AI4Math: How Machines Explore, Conjecture, and Discover Mathematics

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CQF Seminar

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What AI can do for Mathematics? Trends and a concrete example.

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Why? AI is going to change the way of how we do science and mathematics

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Today: Brief overview of approach, two new constructions, and outlook.

What AI can do for Mathematics? Trends and a concrete example.

Why? AI is going to change the way of how we do science and mathematics

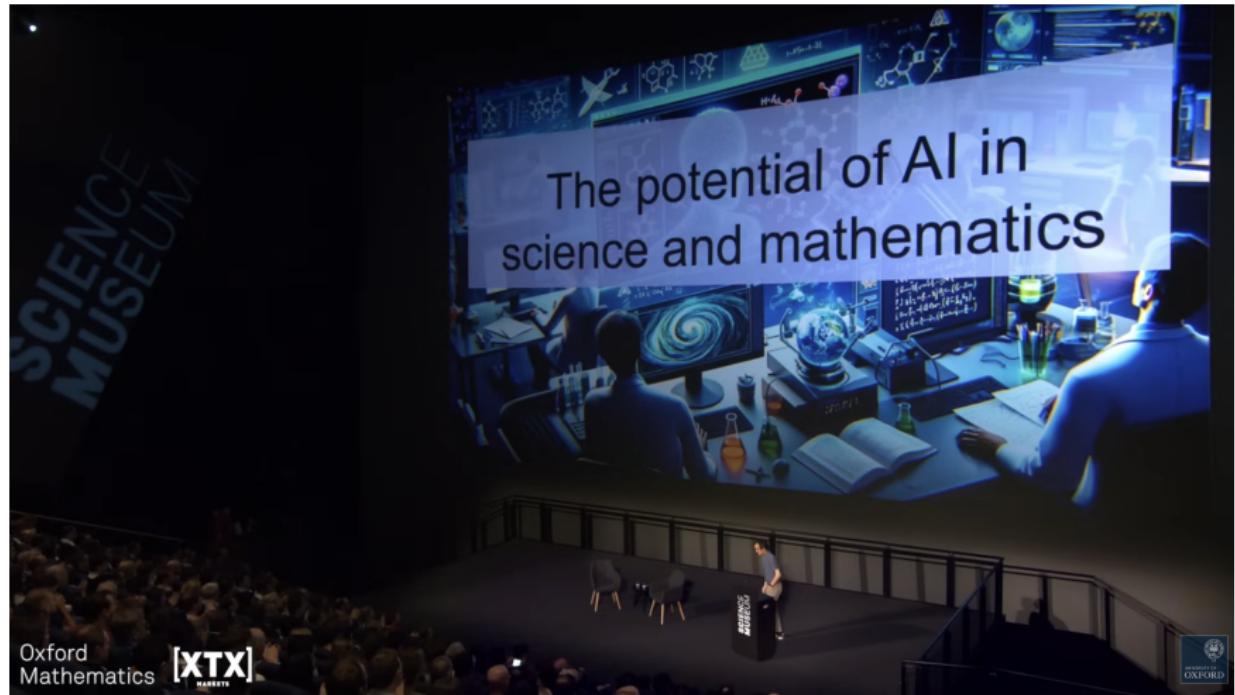**Today:** Brief overview of approach, two new constructions, and outlook.

Outline
- AI and Mathematics
- The Hadwiger-Nelson Problem: formulation and status
- Machine learning approach
- Results a.k.a. constructions

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

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

What is this talk about?

AI and Mathematics

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 - present
- **AI Co-creator**: Fully integrated, autonomous, co-creator   2027(??)

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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 and 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 Hadwiger-Nelson Problem

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

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

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 $\|x - y\| = 1$
$\Rightarrow$ 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]

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 long[18]-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**"

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.

Lower bounds through unit distance graphs

The Hadwiger-Nelson Problem

Find unit distance graphs of large chromatic number.

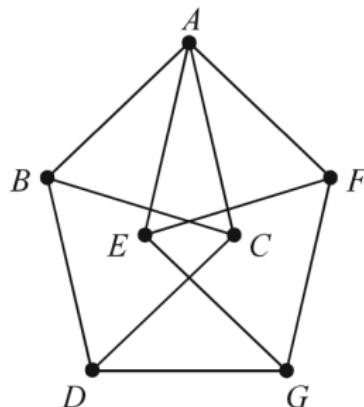## Definition

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 $\{u, v\} \in E$.

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A triangle gives a lower bound of 3.
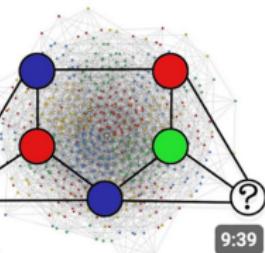
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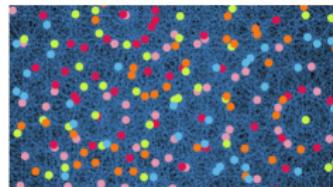The Moser spindle gives a lower bound of 4.

[Moser and Moser, 1961]

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Theorem
There is a unit distance graph on $20\,425$ *vertices with chromatic number* 5.   [De Grey, 2018]

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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...

Quantamagazine

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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Simpler constructions with...

1. 1581 vertices for detail see [De Grey, 2018]
2. 627 vertices [Exoo and Ismailescu, 2020]
3. 553 vertices (as part of `Polymath16`) Marijn Heule, for details see [Mixon, 2021]
4. 509 vertices (as part of `Polymath16`) Jaan Parts, for details see [Mixon, 2021]

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

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
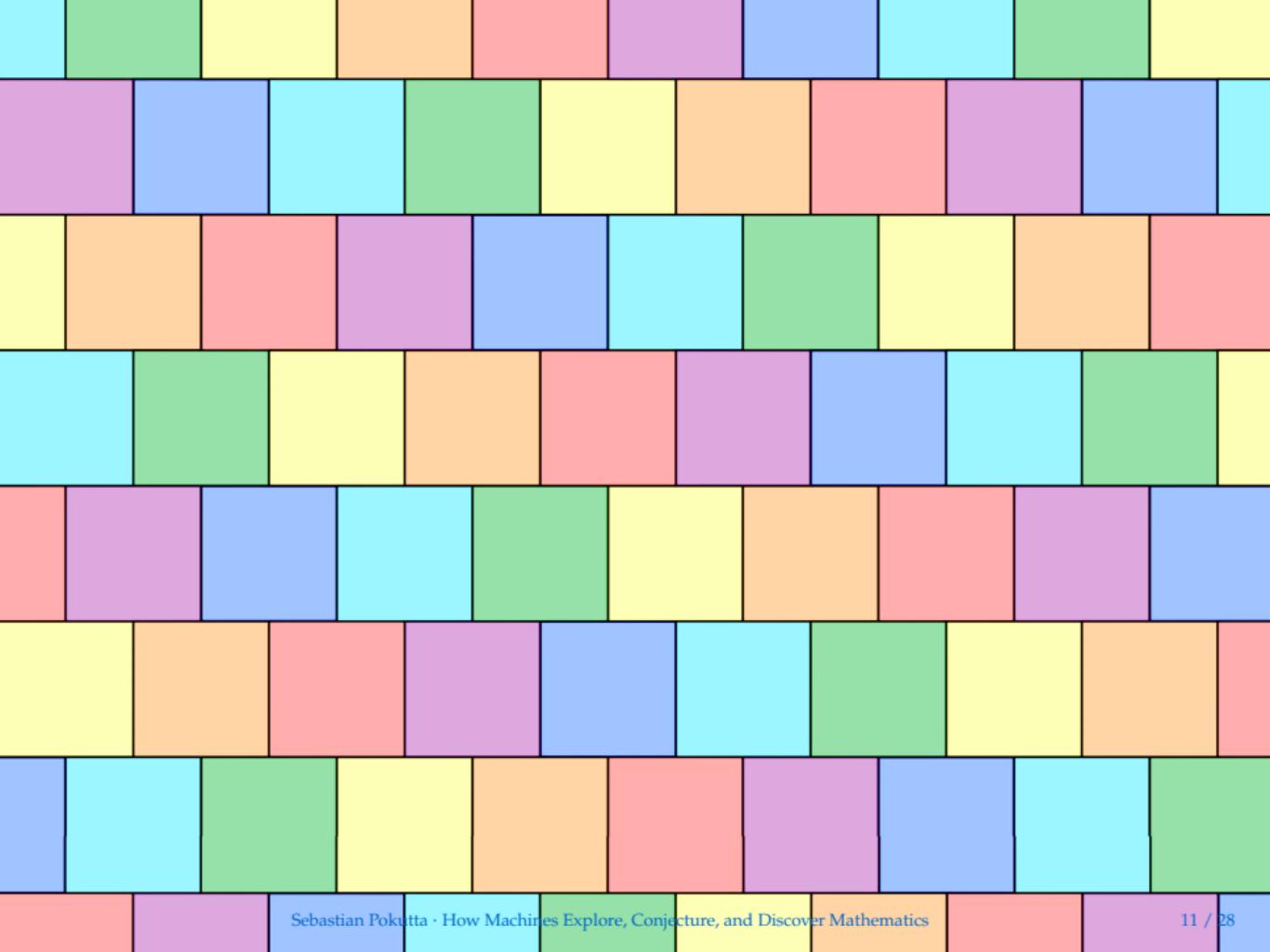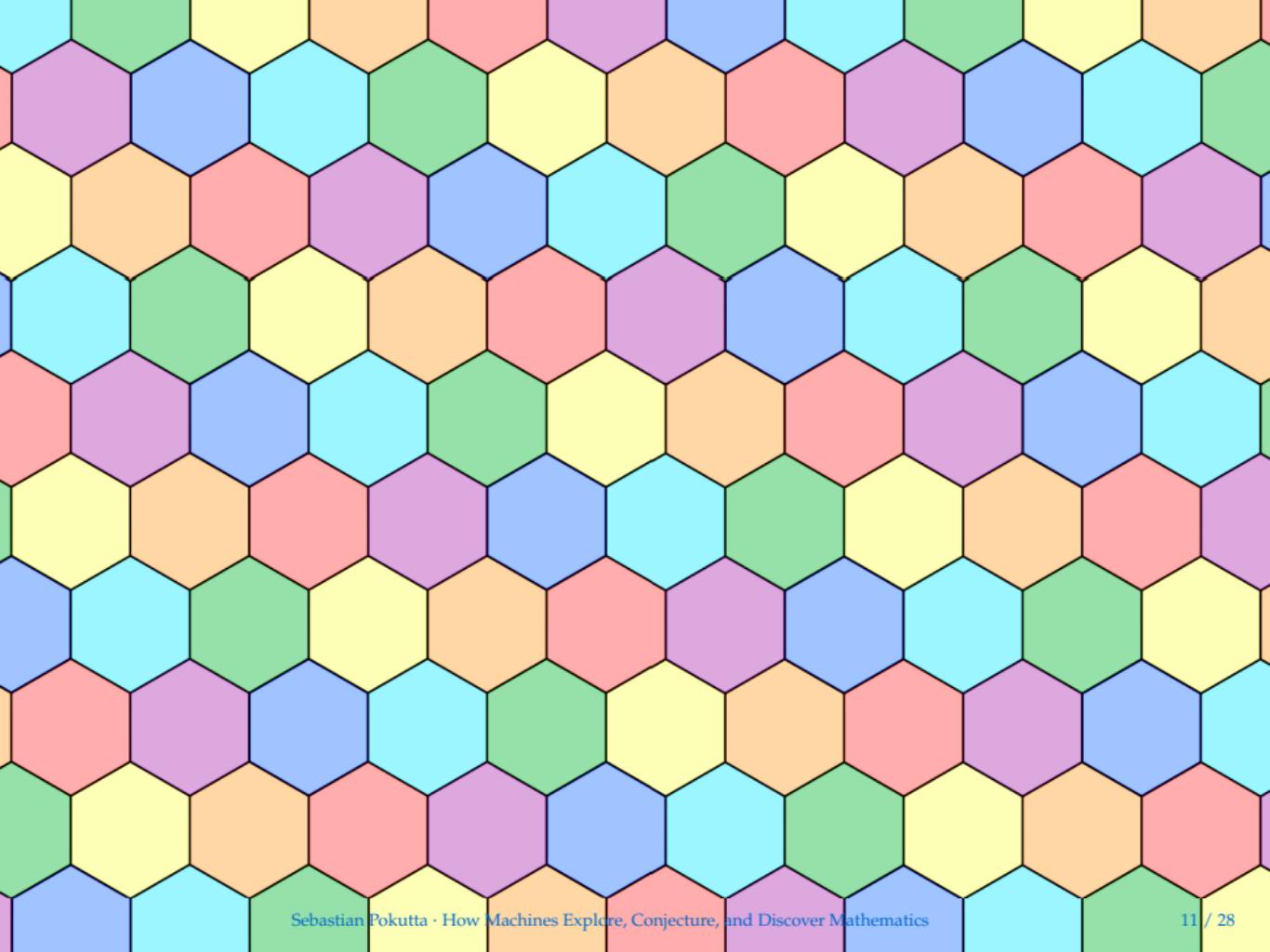
$$5 \leq \chi(\mathbb{E}^2) \leq \ldots$$
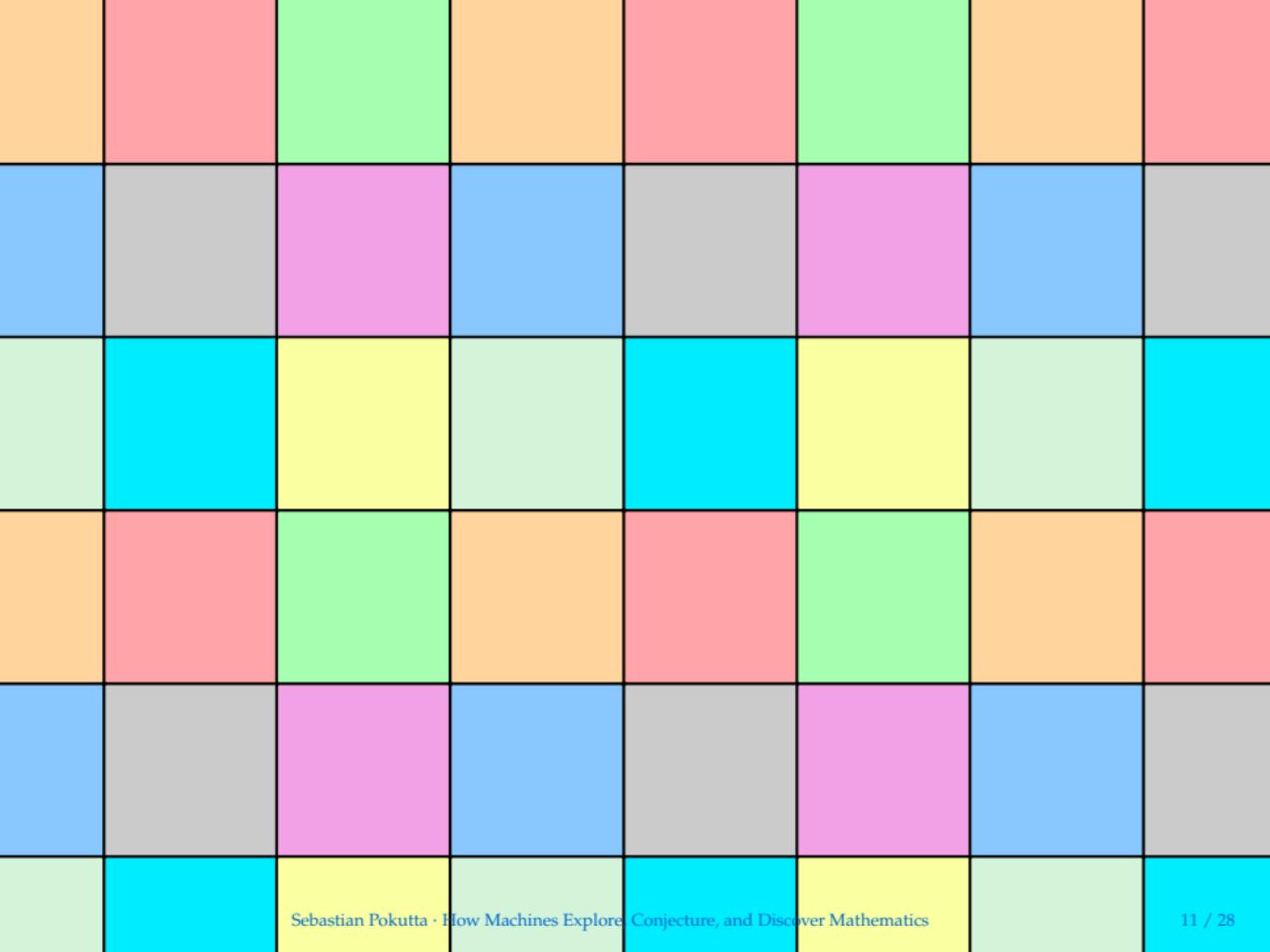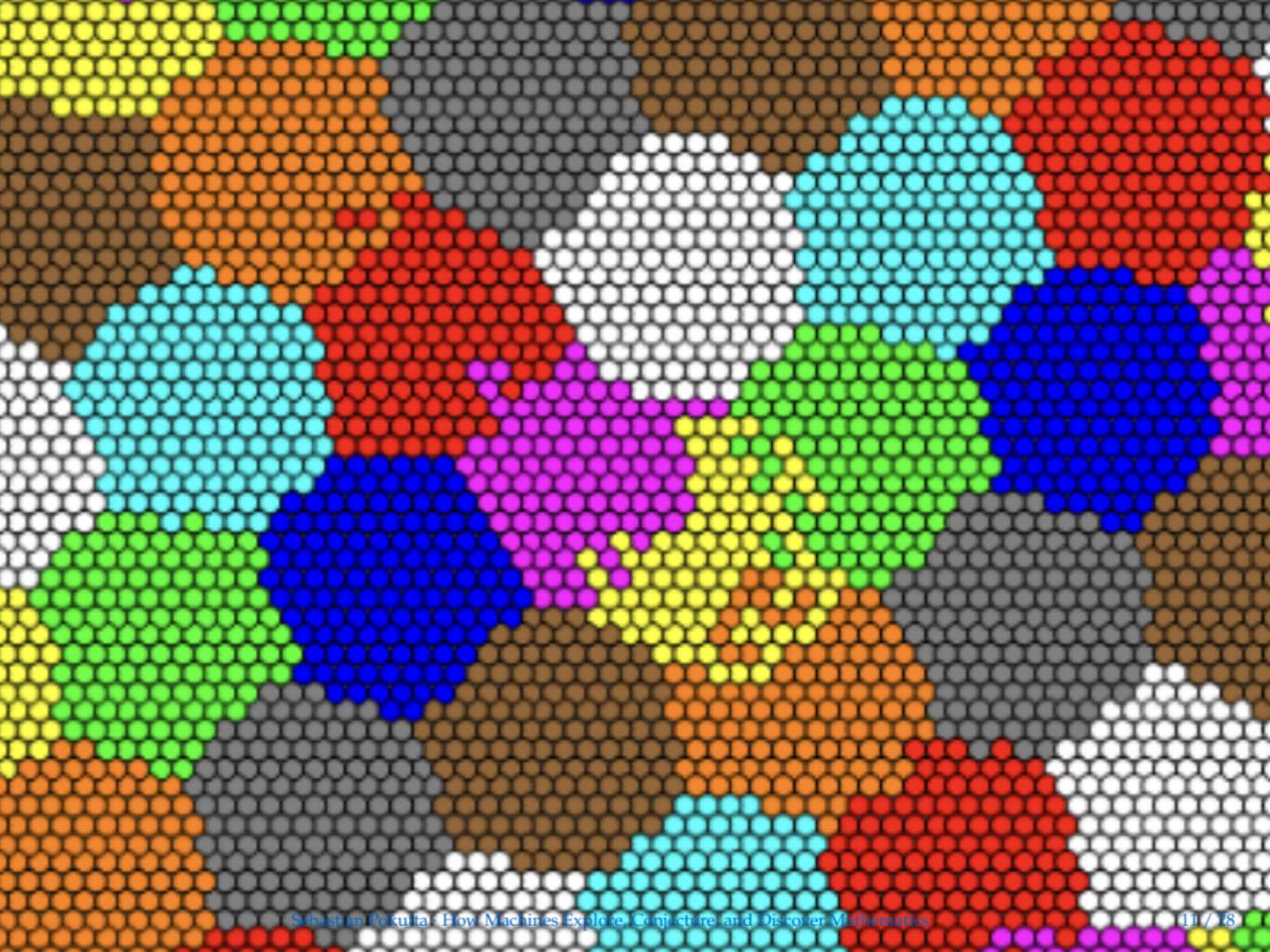
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Explicit colorings $g : \mathbb{E}^2 \to [c] := \{1, \ldots, c\}$, usually derived through tesselations using simple polytopal shapes, give

$$5 \leq \chi(\mathbb{E}^2) \leq 9.$$
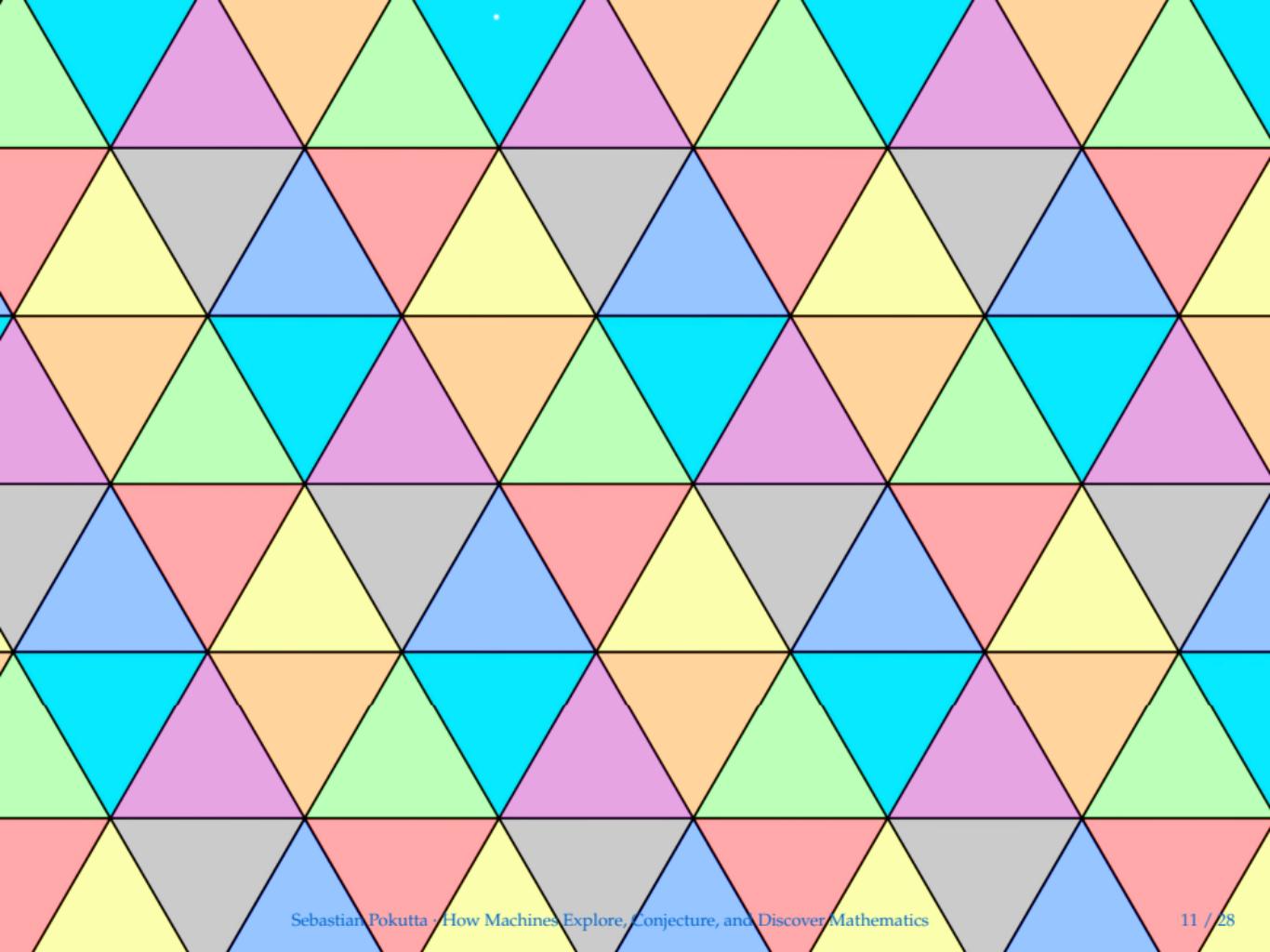
Upper bounds through colorings
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Explicit colorings $g : \mathbb{E}^2 \to [c] := \{1, \dots, c\}$, usually derived through tesselations using simple polytopal shapes, give

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

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

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

Upper bounds through colorings
The Hadwiger-Nelson Problem

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

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

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

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

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

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

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

input $\longrightarrow$

Blackbox

heavily parameterized
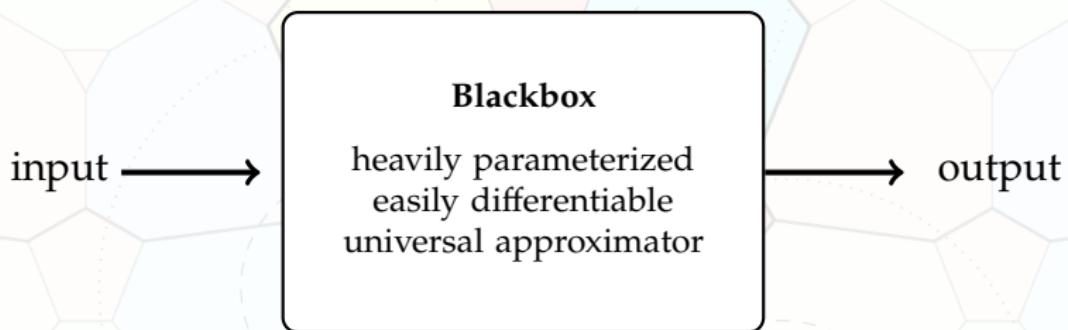easily differentiable
universal approximator

$\longrightarrow$ output

One second recap: Neural Networks

Neural Networks as Colorings

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Blackbox

heavily parameterized
easily differentiable
universal approximator

input $\longrightarrow$ output
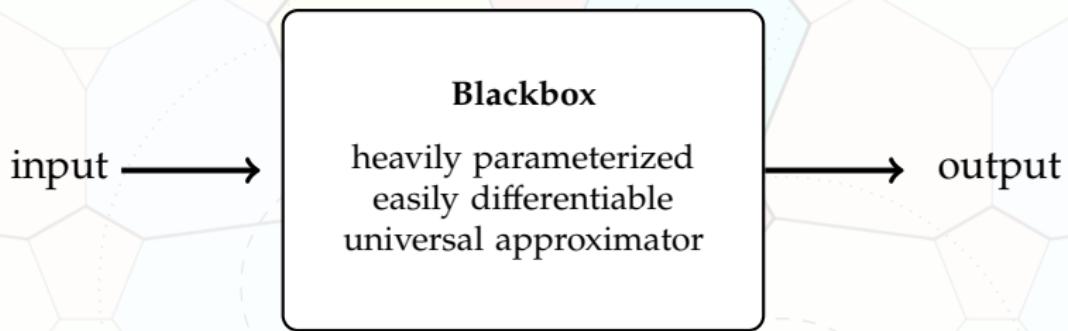
Theorem (Universal Approximation Theorem)

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

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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")
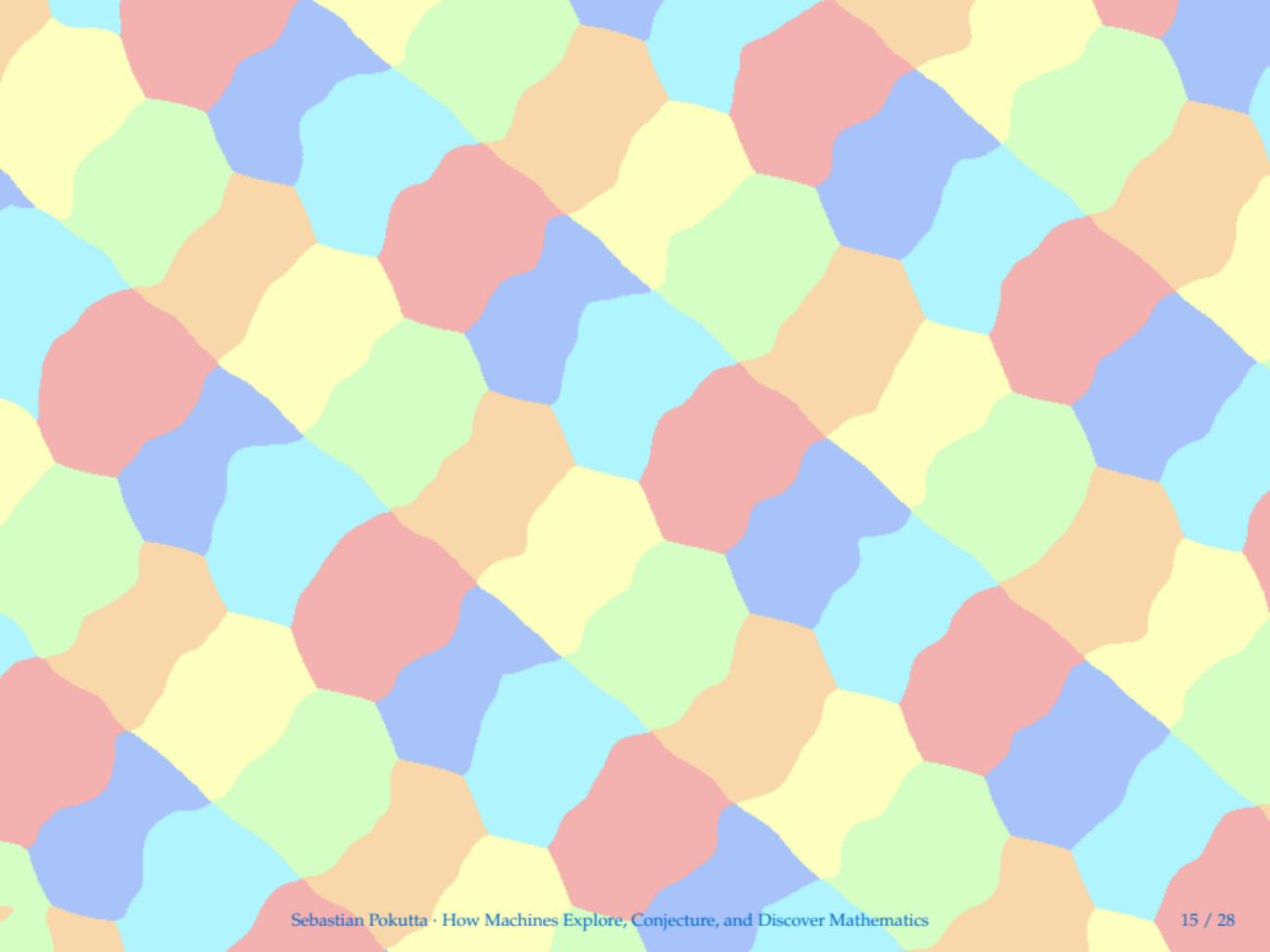
Unfortunately this coloring was already known...
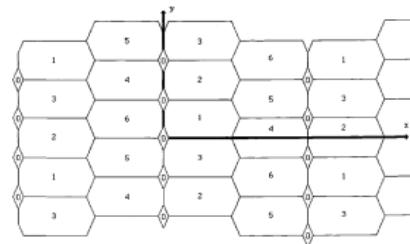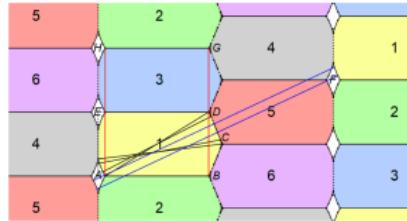
Neural Networks as Colorings

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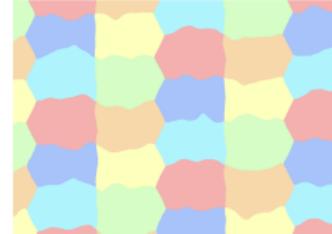
Theorem

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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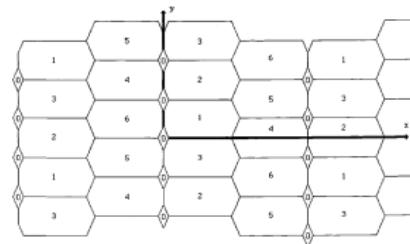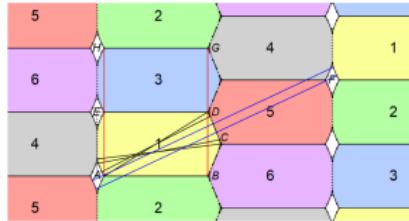
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Corollary

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

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

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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
Neural Networks as Colorings

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

Determine the continuum of six-colorings $X_6 = \{d \mid (1,1,1,1,1,d) \text{ can be realized}\}$.
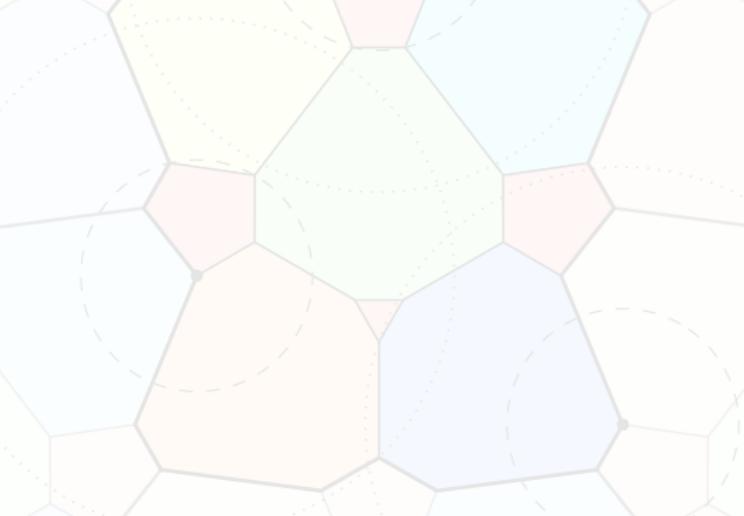
[Soifer, 1994a, Nash and Rassias, 2016]

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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. Part of 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]
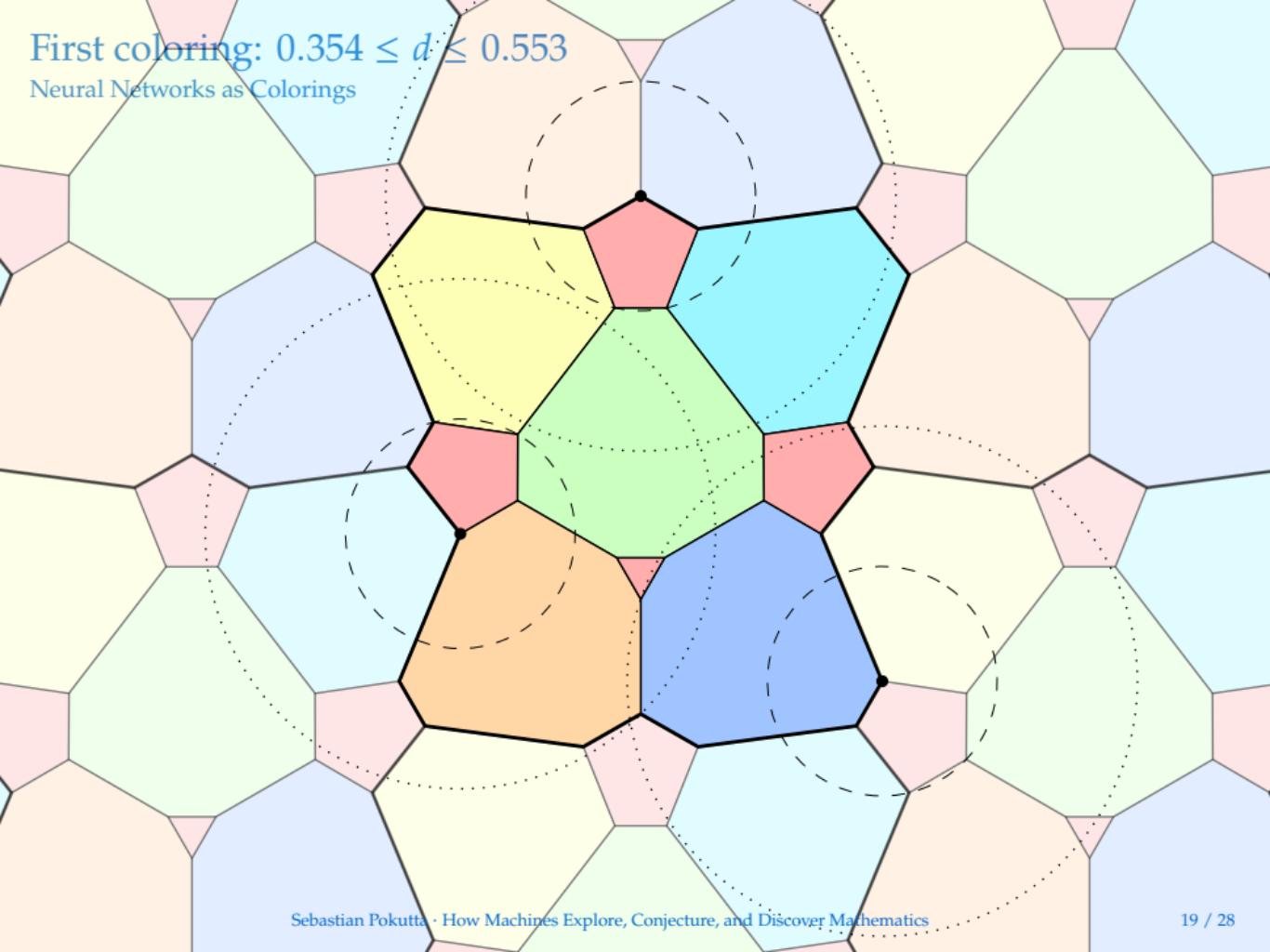
GEOMBINATORICS QUARTERLY

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

Geombinatorics

is a quarterly scientific journal of mathematics. It was established by editor-in-chief Alexander Soifer in 1991 and is published by the University of Colorado at Colorado Springs. The journal covers problems in discrete, convex, and combinatorial geometry, as well as related areas.
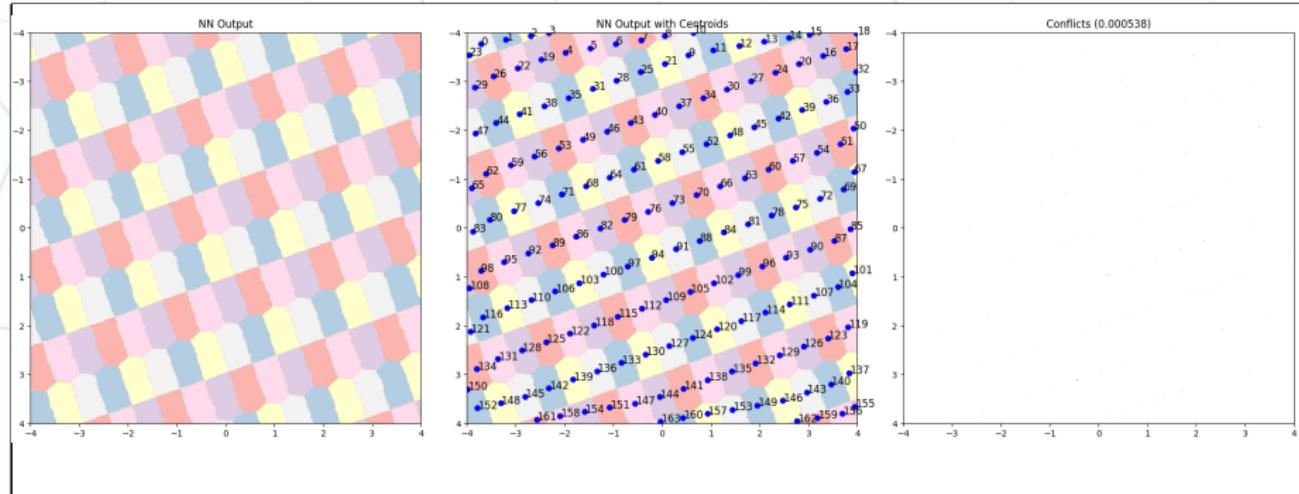
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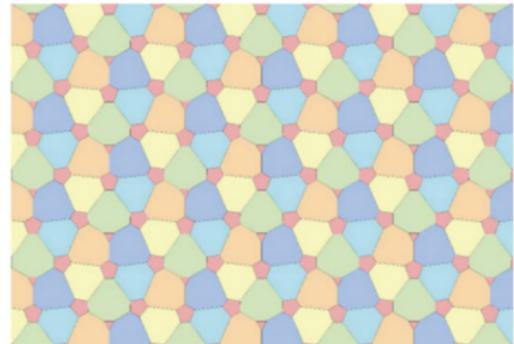
Volume XXXIV   October 2024   Issue 2

Just numerics...?
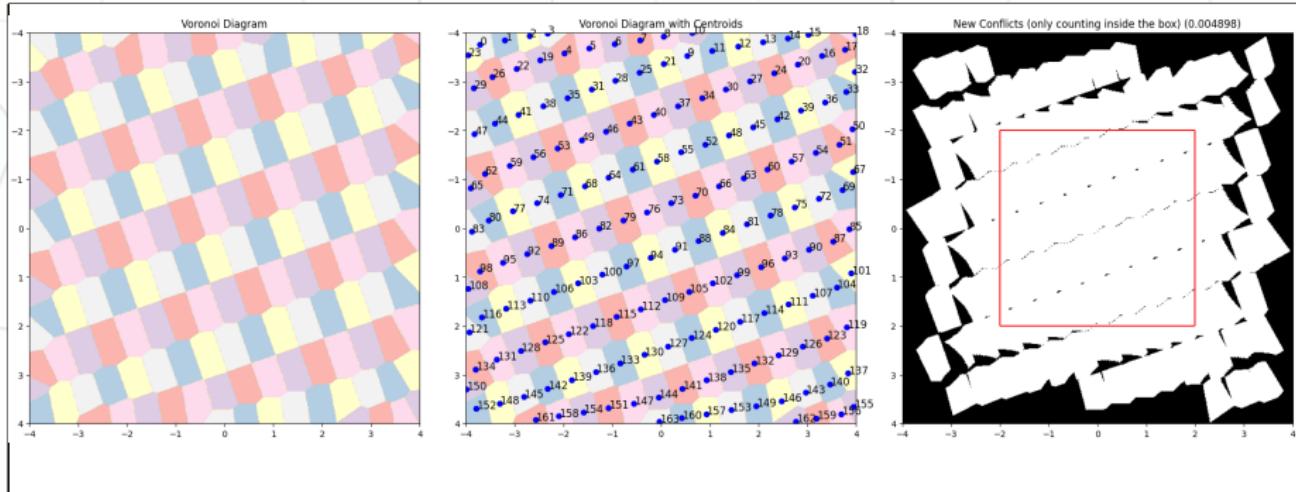## Neural Networks as Colorings

Just numerics...?

Neural Networks as Colorings
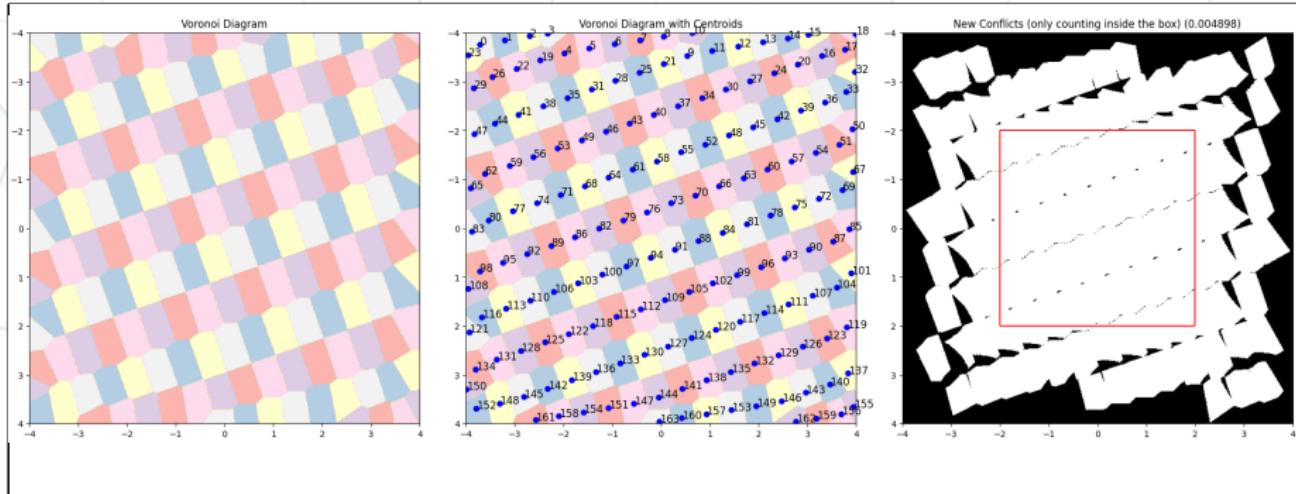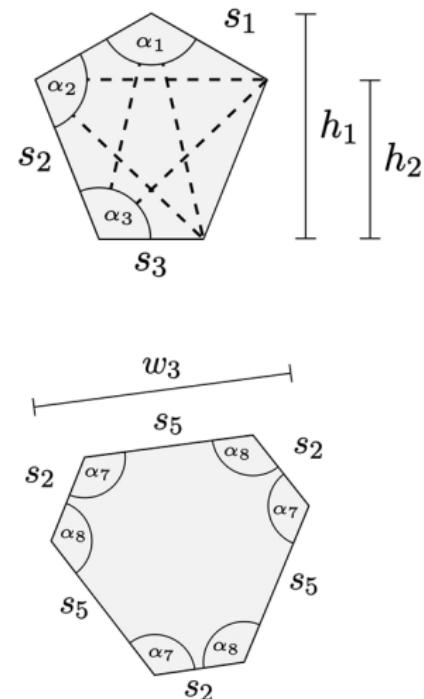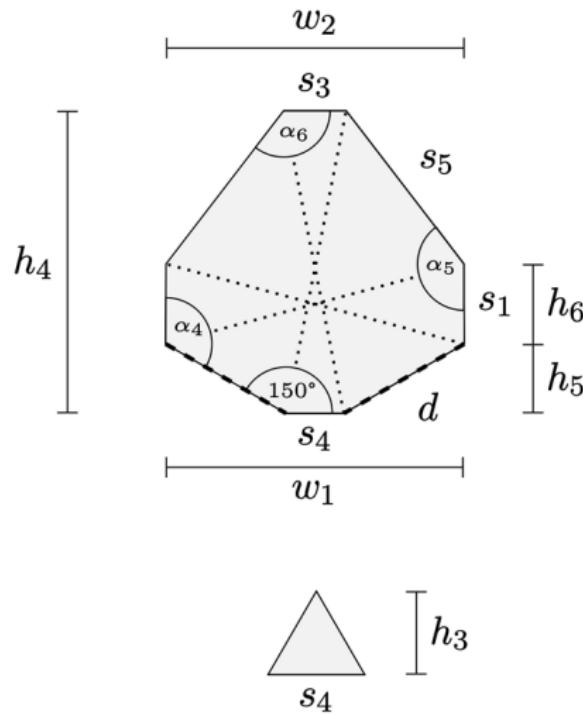
Just numerics...?

Neural Networks as Colorings

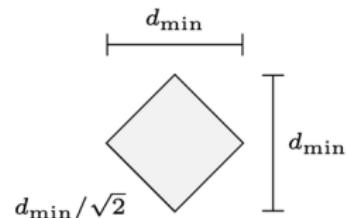Voronoi cell filtering...

⇒ Exact constructions for both colorings.

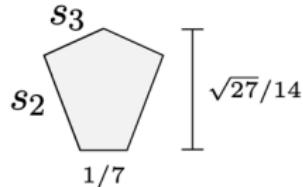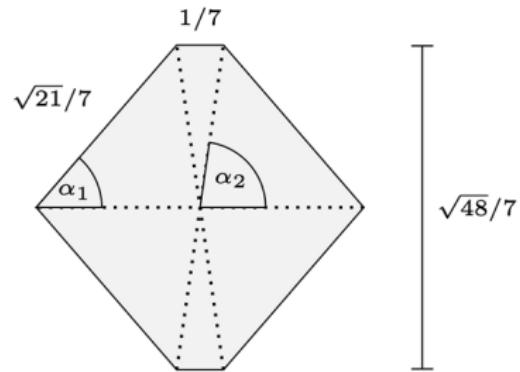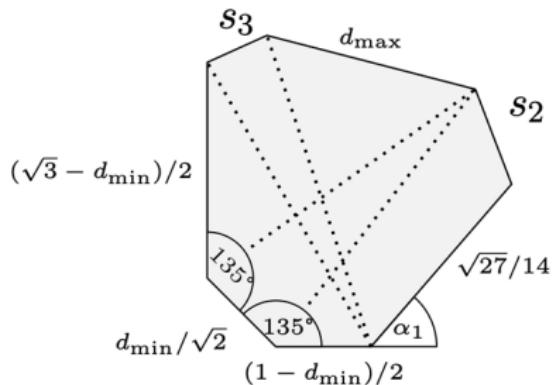Neural Networks as Colorings
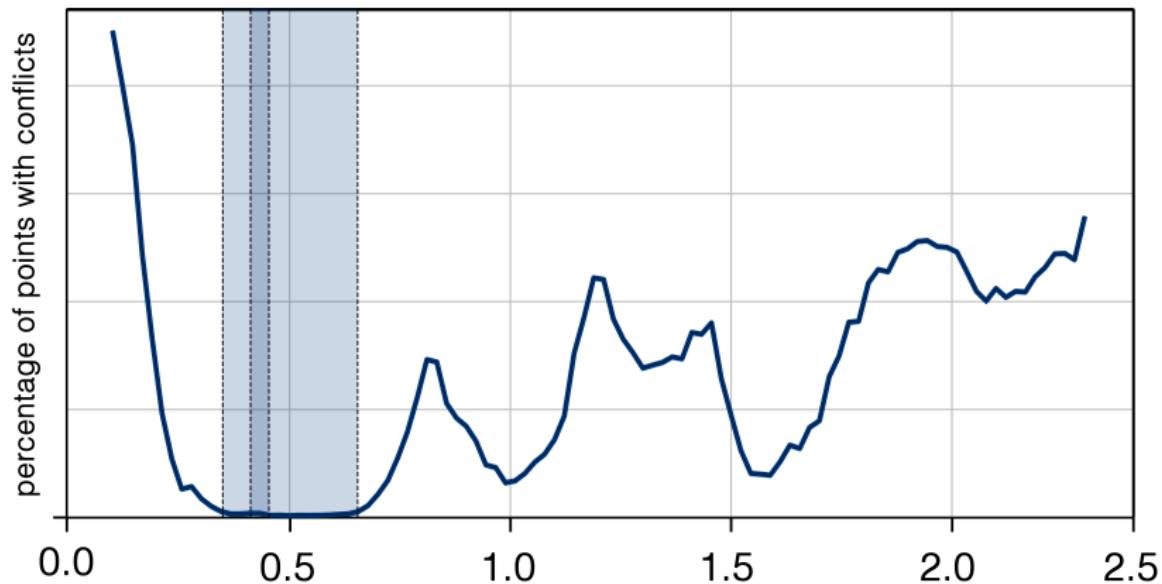
Numerical results showing the percentage of points with some conflict for a given forbidden distance d in the sixth color found over several runs.

Under the hood
Neural Networks as Colorings

External Links.

1. From a bad trip to colorings...
2. Example of system output
3. Coloring 1 for different d in last color

Open Problems and Final Remarks

The underlying optimization approach is very flexible:

1. Can we improve the upper bound of the polychromatic number from 6 to 5?

2. Can we improve the upper bound of the chromatic number of $\mathbb{E}^3$ from 15 to 14?

3. Can we apply the same ideas to generate graphons and other limit structures?

4. Can we use adversarial networks when the objective is non-differentiable?

5. Automatic formal verification of constructions with LEAN?

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4. Can we use adversarial networks when the objective is non-differentiable?

5. Automatic formal verification of constructions with LEAN?

The key question. Are we still working on the 6-coloring?
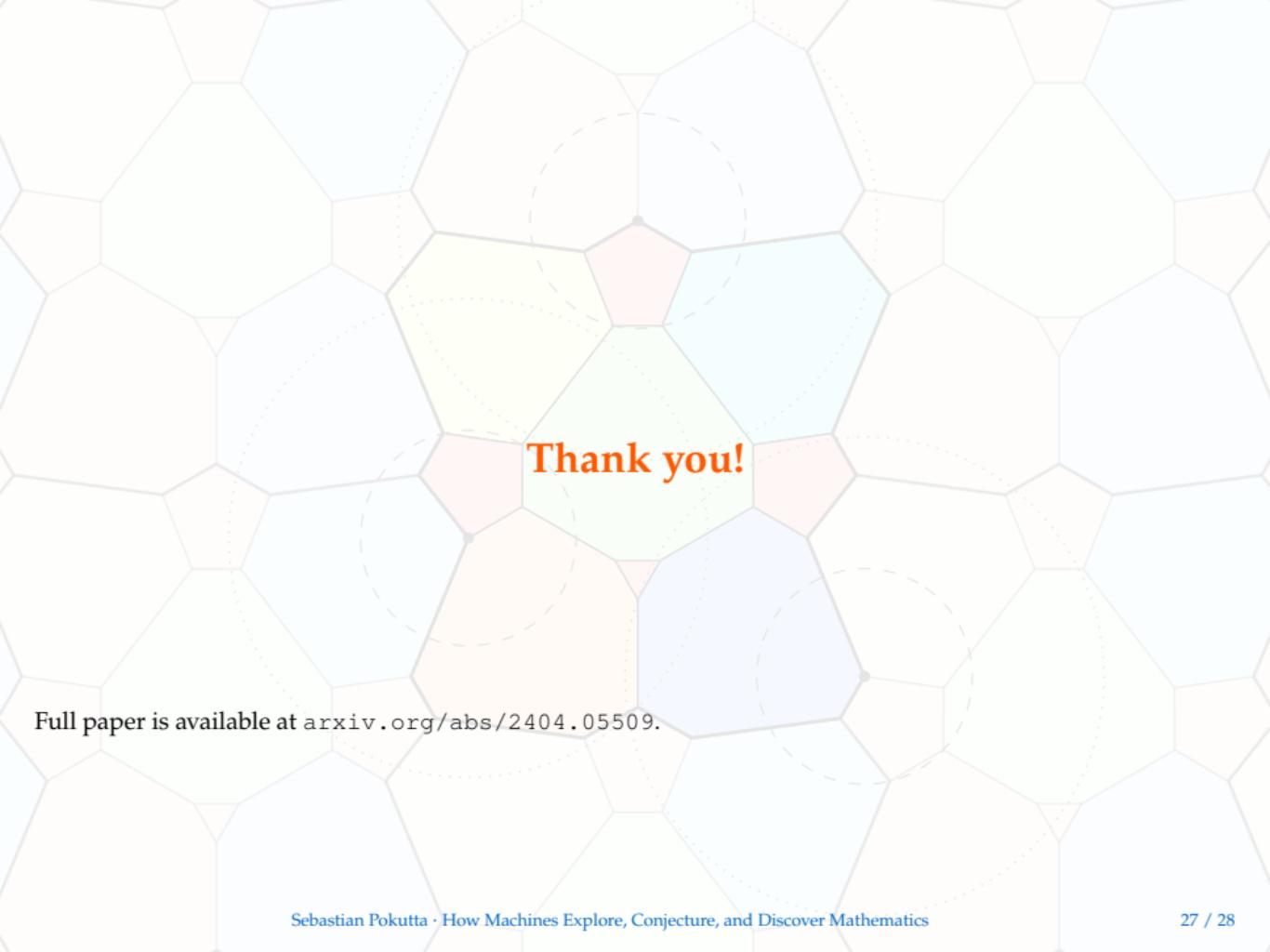
Thank you!

Full paper is available at arxiv.org/abs/2404.05509.

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