

How Machines Explore, Conjecture, and Discover Mathematics

Sebastian Pokutta

Technische Universität Berlin
and
Zuse Institute Berlin

`pokutta@math.tu-berlin.de`
`@spokutta`

Rice University

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Berlin Mathematics Research Center



What is this talk about?

Introduction

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

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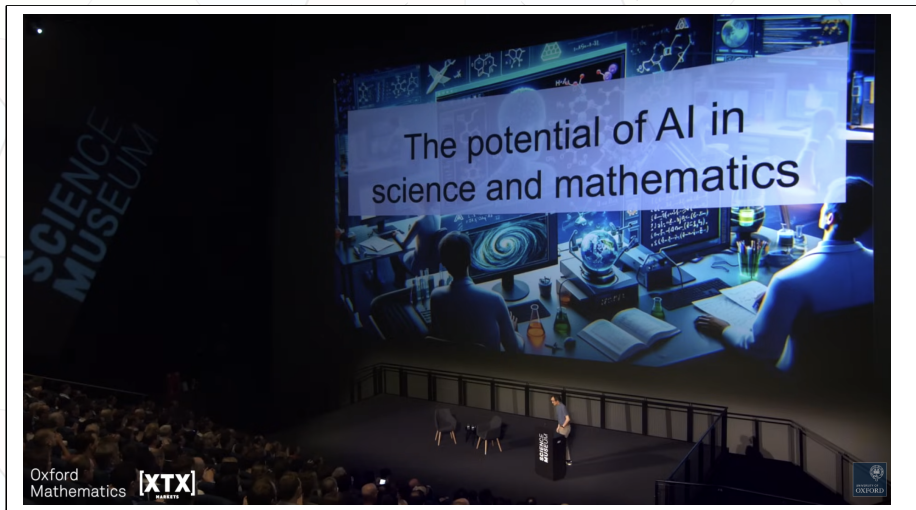
Outline

- 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]

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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

ICML AI4RESEARCH Workshop 2026 (oral)
<https://arxiv.org/abs/2603.15914>

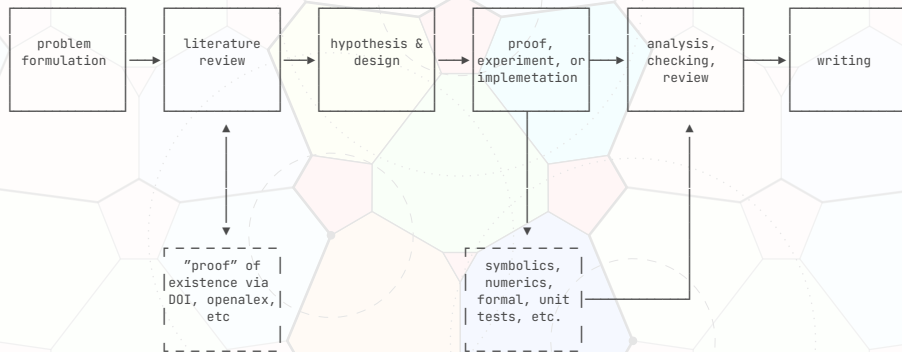
Partially supported by ExC MATH+ Project EF-LiOpt-3
Agent AI in Mathematics

[Zimmer et al., 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 bwrs8ty88

1-hour mid-training status check

Waiting for task (esc to give additional instructions)

+ Bitflying... (8h 39m 19s · ↓ 39.3k tokens · thought for 28s)

↳ 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 --mpr.. (running)
source ~/.bashrc &&CUDA_VISIBLE_DEVICES=5 uv run torchrun --standalone --mpr.. (running)
source ~/.bashrc &&CUDA_VISIBLE_DEVICES=4 uv run torchrun --standalone --mpr.. (running)
source ~/.bashrc &&CUDA_VISIBLE_DEVICES=3 uv run torchrun --standalone --mpr.. (running)
source ~/.bashrc &&CUDA_VISIBLE_DEVICES=2 uv run torchrun --standalone --mpr.. (running)
source ~/.bashrc &&CUDA_VISIBLE_DEVICES=1 uv run torchrun --standalone --mpr.. (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, $\text{\LaTeX}$, and GPU-backed experiments.
- Puts a premium on **verification**: record everything, verify citations, and verify before claiming.

[blog post]

[arXiv]

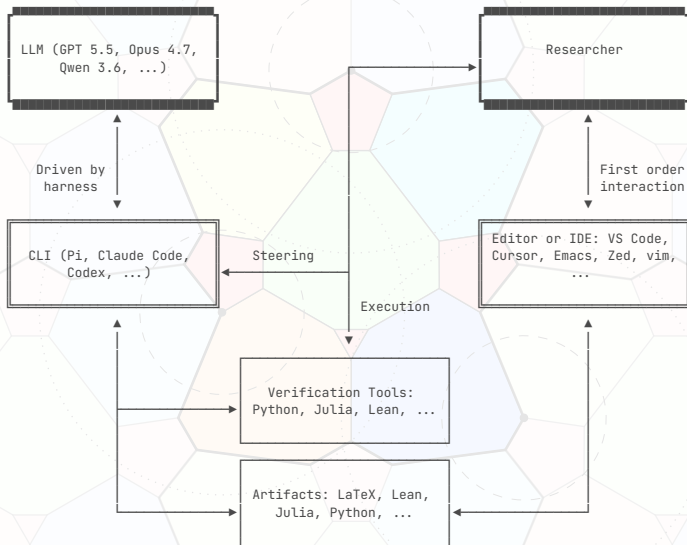
[GitHub]

Does it work? 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. ...

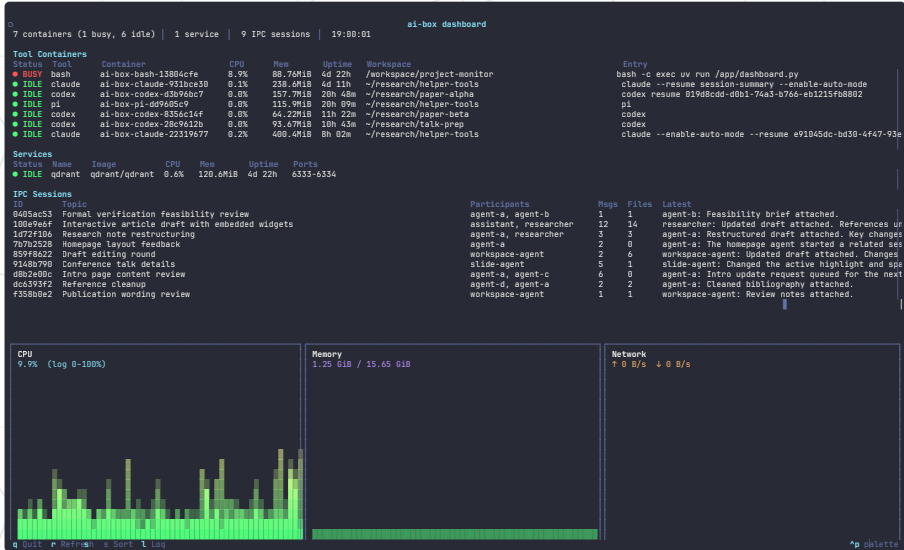
Interacting with the System

The agentic researcher framework



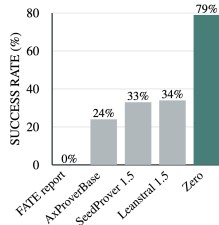
Orchestration Dashboard

The agentic researcher framework

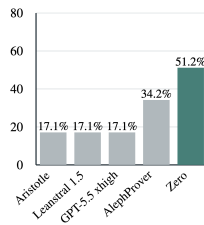


Dashboard showing multiple containerized agents interacting with each other (stylized example).

The agentic researcher framework



(i) FATE-X



(ii) ArXivLean

1. Many recent successes used custom harnesses
2. Doesn't scale to build one harness per problem
3. Solution: add DSL, so that agent can dynamically define its own workflow
4. Significant improvement in overall success rates

[Pelleriti et al., 2026]

Frank-Wolfe Beyond $1/t$ Convergence

NeurIPS 2026

<https://arxiv.org/abs/2604.28006>

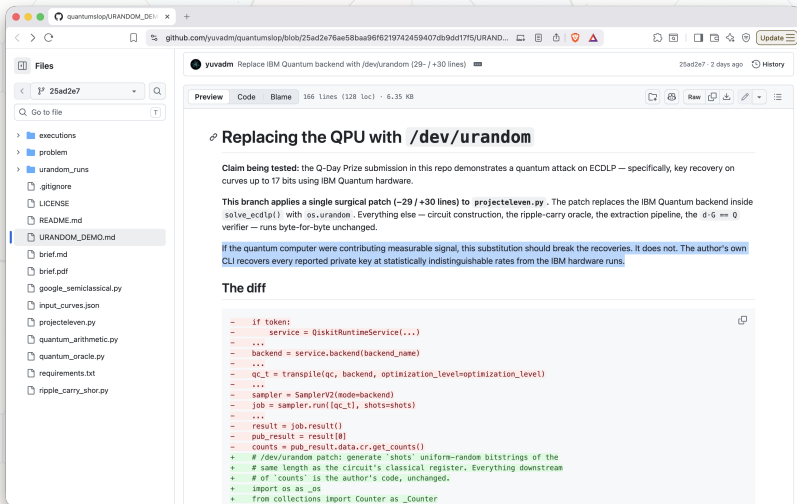
Partially supported by ExC MATH+ Project EF-LiOpt-3

Agent AI in Mathematics

[Pokutta, 2026]

Why Verification is Crucial

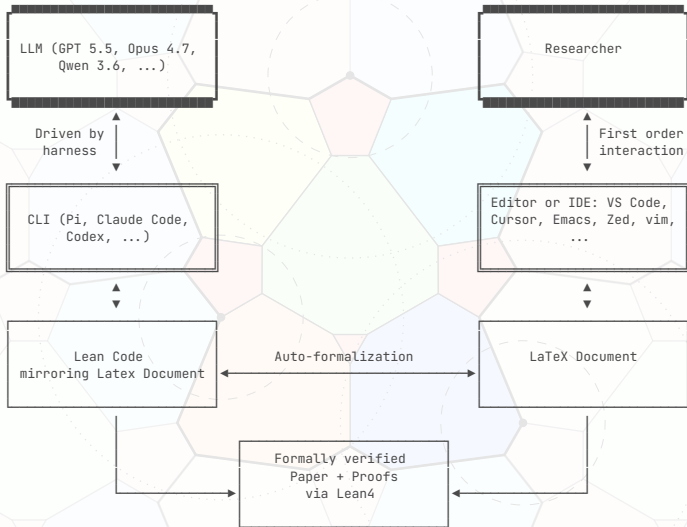
The agentic researcher framework



[GitHub Repository]

End-2-End Formal Verification with Lean 4

The agentic researcher framework



When generation is cheap, verification is everything.

[Pokutta, 2026]

Neural Discovery in Mathematics: Do Machines Dream of Colored Planes?

(a.k.a. 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?

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

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

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Theorem

Assuming Axiom of Choice (AoC):

[Bruijn and Erdos, 1951]

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

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This problem has a long and complicated history...

over 14 pages in [Soifer, 2024]

History

The Hadwiger-Nelson Problem

Table 3.1 Who created the chromatic number of the plane problem?

Publication	Year	Author(s)	Problem creator(s) or source named
[Gar2]	1960	Gardner	“Leo Moser ...writes...”
[Had4]	1961	Hadwiger (after Klee)	Nelson
[E61.22]	1961	Erdős	“I cannot trace the origin of this problem”
[Cro]	1967	Croft	“A long¹⁸-standing open problem of Erdős”
[Woo1]	1973	Woodall	Gardner
[Sim]	1976	Simmons	Erdős, Harary, and Tutte
[E80.38] [E81.23] [E81.26]	1980– 1981	Erdős	Hadwiger and Nelson
[CFG]	1991	Croft, Falconer, and Guy	“Apparently due to E. Nelson”
[KW]	1991	Klee and Wagon	“Posed in 1960–61 by M. Gardner and Hadwiger”

p. 24 in [Soifer, 2024]



Lower bounds on $\chi(\mathbb{E}^2)$

Lower bounds through unit distance graphs

The Hadwiger-Nelson Problem

Find unit distance graphs of large chromatic number.

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Definition

A graph $G = (V, E)$ is a **unit distance graph** if there exists an embedding $f: V \rightarrow \mathbb{E}^2$ of its vertices in the plane s.t. $\|f(u) - f(v)\| = 1$ if and only if $\{u, v\} \in E$.

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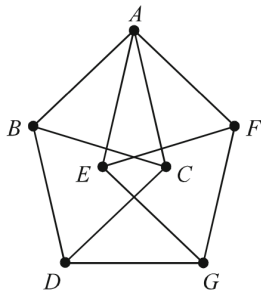
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Theorem

There is a unit distance graph on 20425 vertices with chromatic number 5.

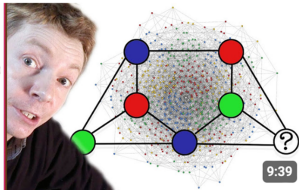
[De Grey, 2018]

Lower bounds through unit distance graphs

The Hadwiger-Nelson Problem

Find unit distance graphs of large chromatic number.

Numberphile



A Colorful Unsolved Problem - Numberphile

681K views • 5 years ago



Numberphile ✓

More links & stuff in full description below ↓↓↓

Numberphile is supported by the Mathematical Science...

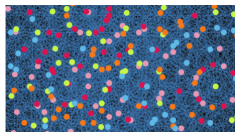
CC



Lower bounds through unit distance graphs

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GRAPH THEORY

Decades-Old Graph Problem Yields to Amateur Mathematician

By EVELYN LAMB | APRIL 17, 2018 | 26 |

...number of vertices? The problem, now known as the Hadwiger-Nelson problem or the problem of finding the chromatic number of the plane, has piqued the interest of many mathematicians, including...



Lower bounds through unit distance graphs

The Hadwiger-Nelson Problem

Find unit distance graphs of large chromatic number.



Aubrey de Grey and Alexander Soifer, *Il Vicino*, January 18, 2020



Ronald L. Graham presents Aubrey D.N.J. de Grey the Prize: \$1000, San Diego, September 22, 2018

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[De Grey, 2018]

Simpler constructions with...

1. 1581 vertices
2. 627 vertices
3. 553 vertices (as part of Polymath16)
4. 509 vertices (as part of Polymath16)

for detail see [De Grey, 2018]

[Exoo and Ismailescu, 2020]

Marijn Heule, for details see [Mixon, 2021]

Jaan Parts, for details see [Mixon, 2021]

Lower bounds through unit distance graphs

The Hadwiger-Nelson Problem

Find unit distance graphs of large chromatic number.

The Euclidean plane is not five-colorable

OpenAI

September 23, 2026

Abstract

We prove that every coloring of the Euclidean plane with five colors has a monochromatic unit-distance pair, with no regularity assumption on the color classes. Consequently, the chromatic number of the plane is either six or seven.

[OpenAI, 2026]

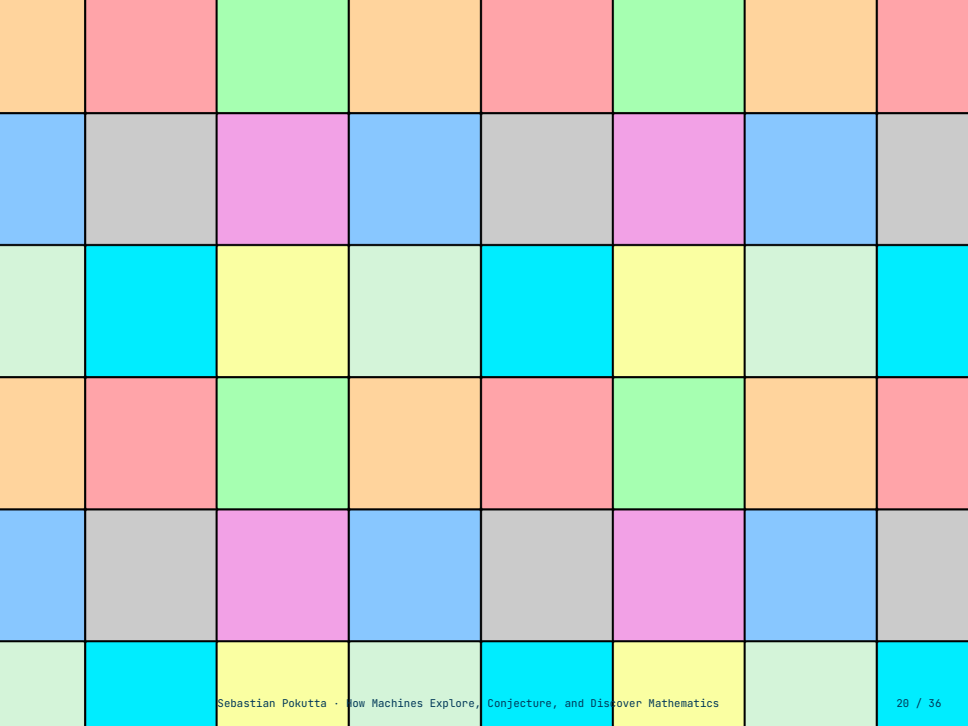
Upper bounds on $\chi(\mathbb{E}^2)$

Upper bounds through colorings

The Hadwiger-Nelson Problem

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

$$6 \leq \chi(\mathbb{E}^2) \leq \dots$$

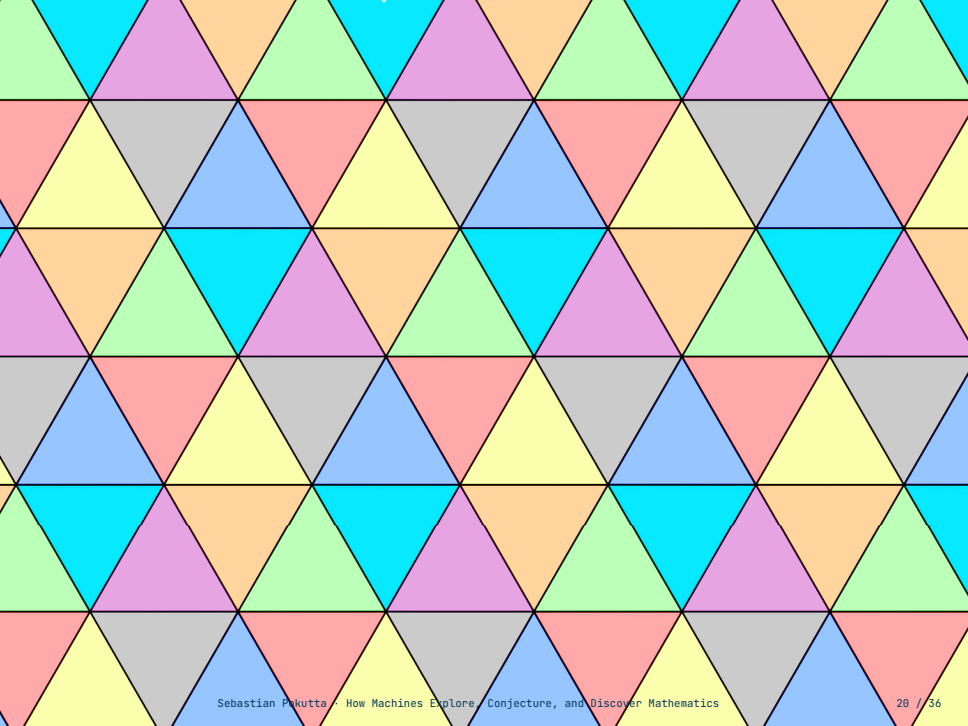


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Explicit colorings $g : \mathbb{E}^2 \rightarrow [c] := \{1, \dots, c\}$, usually derived through tessellations using simple polytopal shapes, give

$$6 \leq \chi(\mathbb{E}^2) \leq 9.$$

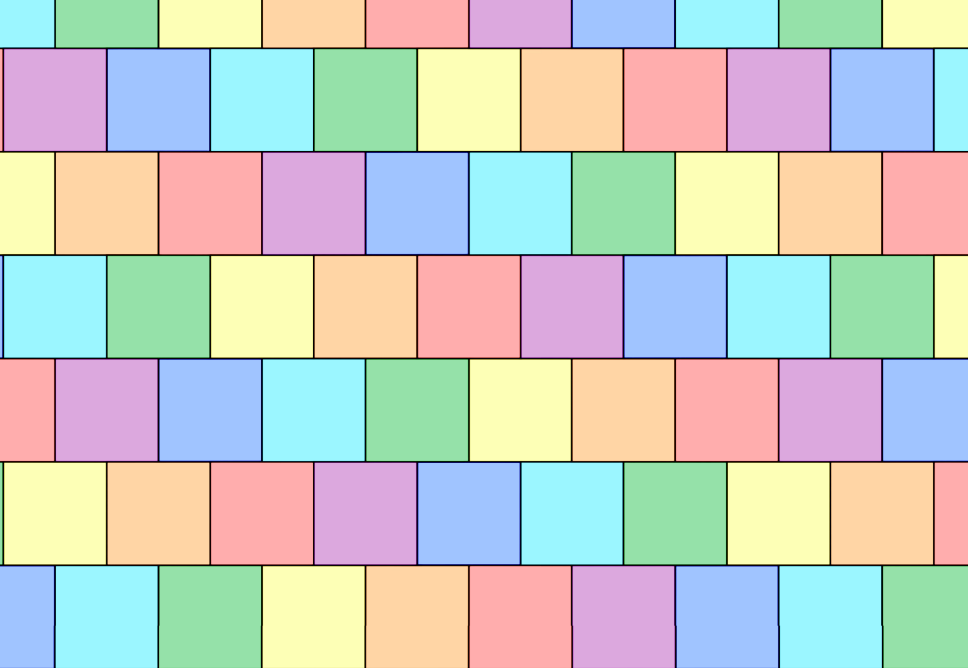


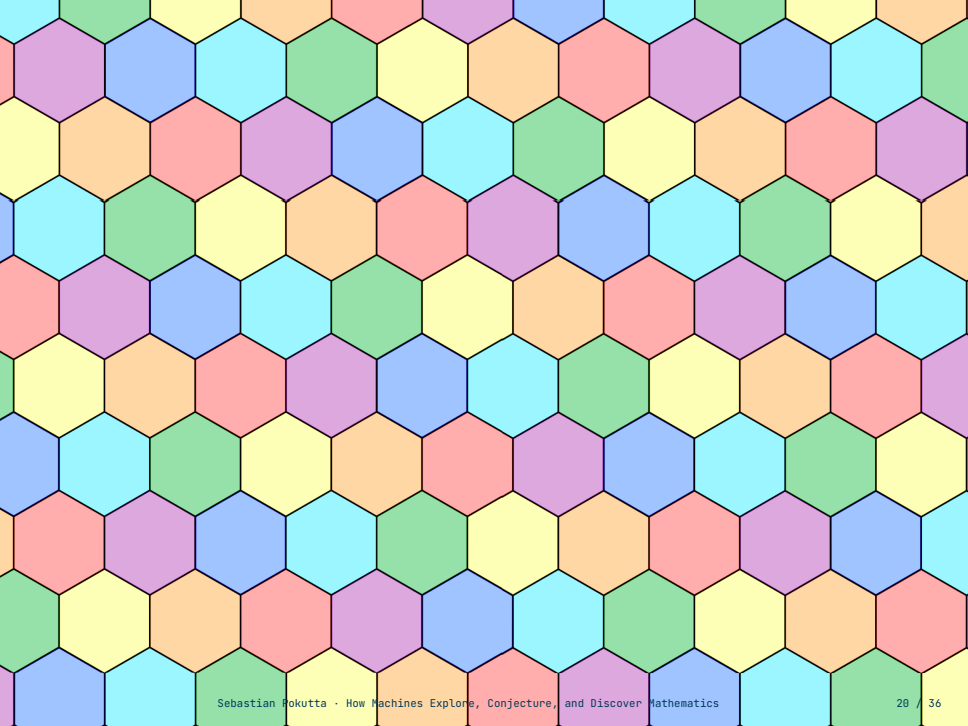
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Explicit colorings $g : \mathbb{E}^2 \rightarrow [c] := \{1, \dots, c\}$, usually derived through tessellations using simple polytopal shapes, give

$$6 \leq \chi(\mathbb{E}^2) \leq 8.$$





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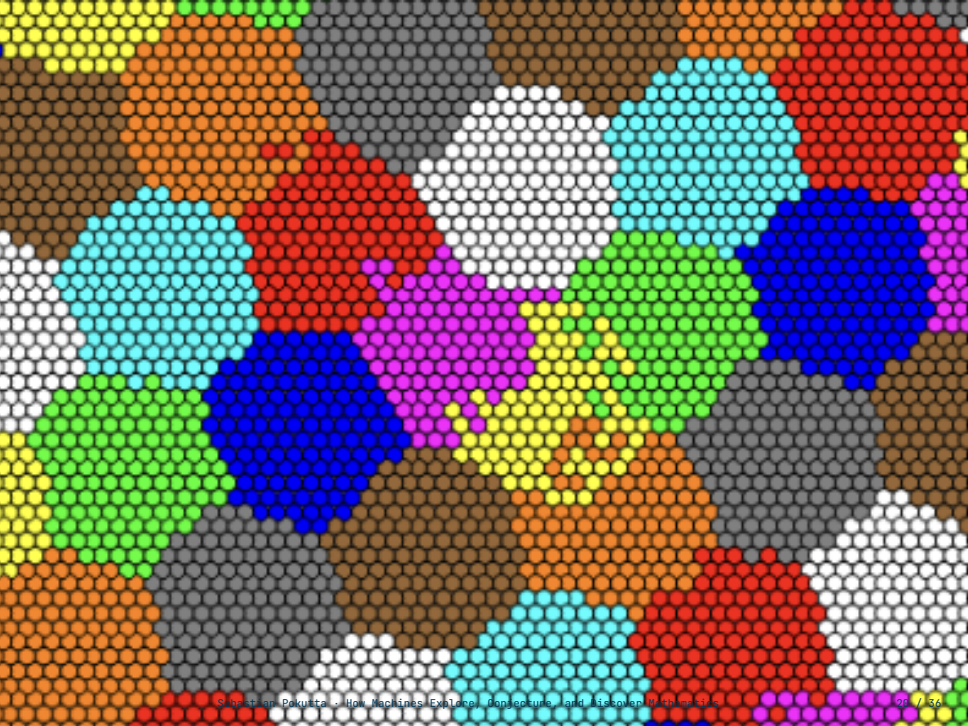
Explicit colorings $g : \mathbb{E}^2 \rightarrow [c] := \{1, \dots, c\}$, usually derived through tessellations using simple polytopal shapes, give

$$6 \leq \chi(\mathbb{E}^2) \leq 7.$$

Question. Can we use computers to find admissible colorings $g : \mathbb{E}^2 \rightarrow [c]$, 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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Idea. Use a parameterized and easily differentiable family $g_\theta : \mathbb{E}^2 \rightarrow \Delta_c$ and find

$$\operatorname{argmin}_{\theta} \mathbb{E} \left[\int_{B_1(x)} g_\theta(x) \cdot g_\theta(y) dy \mid x \in \mathbb{E}^2 \right].$$

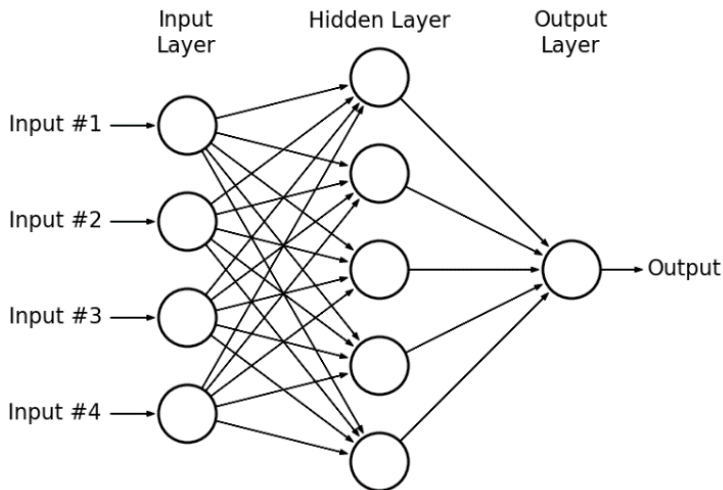
Key Point. Approach is continuous in nature.

The background of the slide is a Voronoi diagram with a repeating pattern of light blue, light green, and light orange/pink cells. In the center, a cluster of cells is highlighted. Three dashed circles are centered on three of the vertices within this cluster. Two dotted circles are also centered on two of the same vertices, with a larger one encompassing a wider area. The text "New upper bounds via machine learning?" is written in orange in the center of the diagram.

**New upper bounds via
machine learning?**

One second recap: Neural Networks

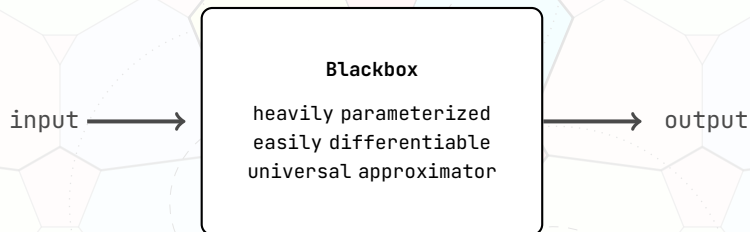
Neural Networks as Colorings



One second recap: Neural Networks

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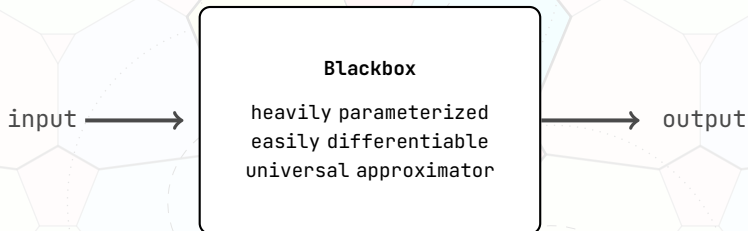
Here. Simply a parameterized continuous function to model the coloring.



One second recap: Neural Networks

Neural Networks as Colorings

Here. Simply a parameterized continuous function to model the coloring.



Theorem (Universal Approximation Theorem)

Feedforward neural networks with certain activation functions are dense (w.r.t. compact convergence) in the space of continuous functions.

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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Problem. Still a continuous problem. How to compute?

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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 $i = 1, \dots, m$

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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 $i = 1, \dots, m$ and use that

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

Can we improve the upper bound?

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

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 $i = 1, \dots, m$ and use that

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

where $\nabla_\theta g_\theta(x^{(i)}) \cdot g_\theta(y^{(i)})$ is easily computed through backpropagation,

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 $b \in \mathbb{R}$?

Problem. Still a continuous problem. How to compute?

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

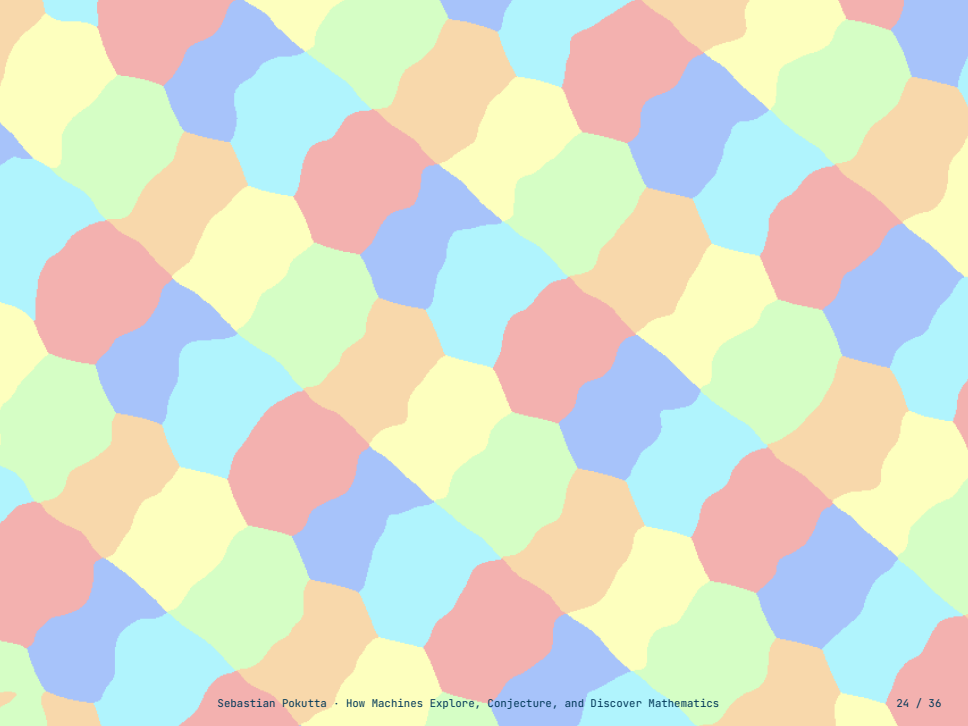
$$\nabla_\theta L(\theta) \approx \hat{\nabla}_\theta L(\theta) \doteq \frac{1}{m} \sum_{i=1}^m \nabla_\theta g_\theta(x^{(i)}) \cdot g_\theta(y^{(i)}),$$

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

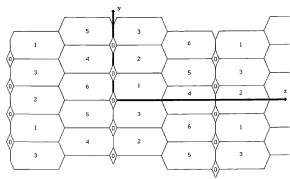
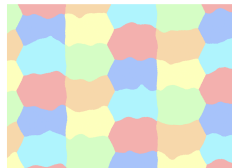
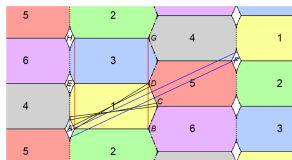


FIG. 3. A good 7-coloring of $(\mathbb{R}^2, 1)$.



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]

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Neural Networks as Colorings

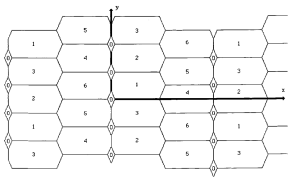
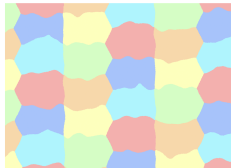
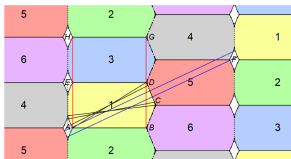


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Corollary

Any unit distance graph with chromatic number 7 must have at least 6992 vertices.

⇒ 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

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

Going off-diagonal

Neural Networks as Colorings

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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. $d = 1/\sqrt{5}$
2. $d = \sqrt{2} - 1$
3. Family with $0.414 \approx \sqrt{2} - 1 \leq d \leq 1/\sqrt{5} \approx 0.447$

[Soifer, 1992]

[Hoffman and Soifer, 1993, 1996]

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

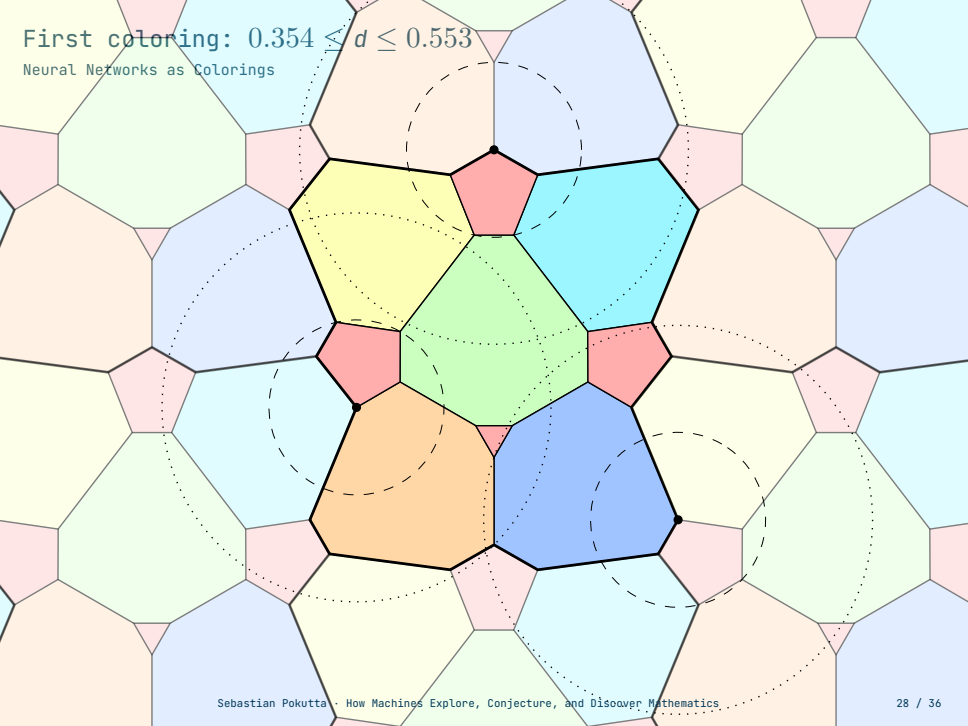
Theorem

X_6 contains the closed interval $[0.354, 0.657]$.

[Mundinger et al., 2024, 2025]

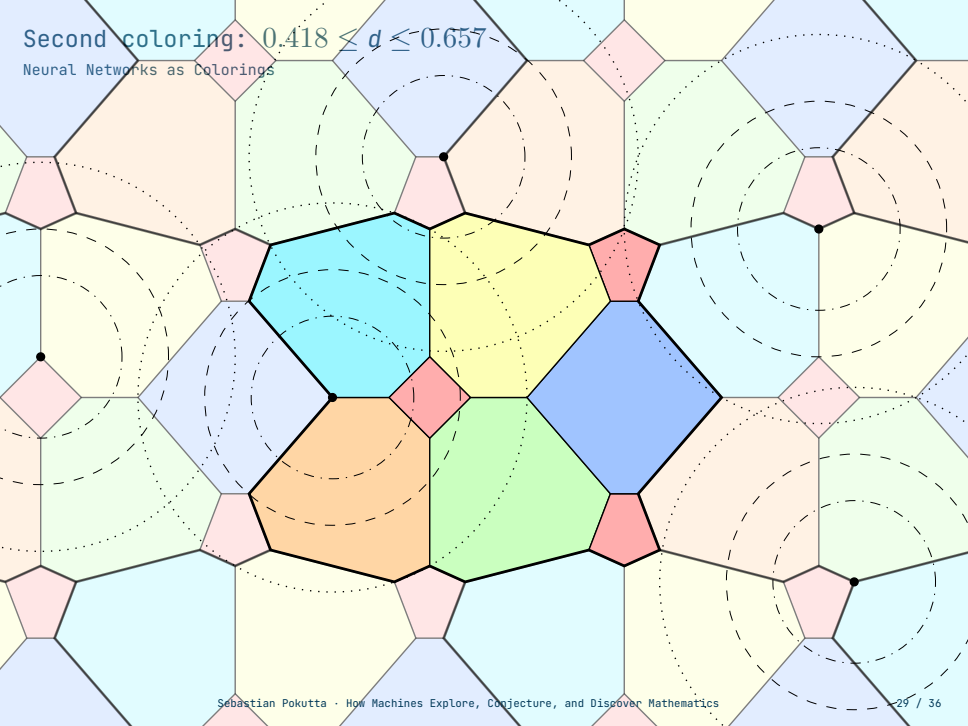
First coloring: $0.354 \leq d \leq 0.553$

Neural Networks as Colorings



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

Neural Networks as Colorings



GEOMBINATORICS QUARTERLY

**Welcome to the journal on open
problems of combinatorial &
discrete geometry and related
areas**

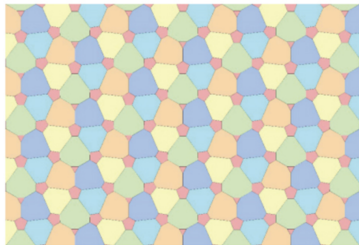
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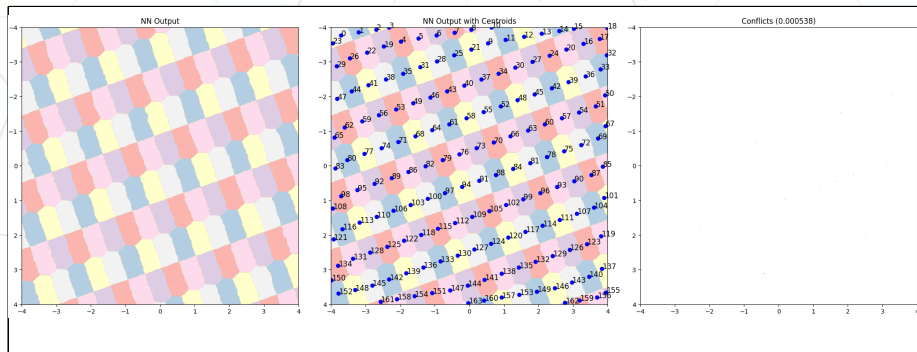
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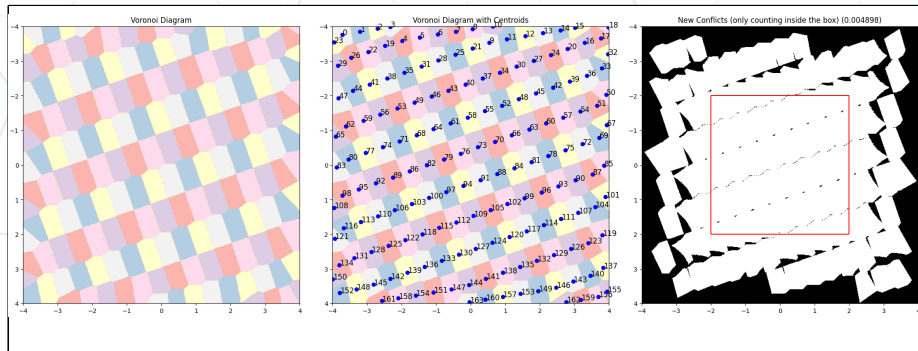
Just numerics...?

Neural Networks as Colorings



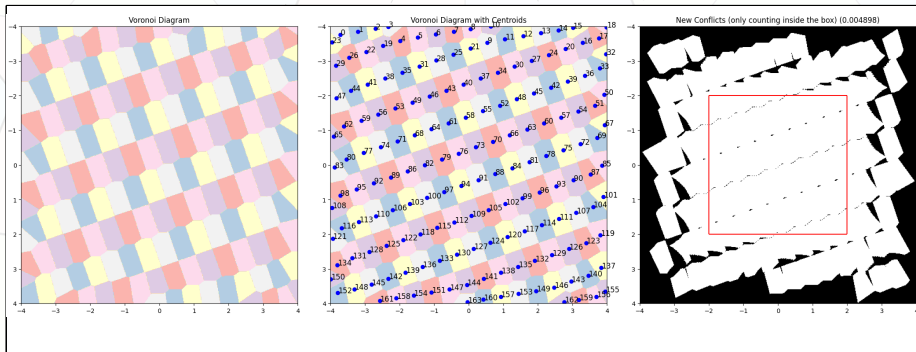
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Neural Networks as Colorings



Just numerics...?

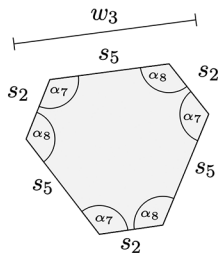
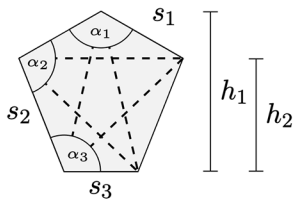
Neural Networks as Colorings



Voronoi cell filtering...

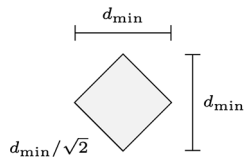
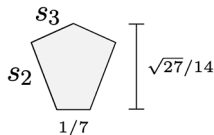
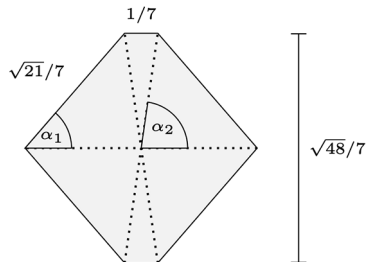
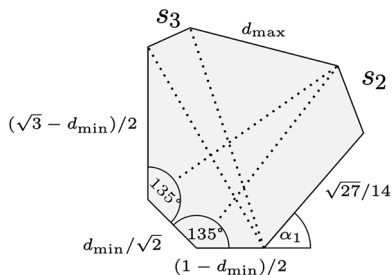
⇒ Exact constructions for both colorings.

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!

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