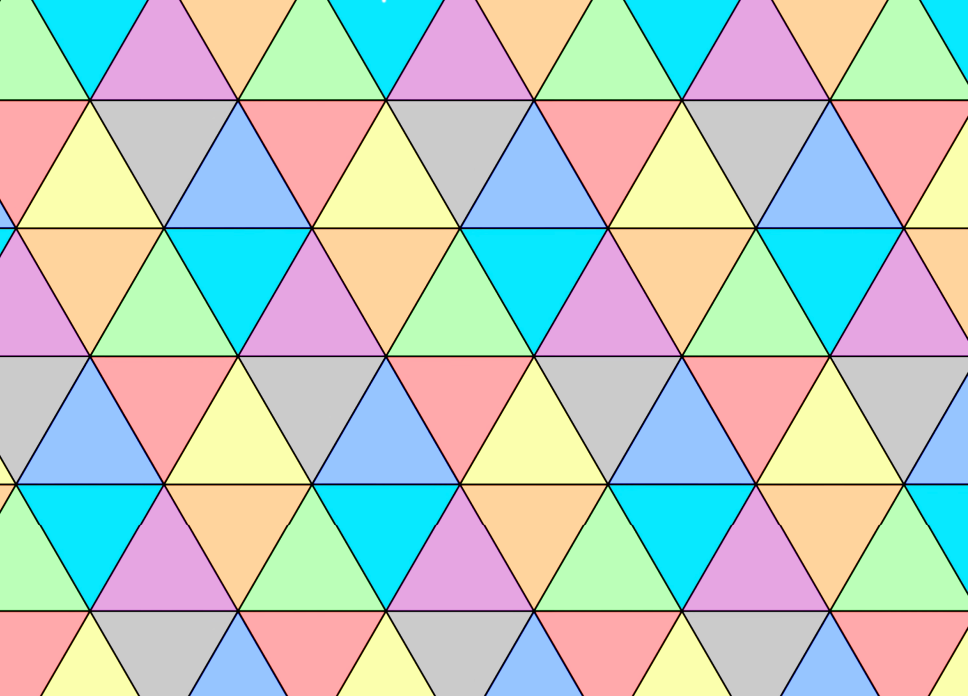
$$5 \leq \chi(\mathbb{E}^2) \leq 9.$$



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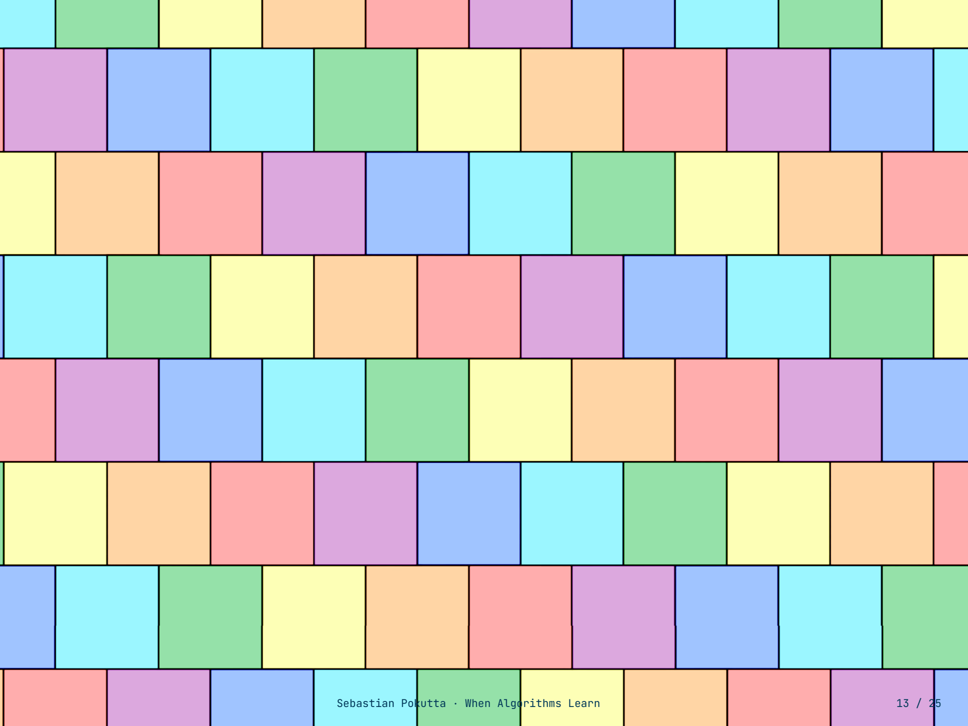
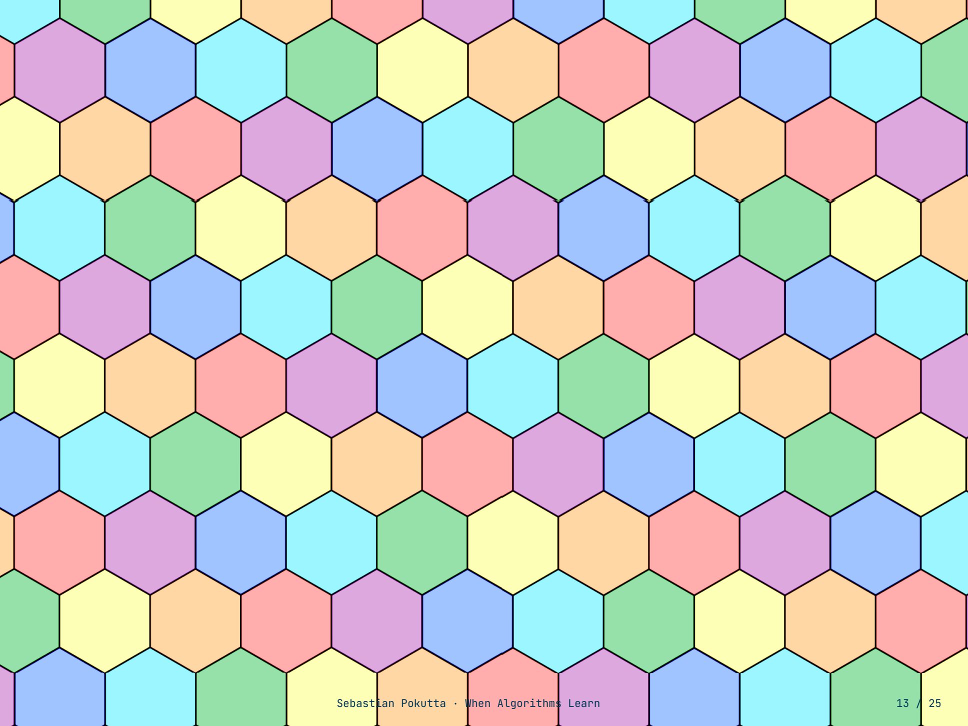
Explicit colorings $g : \mathbb{E}^2 \to [c] := \{1, \ldots, c\}$, usually derived through tesselations using simple polytopal shapes, give

$$5 \leq \chi(\mathbb{E}^2) \leq 8.$$





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Explicit colorings $g : \mathbb{E}^2 \to [c] := \{1, \ldots, c\}$, usually derived through tesselations using simple polytopal shapes, give

$$5 \leq \chi(\mathbb{E}^2) \leq 7.$$

Upper bounds through colorings

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Explicit colorings $g : \mathbb{E}^2 \to [c] := \{1, \dots, c\}$, usually derived through tesselations using simple polytopal shapes, give

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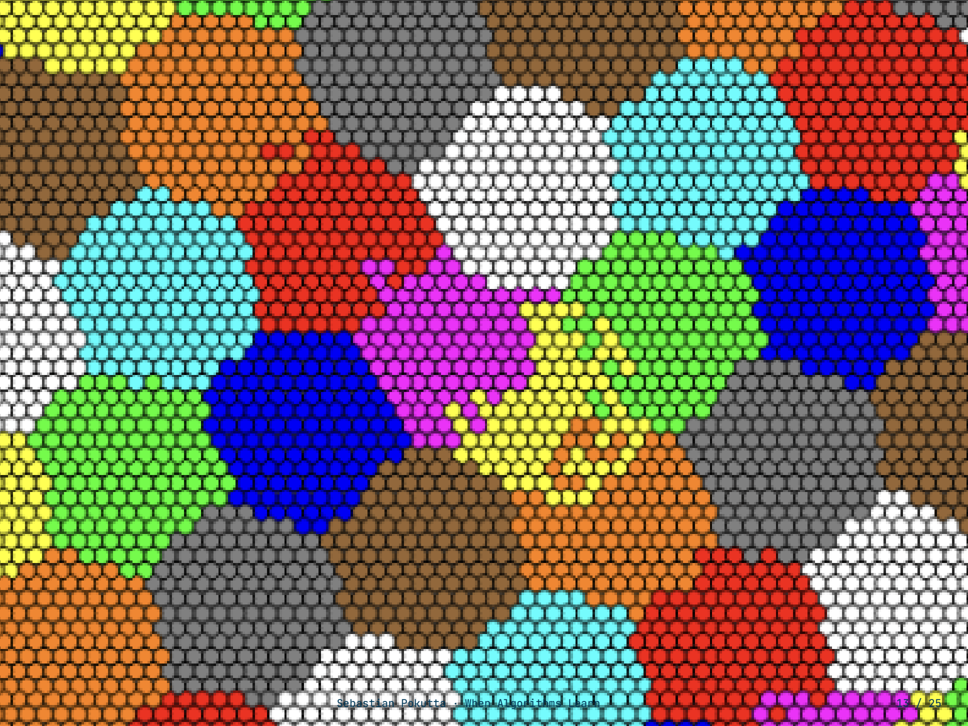
Question. Can we use computers to find admissible colorings $g : \mathbb{E}^2 \to [c]$, i.e.,

$$\{x \in \mathbb{E}^2 \mid \exists y \in B_1(x) : g(x) = g(y)\} = \emptyset?$$

... attempts, e.g., via discretization and SAT solvers...



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... attempts, e.g., via discretization and SAT solvers...

Idea. Use a parameterized and easily differentiable family $g_\theta : \mathbb{E}^2 \to \Delta_c$ and find

$$\arg\min_\theta \mathbb{E}\left[\int_{B_1(x)} g_\theta(x) \cdot g_\theta(y)\, dy \,\middle|\, x \in \mathbb{E}^2\right].$$

Key Point. Approach is continuous in nature.

New upper bounds via machine learning?

Can we improve the upper bound?

Neural Networks as Colorings

Idea. Use gradient descent to train a feedforward network g_θ to minimize

$$L(\theta) = \int_{[-b,b]\times[-b,b]} \int_{B_1(x)} g_\theta(x) \cdot g_\theta(y)\, dy\, dx$$

for some reasonable $b \in \mathbb{R}$?

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Stochastic (Batch) Gradient Descent. Sample point $x^{(i)} \in [-b, b] \times [-b, b]$ and $y^{(i)} \in B_1(x)$ for $i = 1, \ldots, m$

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$$\nabla_\theta L(\theta) \approx \hat{\nabla}_\theta L(\theta) \doteq \frac{1}{m} \sum_{i=1}^{m} \nabla_\theta \, g_\theta(x^{(i)}) \cdot g_\theta(y^{(i)}),$$

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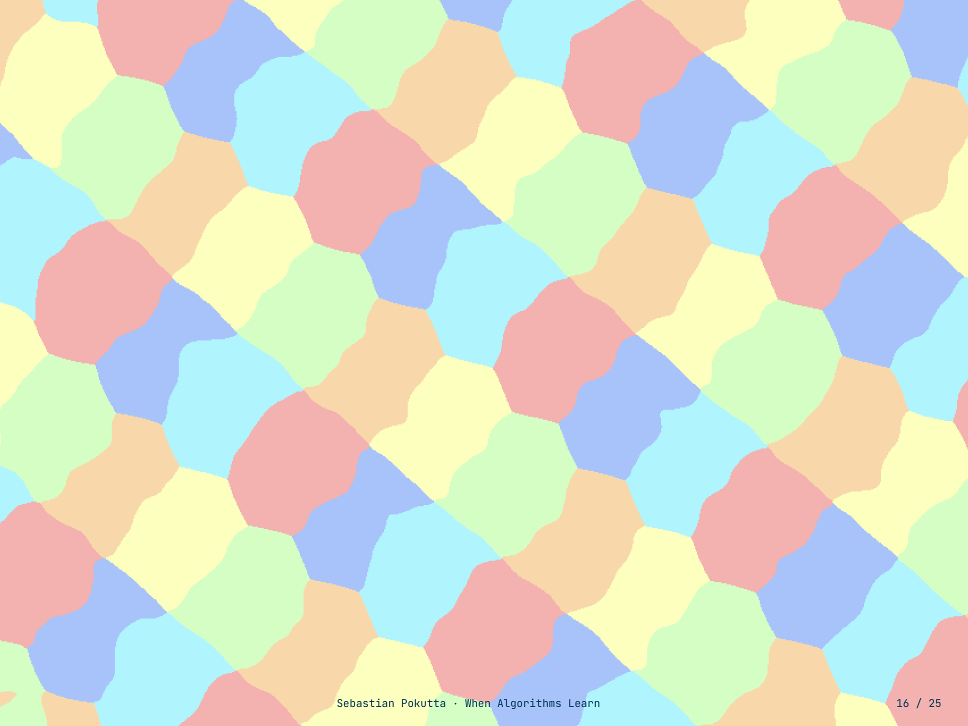
where $\nabla_\theta \, g_\theta(x^{(i)}) \cdot g_\theta(y^{(i)})$ is easily computed through backpropagation, to adjust the parameters θ with an appropriate step size α_k through

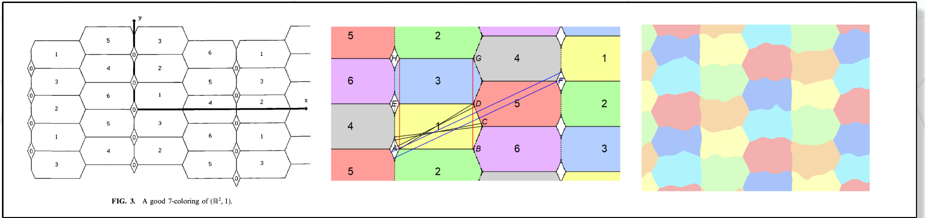
$$\theta_{k+1} = \theta_k - \alpha_k \, \hat{\nabla}_\theta L(\theta).$$

⇒ Very flexible approach “Deep Annealing”
(also: tropicalization of loss function aka softmax... “minimize the max”)



Unfortunately this coloring was already known...

Neural Networks as Colorings



Theorem

99.985% of the plane can be colored with 6 colors such that no two points of the same color are a unit distance apart. [Pritikin, 1998, Parts, 2020]

Corollary

Any unit distance graph with chromatic number 7 must have at least $6\,992$ vertices.

$\Rightarrow$ While coloring was known already maybe on the right track?

Off-diagonal variant

Going off-diagonal

Neural Networks as Colorings

If we cannot solve the original problem, we study variants of it:

Going off-diagonal

Neural Networks as Colorings

If we cannot solve the original problem, we study variants of it:

A c-coloring of the plane has **type** $(d_1, \ldots, d_c)$
if color i does not contain any points at distance d_i.

Going off-diagonal

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Problem (Soifer in Nash and Rassias' *Open Problems in Mathematics*)

Determine the continuum of six-colorings

$$X_6 = \{d \mid (1,1,1,1,1,d) \text{ can be realized}\}.$$

[Soifer, 1994a, Nash and Rassias, 2016]

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Status. Six-colorings exist for:

1. $d = 1/\sqrt{5}$ [Soifer, 1992]
2. $d = \sqrt{2} - 1$ [Hoffman and Soifer, 1993, 1996]
3. Family with $0.414 \approx \sqrt{2} - 1 \leq d \leq 1/\sqrt{5} \approx 0.447$ [Hoffman and Soifer, 1996, Soifer, 1994b, 2009]

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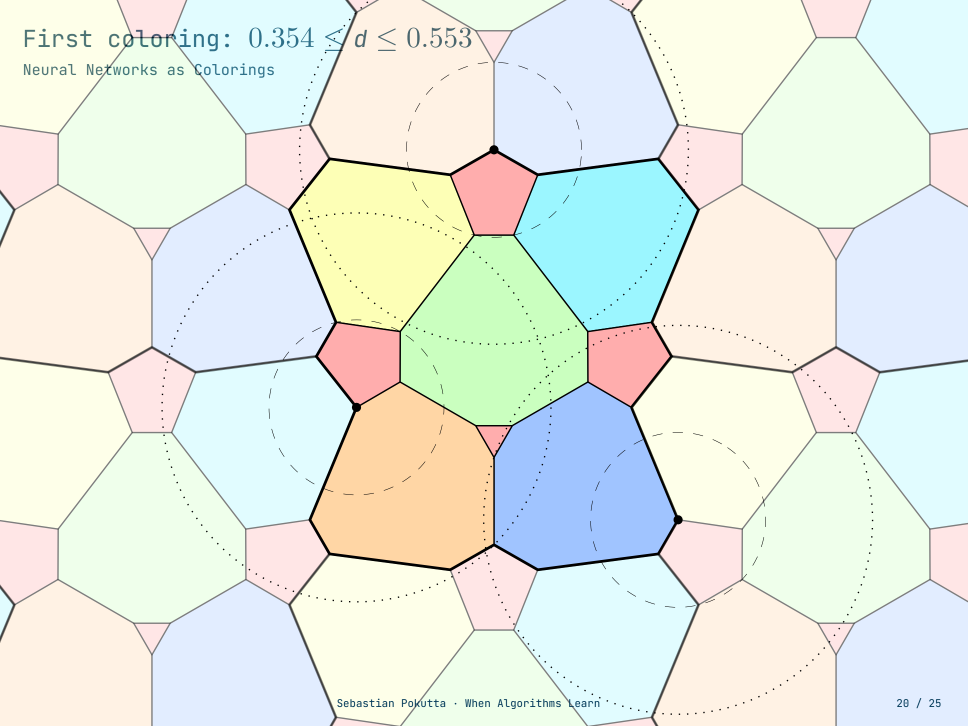
Deep Annealing approach provides two new colorings leading to...

Theorem

X_6 contains the closed interval [0.354, 0.657]. [Mundinger et al., 2024, 2025]

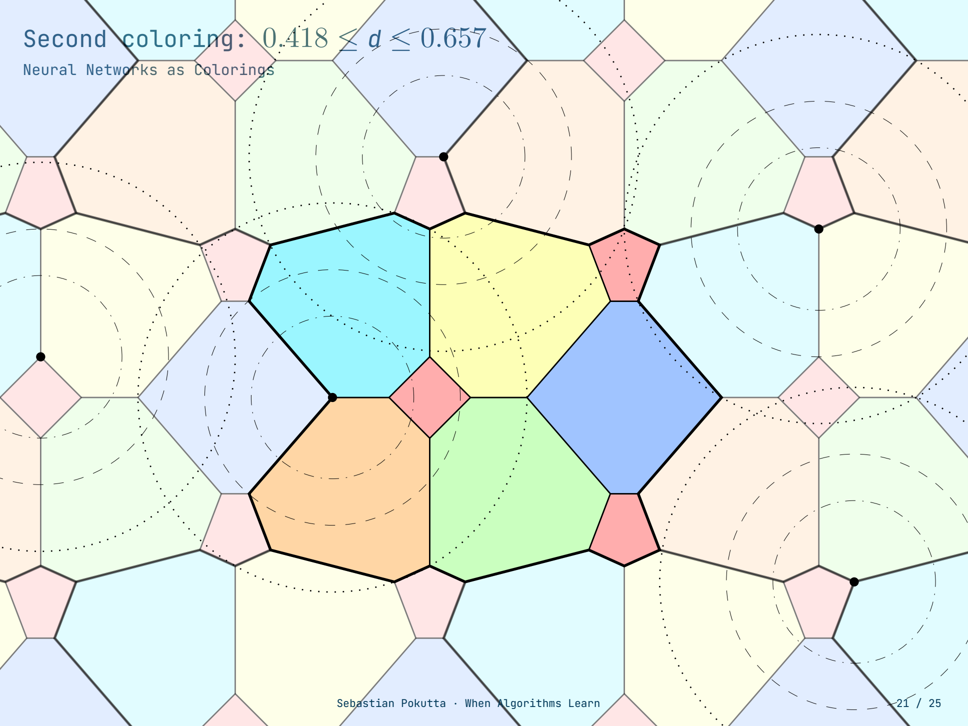
First coloring: $0.354 \leq d \leq 0.553$

Neural Networks as Colorings



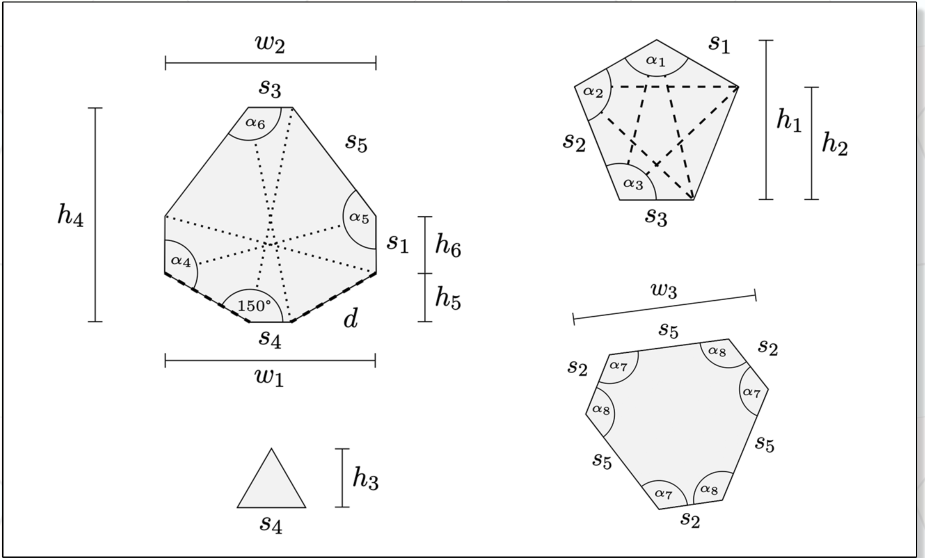
Second coloring: $0.418 \leq d \leq 0.657$

Neural Networks as Colorings



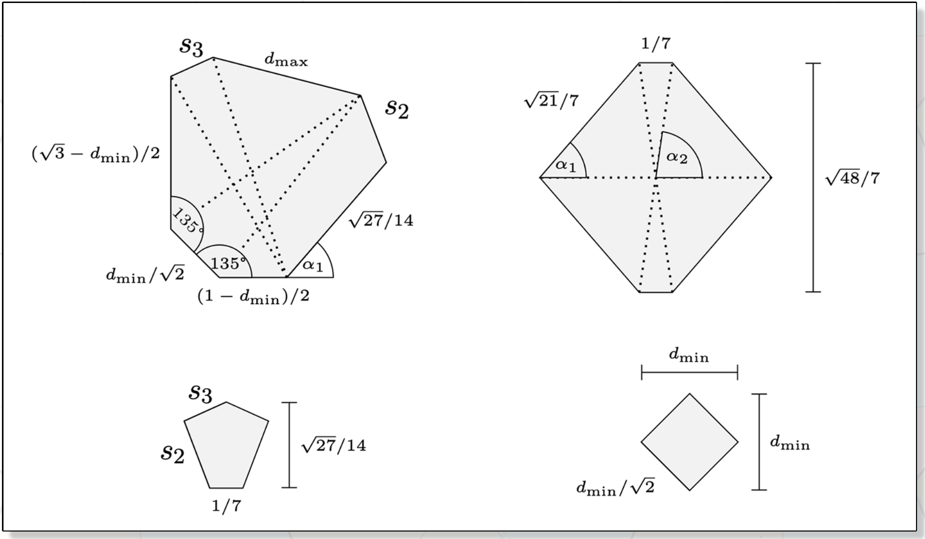
First coloring: exact components

Neural Networks as Colorings



Second coloring: exact components

Neural Networks as Colorings



Final Remarks

1. AI can be used in various ways in modern mathematical research workflows (actual discovery, verification, etc); beyond simple black-box prompting
2. Fully-automatic discovery of new mathematics might be possible in the future but relies on *strong* verification approaches
3. The agentic harness seems to be key: how does the agent receive feedback on its work, how is it guided, and which tools are available?
4. Empirically: the human-in-the-loop is crucial to guide the search

The promises of AI4MATH are great but need to go beyond simple black-box prompting “your favorite Erdős problem” (which then turns out having a solution that is already known)...

Thank you!

Mundinger, K., Pokutta, S., Spiegel, C., and Zimmer, M. (2024). Extending the Continuum of Six-Colorings. Geombinatorics Quarterly. Available at https://arxiv.org/abs/2404.05509.

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