Automated Discovery of Extremal Unit-Distance Graphs

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MIT PRIMES-USA
Under the Direction of Andrew Gritsevskiy & Dr. Jesse Geneson

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About Me


SMITH


Weak Error Analysis and Small-Noise Optimization of Stochastic Linear Multistep Methods (SLMMs) for Itô and Lévy SDEs
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Under the Direction of Joonsoo Lee[1]
July 30, 2025
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About MIT PRIMES-USA



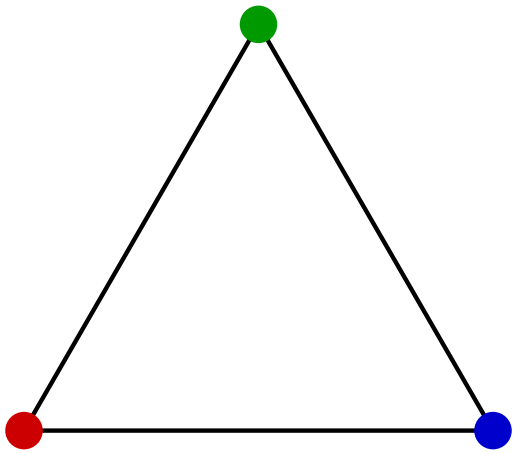
PRIMES: Program for Research in Mathematics, Engineering and Science for High School Students

The Hadwiger-Nelson Problem

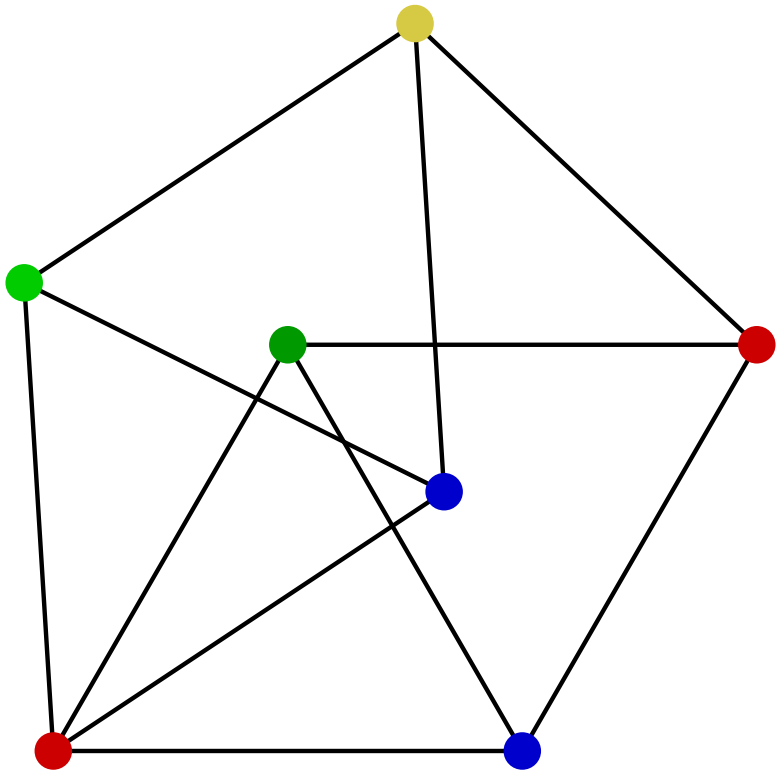
What is the minimum number of colors c required to color each point in the plane such that no two points at a distance 1 have the same color?

Asked by Nelson in 1950.

The Hadwiger–Nelson Problem: $c \geq 3$

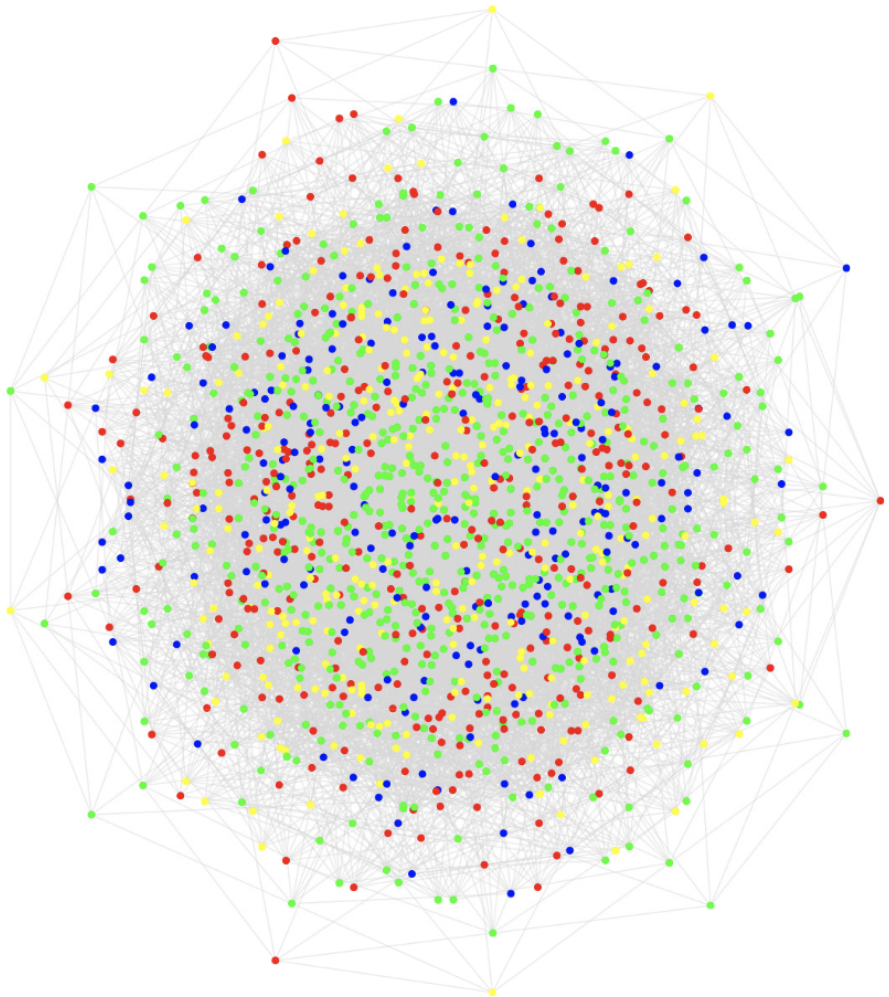


The Hadwiger–Nelson Problem: $c \geq 4$



Moser Spindle

The Hadwiger–Nelson Problem: $c \geq 5$



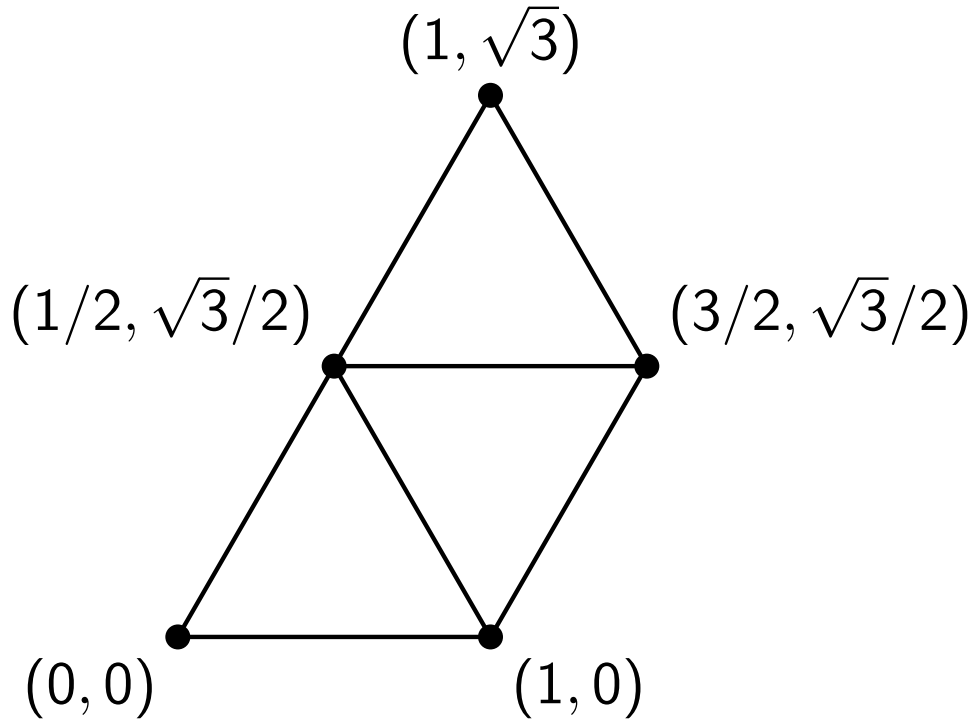
De Grey Graph (2018), 1581 vertices.

An Equivalent Question

- Let a *unit-distance graph* (UDG) be a graph with vertices being points in the plane, and edges between points with distance 1.

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- Over all finite UDGs, what is the maximum chromatic number?



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- How many edges can UDGs in $\mathbb{R}^d$ have, for $d \geq 2$?
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- **Dense UDGs give us information about many types of extremal UDGs.**

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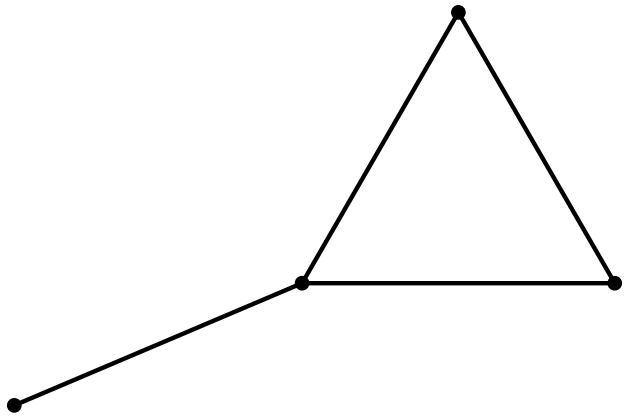
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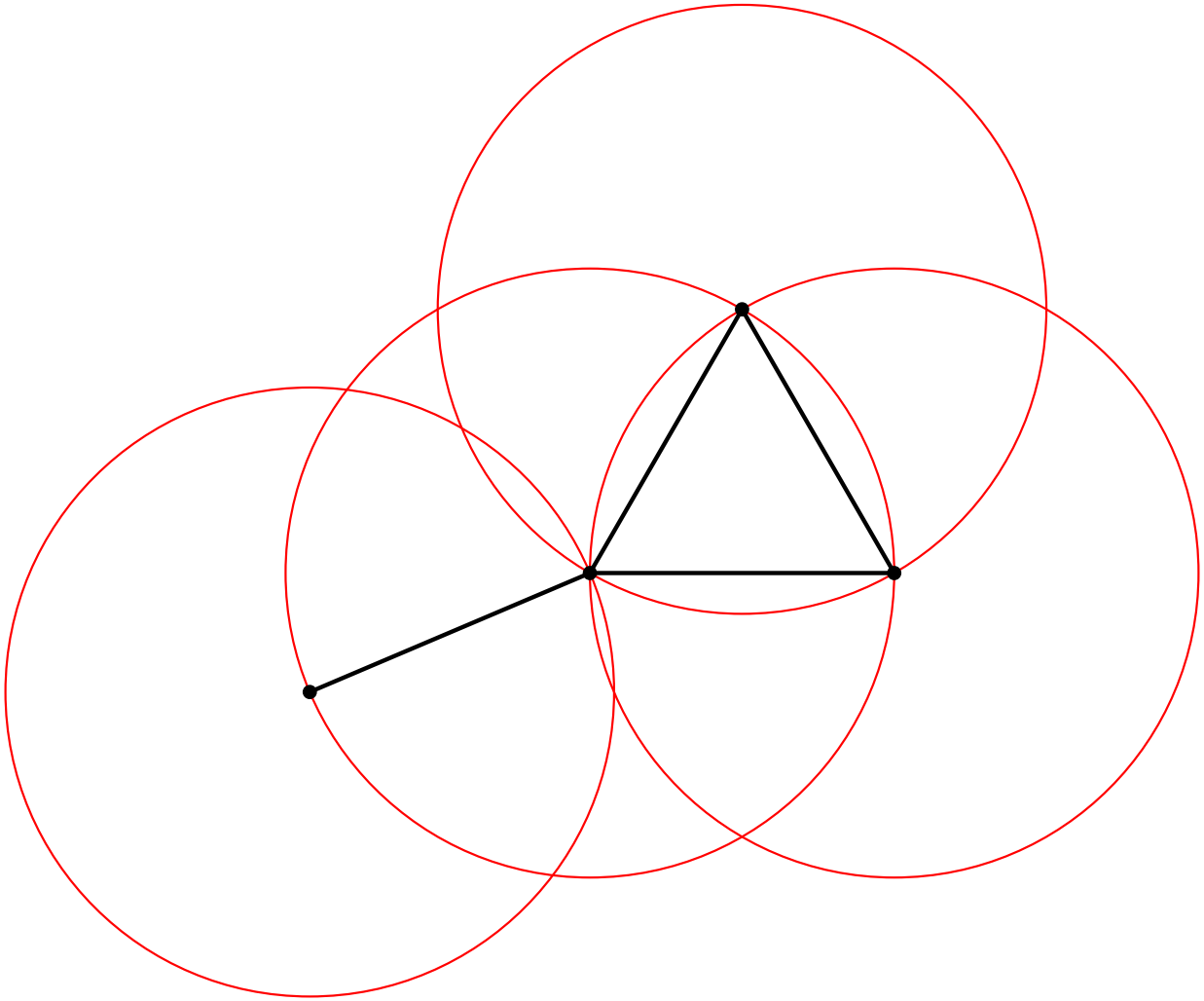
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- For $d = 2$, the densest UDGs on up to 21 vertices are known. It is suspected that we have discovered the densest possible UDGs on up to ≈ 30 vertices.
- For $d = 3$, little to no work has been done on computational discovery. Complexity increases greatly.

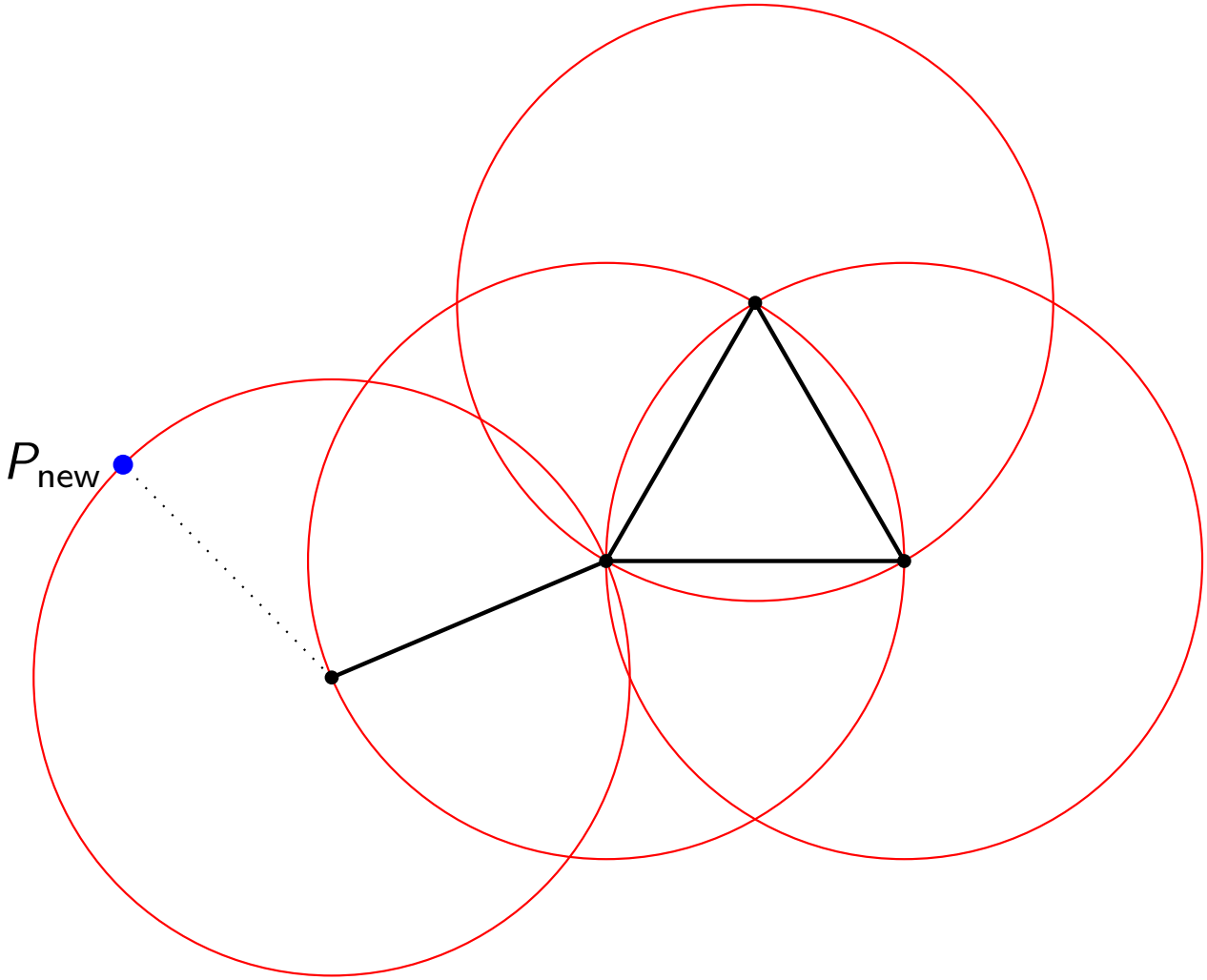
Searching For a UDG



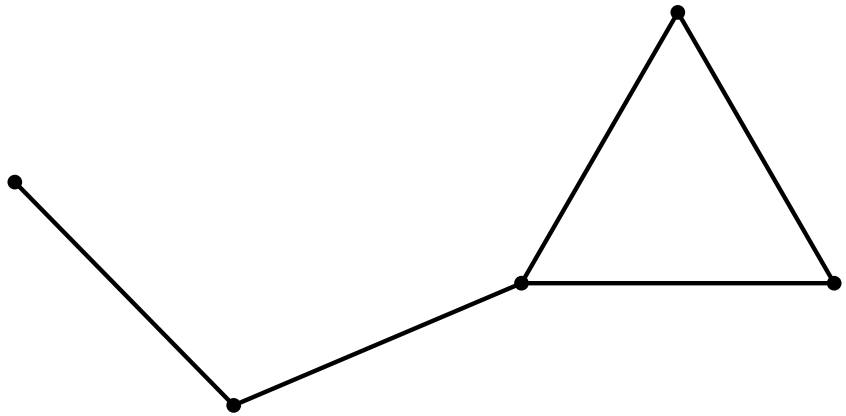
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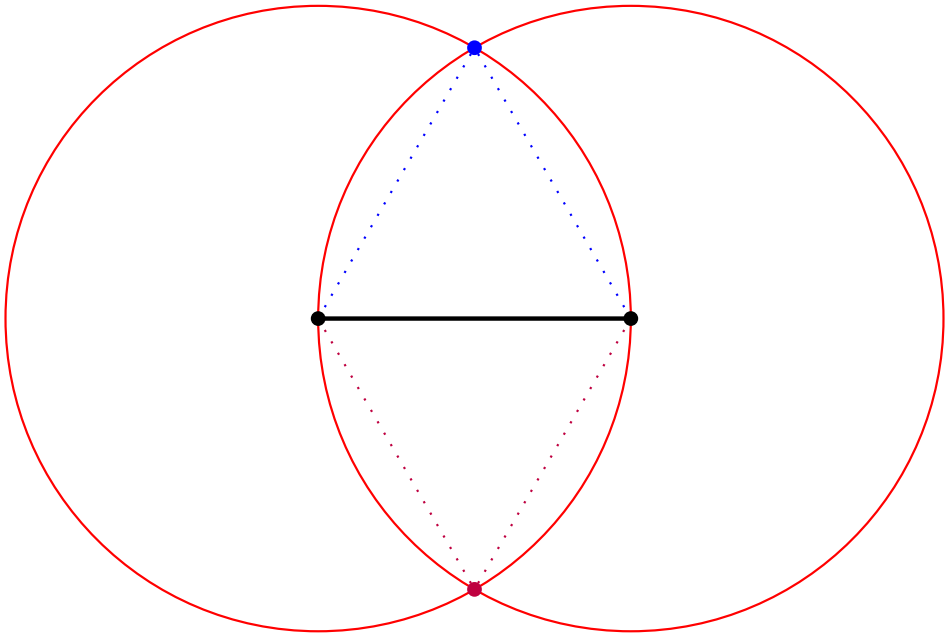
The Two Approaches

- **Continuous**: Use the whole circle.
- **Discrete**: Only use a (carefully selected) finite subset of each circle.

The Continuous Approach

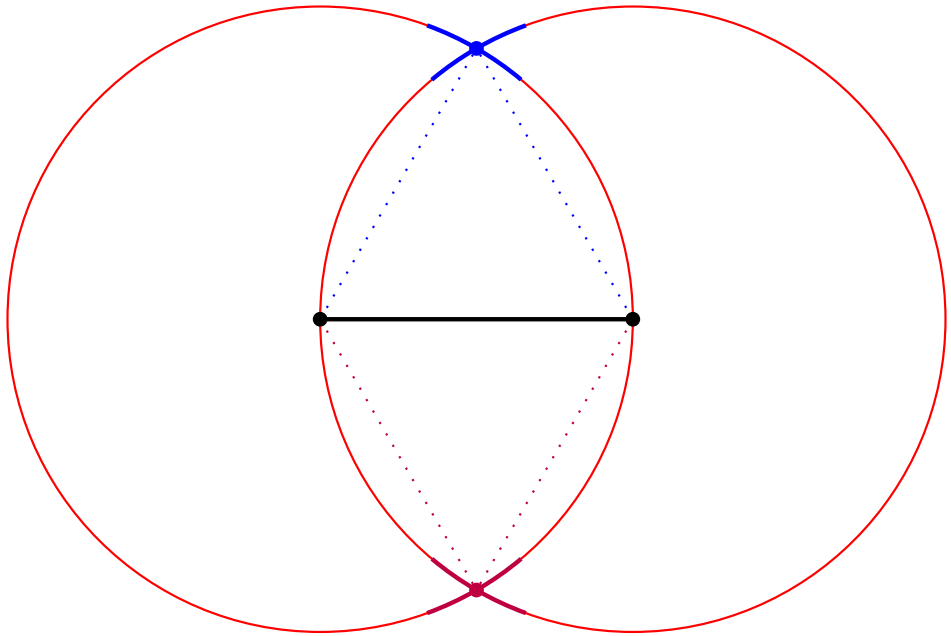
The Continuous Approach: The Issue

Infinite action space $\implies$ probability 0 of anything "useful"



The Continuous Approach: Potential Fix

Relax definition to ε-**UDGs**: include edges between points at distance 1 with a tolerance ε. In other words, edges are drawn between points with distance in $[1-\varepsilon, 1+\varepsilon]$.



The Continuous Approach: Another Issue

The following is an ε-UDG but not a UDG.



The Continuous Approach: A Final Fix

Let a (ε, δ)-**UDG** be an ε-UDG such that no two vertices are within a distance δ from each other.

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Theorem (Aggarwal, 2025)

There exist functions $\varepsilon(n, d), \delta(n, d) > 0$ such that any $(\varepsilon(n, d), \delta(n, d))$ unit-distance graph in $\mathbb{R}^d$ on n vertices is a unit-distance graph.

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The Discrete Approach

The Discrete Approach: Main Idea



Tangent: Algebraic Number Theory

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- Number Theory, the study of the integers $\mathbb{Z}$
- Primes, GCDs, LCMs, etc.
- The rational numbers $\mathbb{Q}$ help us study $\mathbb{Z}$ (it is useful to allow division).
- How do we study $\mathbb{Q}$?

Tangent: What is a Number Field?

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- Over $\mathbb{Q}$, $x^2 - 2$ does not factor (it is irreducible).
- If we **add** $\sqrt{2}$ **to** $\mathbb{Q}$, then it does factor!

$$x^2 - 2 = (x - \sqrt{2})(x + \sqrt{2}).$$

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- $\mathbb{Q}(7^{1/3}, \sqrt{-3}, \alpha)$, where $\alpha^5 + \alpha + 1 = 0$,
- NOT $\mathbb{Q}(\pi)$.

Tangent: Rings of Integers

- $O_{\mathbb{Q}} = \mathbb{Z}$
- $O_{\mathbb{Q}(\sqrt{2})} = \mathbb{Z}[\sqrt{2}]$, the set of $a + b\sqrt{2}$ for $a, b \in \mathbb{Z}$,
- $O_{\mathbb{Q}(i)} = \mathbb{Z}[i]$, the set of $a + bi$ for $a, b \in \mathbb{Z}$.

The Discrete Approach: Main Idea

Unit-distance graphs live in number fields!

Theorem (Aggarwal, 2025)

Let G be a finite unit-distance graph G in $\mathbb{R}^d$. Then there exists a number field $K \subset \mathbb{R}$ such that there exists a finite unit-distance graph G' in K^d such that G is a subgraph of G'.

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Theorem (Aggarwal, 2025)

Let $K \subset \mathbb{R}$ be a number field which is finite over $\mathbb{Q}$. Let $m \in \mathbb{N}$ and O_K be the ring of integers of K. Then there are finitely many vectors $\mathbf{v} \in \left(\frac{1}{m} \cdot O_K\right)^2$ such that $||\mathbf{v}|| = 1$.

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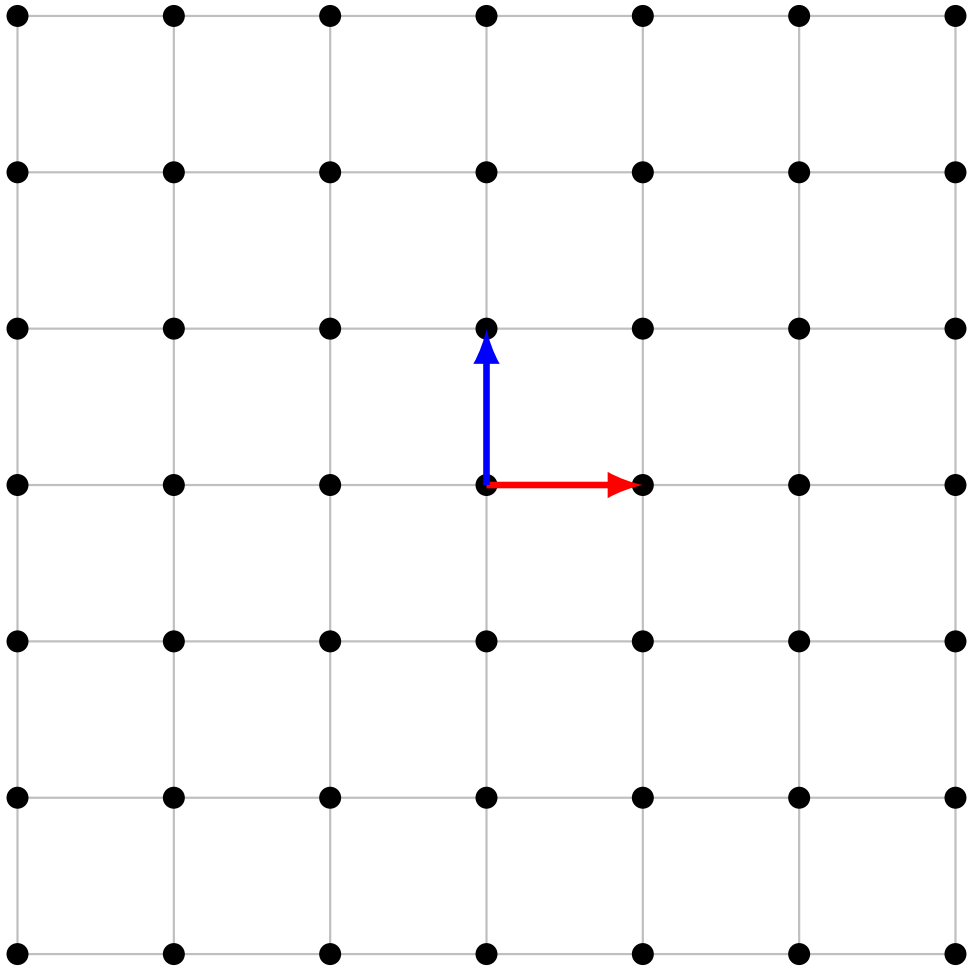
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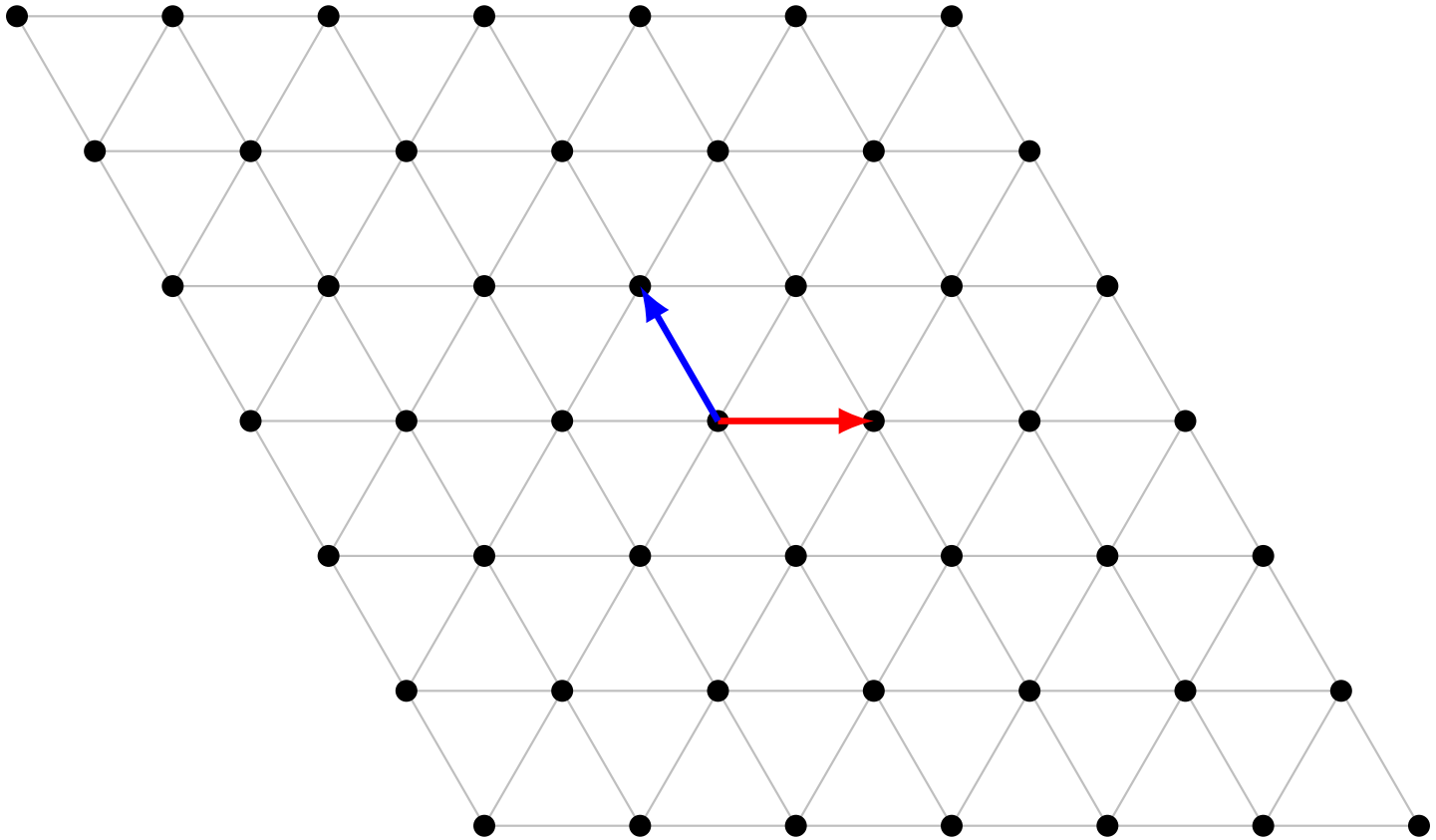
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It suffices to look at lattices!

Example: $\mathbb{Z}[i]$ as a lattice



Example: $\mathbb{Z}\left[\frac{1+i\sqrt{3}}{2}\right]$ as a lattice



The Discrete Approach: A New Question

How do we pick the right magnifying glass?



The Discrete Approach: A New Question

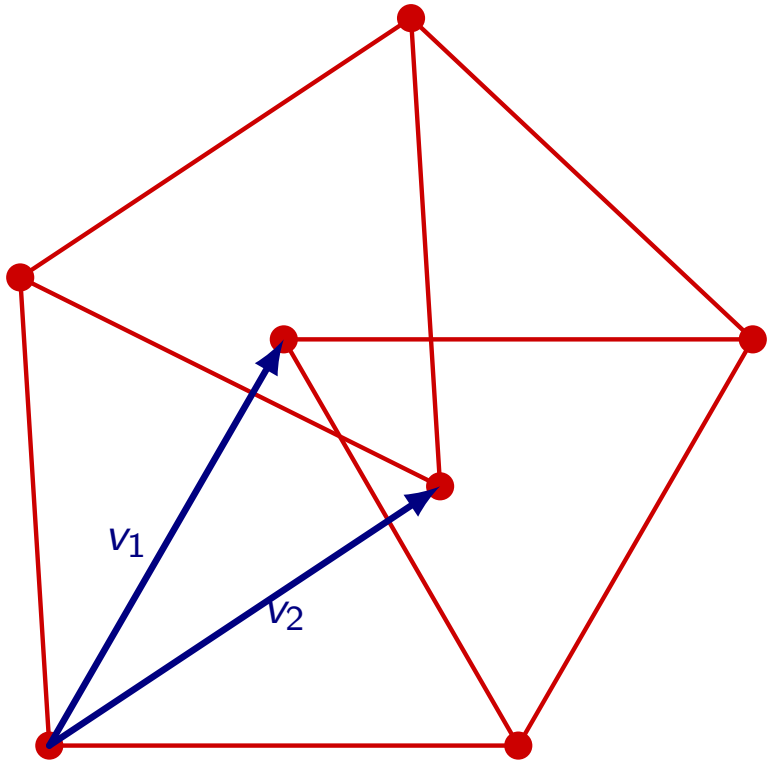
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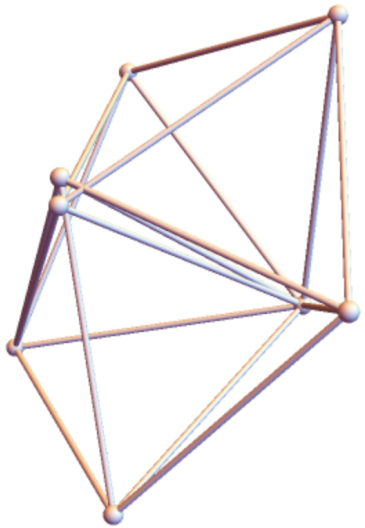
Bonus: Answering this question was the key to ChatGPT's resolution of the unit-distance conjecture!

The Discrete Approach: The Moser Lattice

The lattice the Moser Spindle lives in is $\mathbb{Z}\left[\frac{1+i\sqrt{3}}{2}, \frac{5+i\sqrt{11}}{6}\right]$:

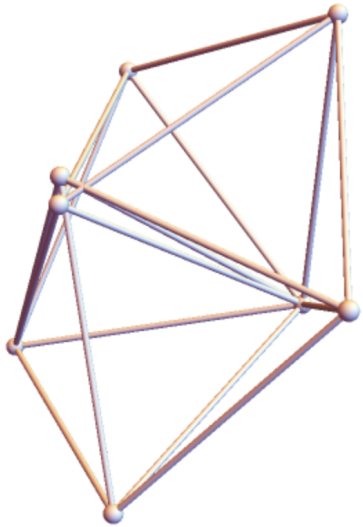


The Discrete Approach: The Raiskii Spindle



Raiskii Spindle in $\mathbb{R}^3$

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Raiskii Spindle in $\mathbb{R}^3$

Theorem (Aggarwal, 2025)

The lattice generated by the $\mathbb{R}^d$ Raiskii Spindle is a subset of $\mathbb{Q}[\sqrt{7d^2+8d}, \sqrt{2}, \sqrt{d+1}]^d$ and is generated by at most $2(d-1)$ vectors.

Recap

Continuous Approach:

- Be tolerant within a certain window $[1-\varepsilon, 1+\varepsilon]$.
- Make sure vertices are at least a distance δ away from each other.
- Search.

Discrete Approach:

- Search only within a lattice.
- Pick the Moser lattice in 2 dimensions and the Raiskii lattice in higher dimensions.

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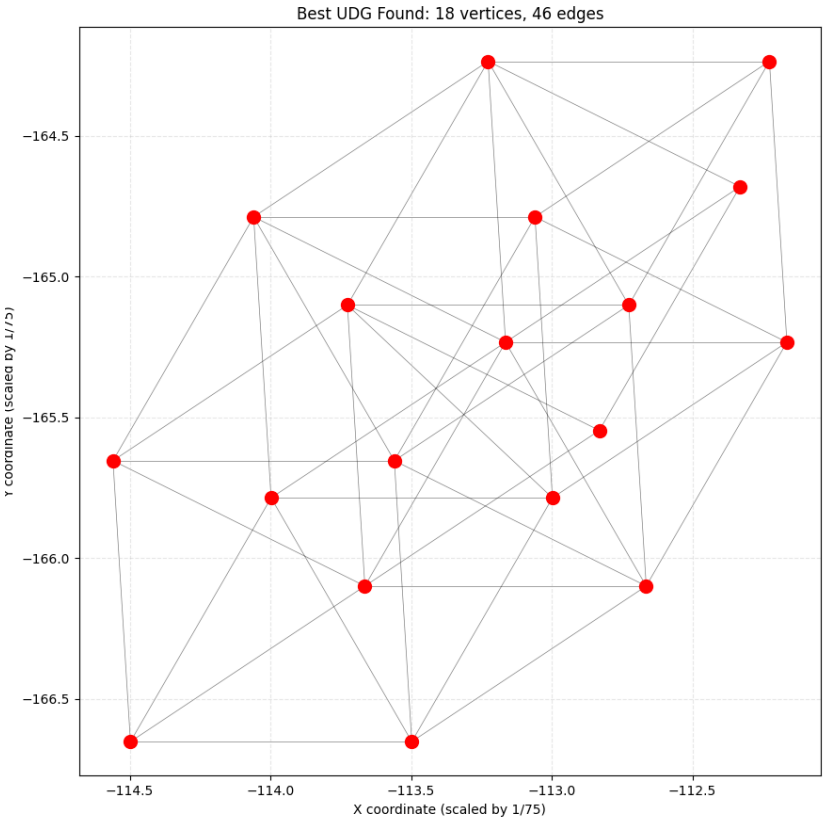
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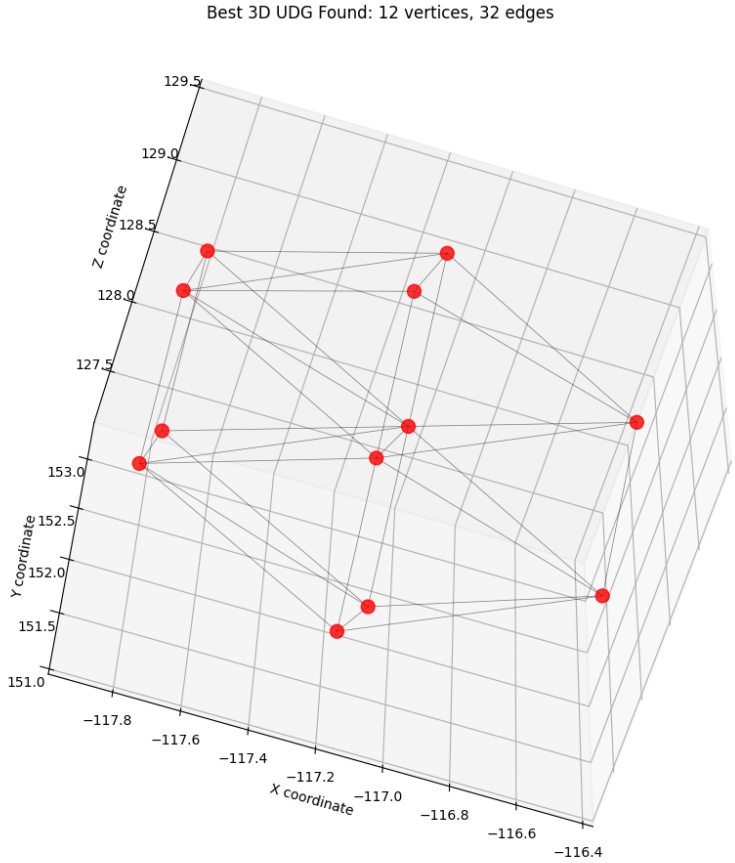
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Computational Results: Examples



Densest 18 vertex UDG in $\mathbb{R}^2$



Densest 12 vertex UDG in $\mathbb{R}^3$

Computational Results

n	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15
$u_3(n) \geq$	0	1	3	6	8	12	15	18	21	25	28	32	36	40	44

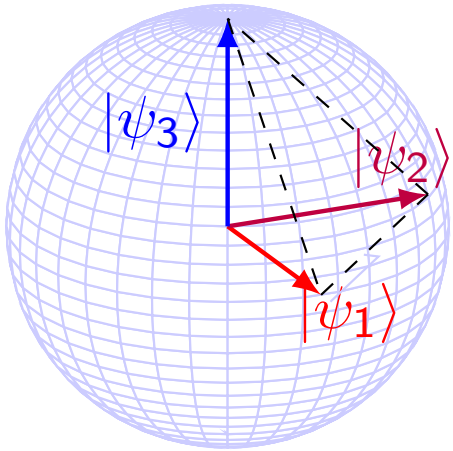
From Geometry to Quantum Logic

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- UDGs also arise in **quantum mechanics** through their special case: **orthogonality graphs**.
- Specifically, they model relationships between **quantum measurements** that can or cannot be simultaneously assigned definite outcomes.



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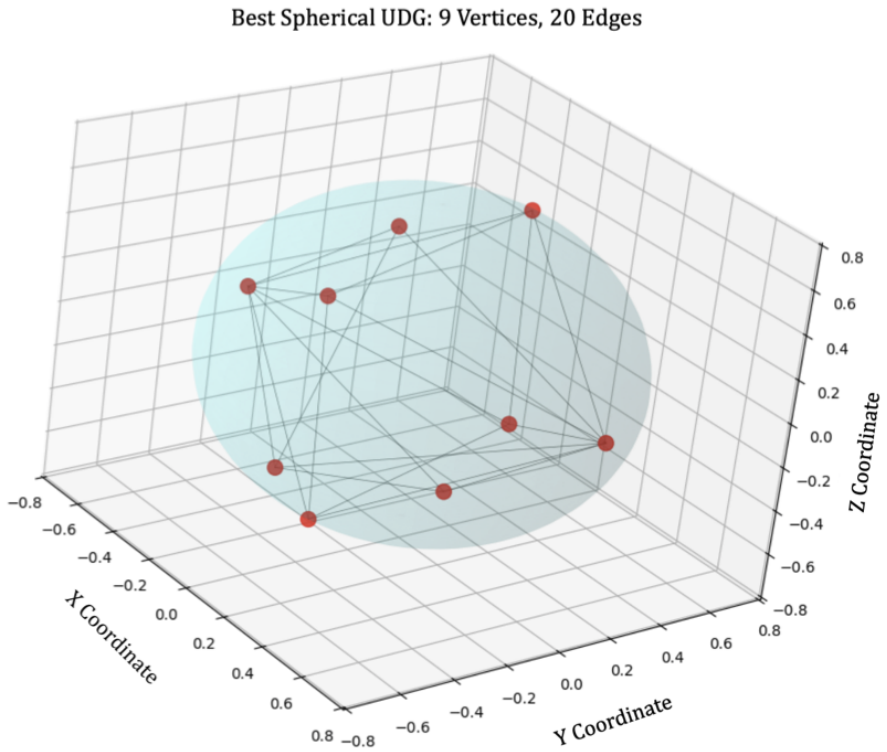
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  - 18-vector set in $\mathbb{R}^4$ (Cabello et al., 1996)

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- Computational discovery of Kochen-Specker Sets?



Thanks to:

- My wonderful mentors Andrew Gritsevskiy and Dr. Jesse Geneson,
- The MIT PRIMES-USA program for this opportunity to conduct research,
- My family and friends for their support throughout this process.

References I

[1] Peter Engel et al. *Diverse beam search to find densest-known planar unit distance graphs*. 2024. arXiv: 2406.15317 [math.CO]. URL: https://arxiv.org/abs/2406.15317.

[2] Leo Moser and William Moser. "Solution to problem 10". In: *Canadian Mathematical Bulletin* 4 (1961), pp. 187–189. DOI: 10.1017/S0008439500025753.

[3] Aubrey D. N. J. de Grey. *The chromatic number of the plane is at least 5*. 2018. arXiv: 1804.02385 [math.CO]. URL: https://arxiv.org/abs/1804.02385.

[4] A Peres. "Two simple proofs of the Kochen-Specker theorem". In: *Journal of Physics A: Mathematical and General* 24.4 (Feb. 1991), p. L175. DOI: 10.1088/0305-4470/24/4/003. URL: https://dx.doi.org/10.1088/0305-4470/24/4/003.

References II

[5] Adán Cabello, JoséM. Estebaranz, and Guillermo García-Alcaine. "Bell-Kochen-Specker theorem: A proof with 18 vectors". In: *Physics Letters A* 212.4 (Mar. 1996), pp. 183–187. ISSN: 0375-9601. DOI: 10.1016/0375-9601(96)00134-x. URL: http://dx.doi.org/10.1016/0375-9601(96)00134-X.

[6] Boris Alexeev, Dustin G. Mixon, and Hans Parshall. *The Erdős unit distance problem for small point sets*. 2025. arXiv: 2412.11914 [math.CO]. URL: https://arxiv.org/abs/2412.11914.

[7] Simon Kochen and Ernst P. Specker. "The Problem of Hidden Variables in Quantum Mechanics". In: *Journal of Mathematics and Mechanics* 17.1 (1967), pp. 59–87.