

Conjecture generation using Machine Intelligence



Challenger Mishra, Computer Laboratory, Cambridge: July 2023

Hilbert's 23 problems



The thirteenth problem:

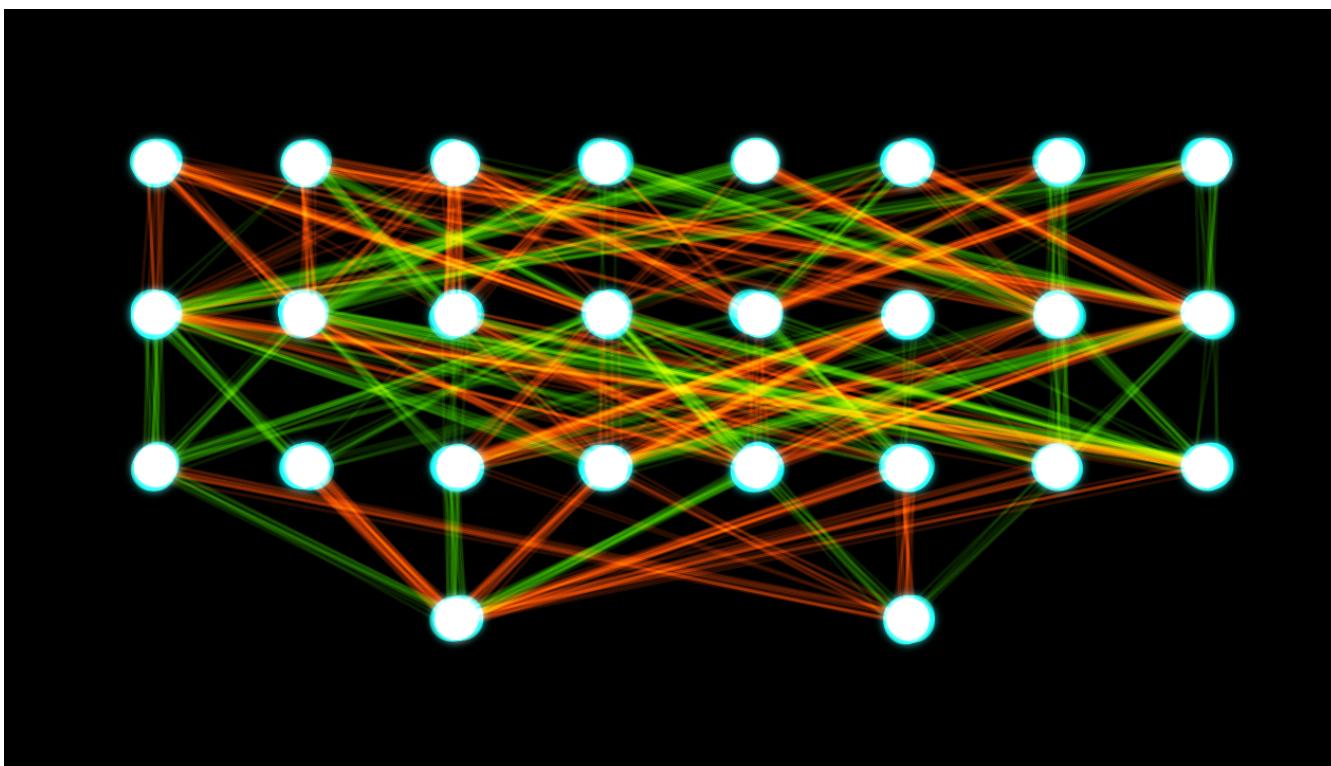
$$x^7 + a x^3 + b x^2 + c x + 1 = 0.$$

Can one write down the solution (x) as a composition of a finite number of 2 variable algebraic/continuous functions? – Hilbert (1900)

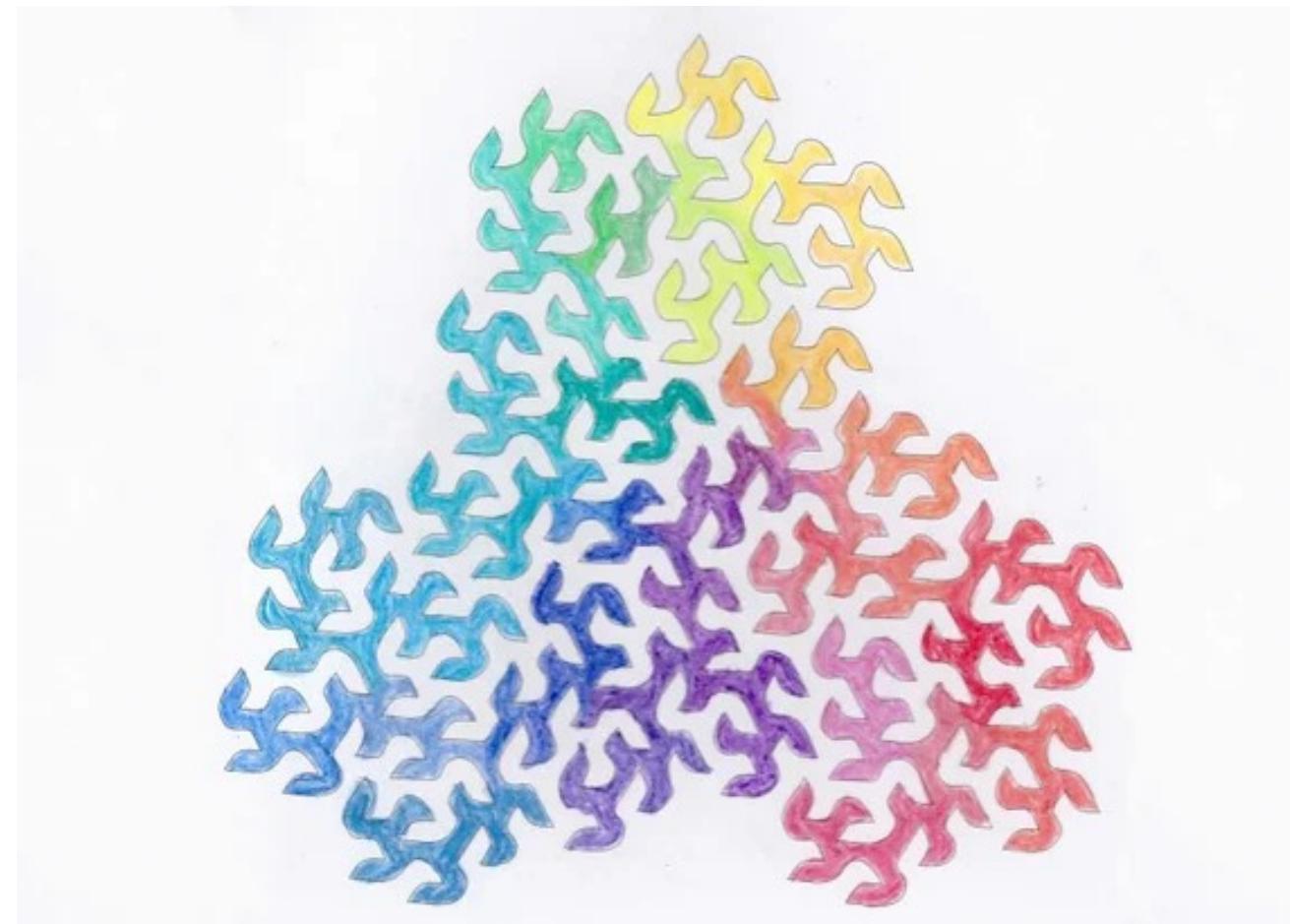
It is possible to construct any continuous function involving multiple variables using a finite set of three-variable functions
[Kolmogorov, 1956]

Only two variable functions are required!
[Arnold, 1957 (aged 19)]

A mathematical supernova



Neurocomputing



Kolmogorov Arnold representation

$$f(\mathbf{x}) = f(x_1, \dots, x_n) = \sum_{q=0}^{2n} \Phi_q \left(\sum_{p=1}^n \phi_{q,p}(x_p) \right).$$

$$f(\mathbf{x}) = \sum_{q=0}^{2n} \Phi \left(\sum_{p=1}^n \lambda_p \phi(x_p + \eta q) + q \right).$$

"The Kolmogorov theorem was discovered during a friendly mathematical duel between Kolmogorov and fellow Soviet Mathematician V.I. Arnold ... Kolmogorov won." - Robert Hecht-Nielsen

Hilbert's conjectures beg the question what constitutes a good conjecture?



Geometric Sampling Techniques –
Theo Long, MPhil, Cambridge

The subtle art of making Conjectures



Conway: Oberwolfach 1987
(with Hirzebruch)

Robbert Dijkgraaf: [https://
www.quantamagazine.org/the-
subtle-art-of-the-mathematical-
conjecture-20190507/](https://www.quantamagazine.org/the-subtle-art-of-the-mathematical-conjecture-20190507/)

Good conjectures are milestones in mathematics. They are

1. nontrivial;
2. with potentially substantial evidence in favour of it (e.g., Goldbach's conjecture);
3. terse (e.g., Collatz conjecture);
4. can potentially unlock new theorems (e.g., RH);
5. "outrageous" – John Conway.

If a conjecture is proved within a few months, then perhaps its creator should have pondered it a bit longer before announcing it to the world. – Robbert Dijkgraaf (we might ignore this sagely advice atm).

Let's consider a class of conjectures ...

Conjectures on Inequalities

INEQUALITIES

By

G. H. HARDY

J. E. LITTLEWOOD

G. PÓLYA

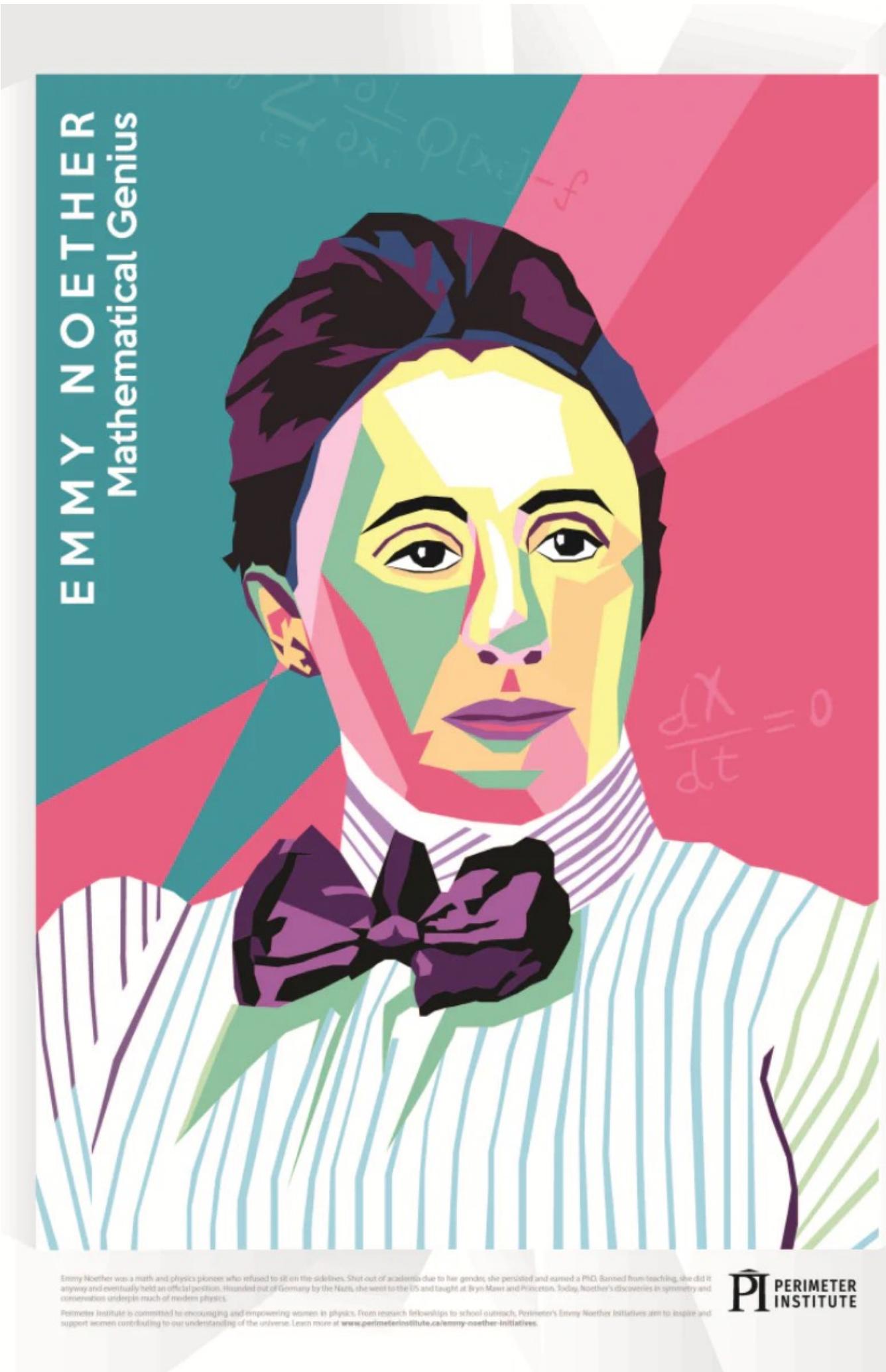
It is often really difficult to trace the origin of a familiar inequality. It is quite likely to occur first as an auxiliary proposition, often without explicit statement, in a memoir on geometry or astronomy; it may have been rediscovered, many years later, by half a dozen different authors; and no accessible statement of it may be quite complete. We have almost always found, even with the most famous inequalities, that we have a little new to add.

CAMBRIDGE
AT THE UNIVERSITY PRESS
1934

$$f < g$$

Wide ranging applications result from an ability to bound functions in mathematics.

We aim to build an oracle that interacts with mathematicians to generate novel conjectures about inequalities which agree on a large amount of data. First we address the question: is there any structure in this space of relations?

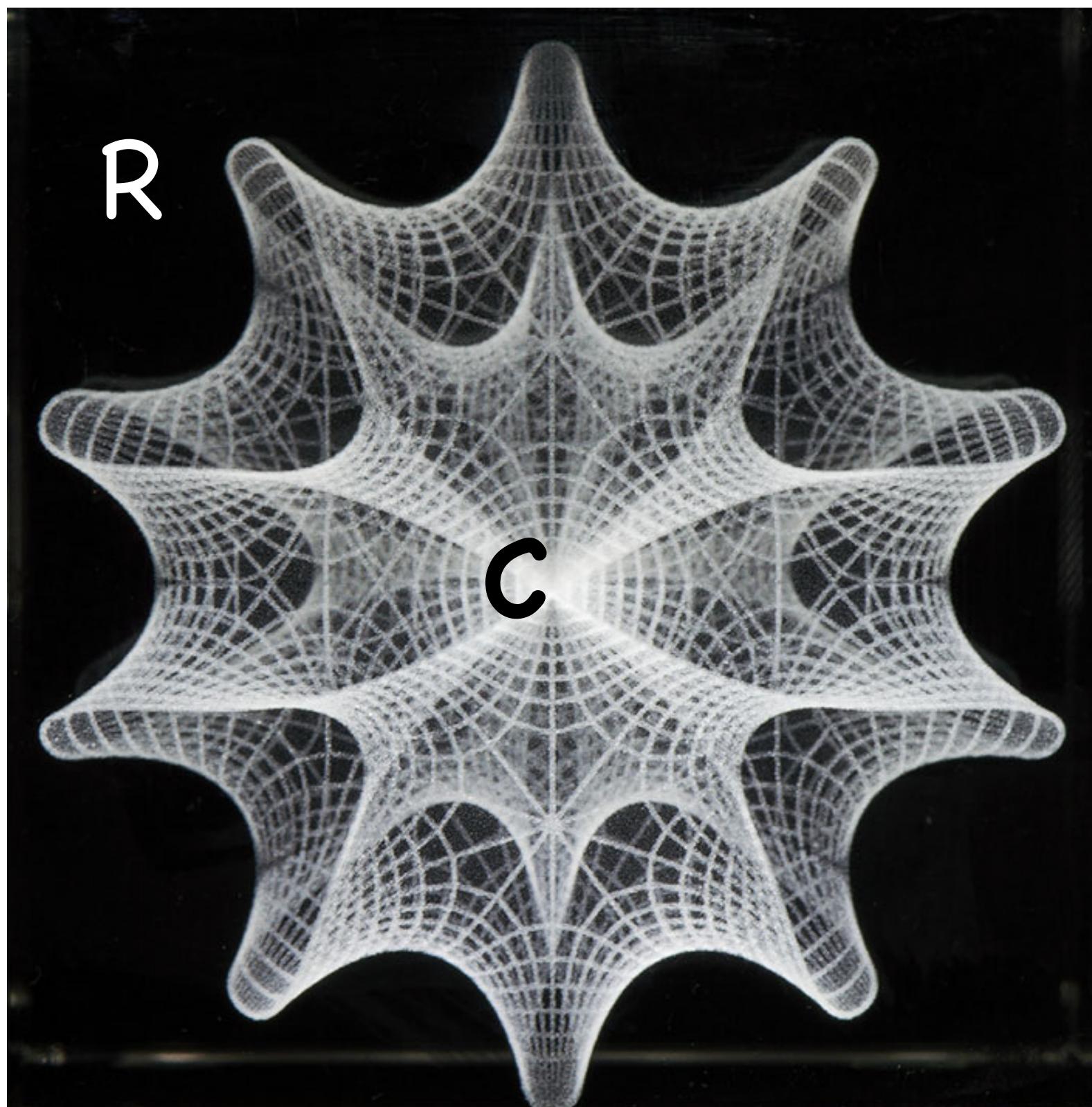


Symmetry as an organising principle for conjectures

Symmetries are a guiding principle for understanding nature through modern theoretical physics.

We now seek to understand whether tools from classical invariant theory help us give structure to a space of inequality relations.

The space of Relations and Conjectures



Let f, g be continuous real valued functions over a compact set D .

Space of relations (R): tuples (f, g) .

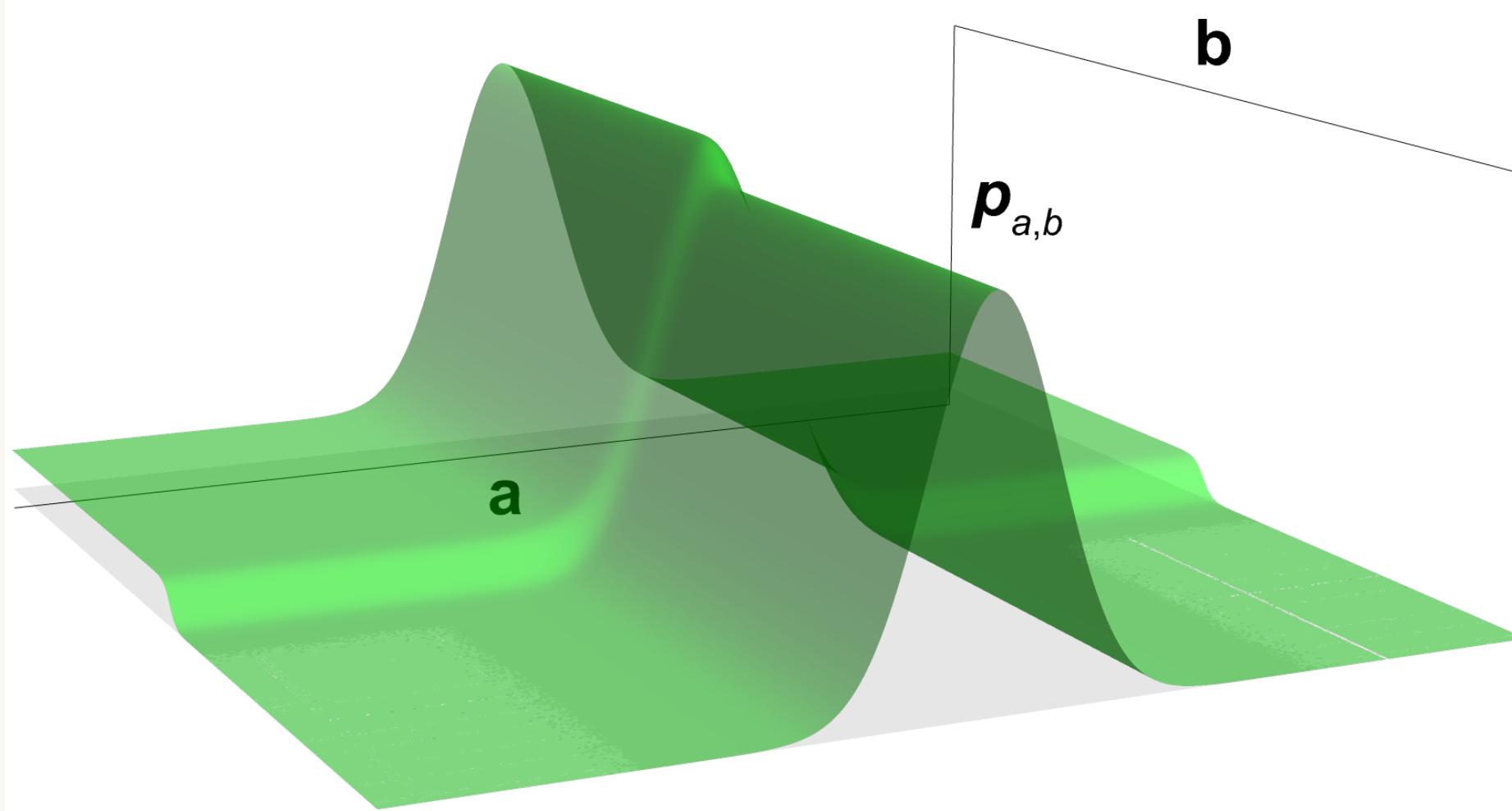
Space of conjectures (C): tuples (f, g) such that $f < g$ over D .

Note $(0,0) \in R$ but $(0,0) \notin C$.

We pose the following questions:

1. What is the largest group acting linearly on C ?
2. Are there any free group actions on this space?

The space of conjectures (\mathcal{C})



A visualisation of a smooth approximation of $p(a,b) := 1 + \delta(a) - \text{sgn}(b)$. When the smooth approximation approaches $p(a,b)$, the conditions $a \neq 0$ and $b > 0$ are met strictly.

Consider a set of linear transformations acting on \mathcal{C} .

$$\mathcal{G} := \{A \in \mathbf{GL}(2, \mathbb{R}) : A(f, g) \in \mathcal{C}, \forall (f, g) \in \mathcal{C}\}, \text{ where}$$

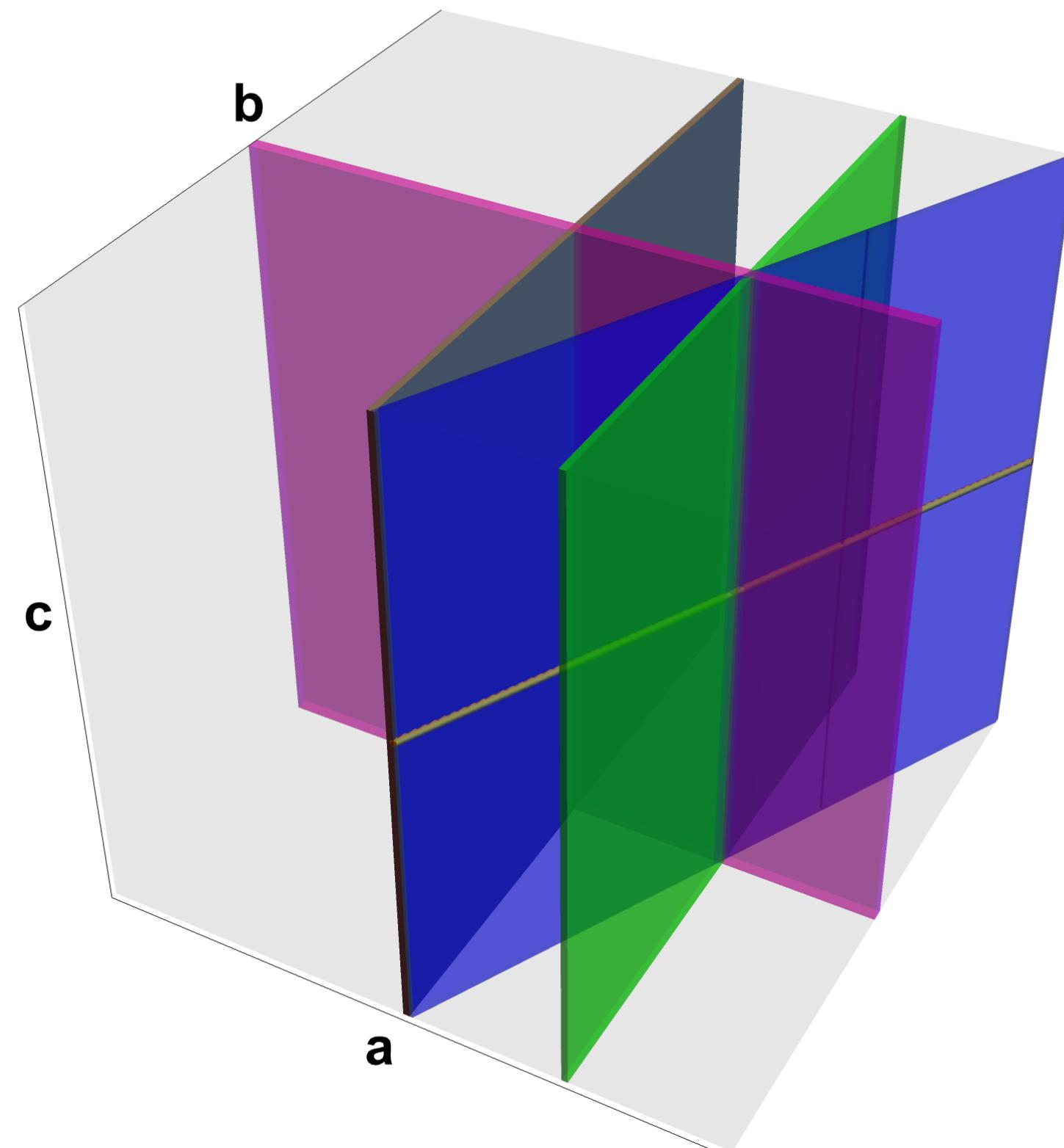
$$A = \begin{pmatrix} 1 & -1 \\ 1 & 1 \end{pmatrix} \begin{pmatrix} a & c \\ 0 & b \end{pmatrix} \begin{pmatrix} 1 & 1 \\ -1 & 1 \end{pmatrix}; \quad a, b, c \in \mathbb{R}, a \neq 0, b > 0.$$

This forms a group and admits a semi direct product structure: $\mathcal{G} = \mathcal{T} \rtimes \mathcal{H}$, where \mathcal{T} is a group of positive dilations parameterised by b , and \mathcal{H} is the subgroup corresponding to $b=1/2$.

Group elements can be thought of as zeroes of the function $p(a, b) := 1 + \delta(a) - \text{sgn}(b)$.

Does this group or any subgroup act freely on \mathcal{C} ? If so, perhaps we could study quotients of \mathcal{C} .

The space of conjectures (C)



Various subgroups of G .

$$\mathcal{H} := \mathcal{G} |_{b=1/2}$$

$$\mathcal{J}_1 := \mathcal{G} |_{a=b}$$

$$\mathcal{J}_2 := \mathcal{G} |_{a=\frac{1}{2}}$$

$$\mathcal{T} := \mathcal{G} |_{a=b, c=0}$$

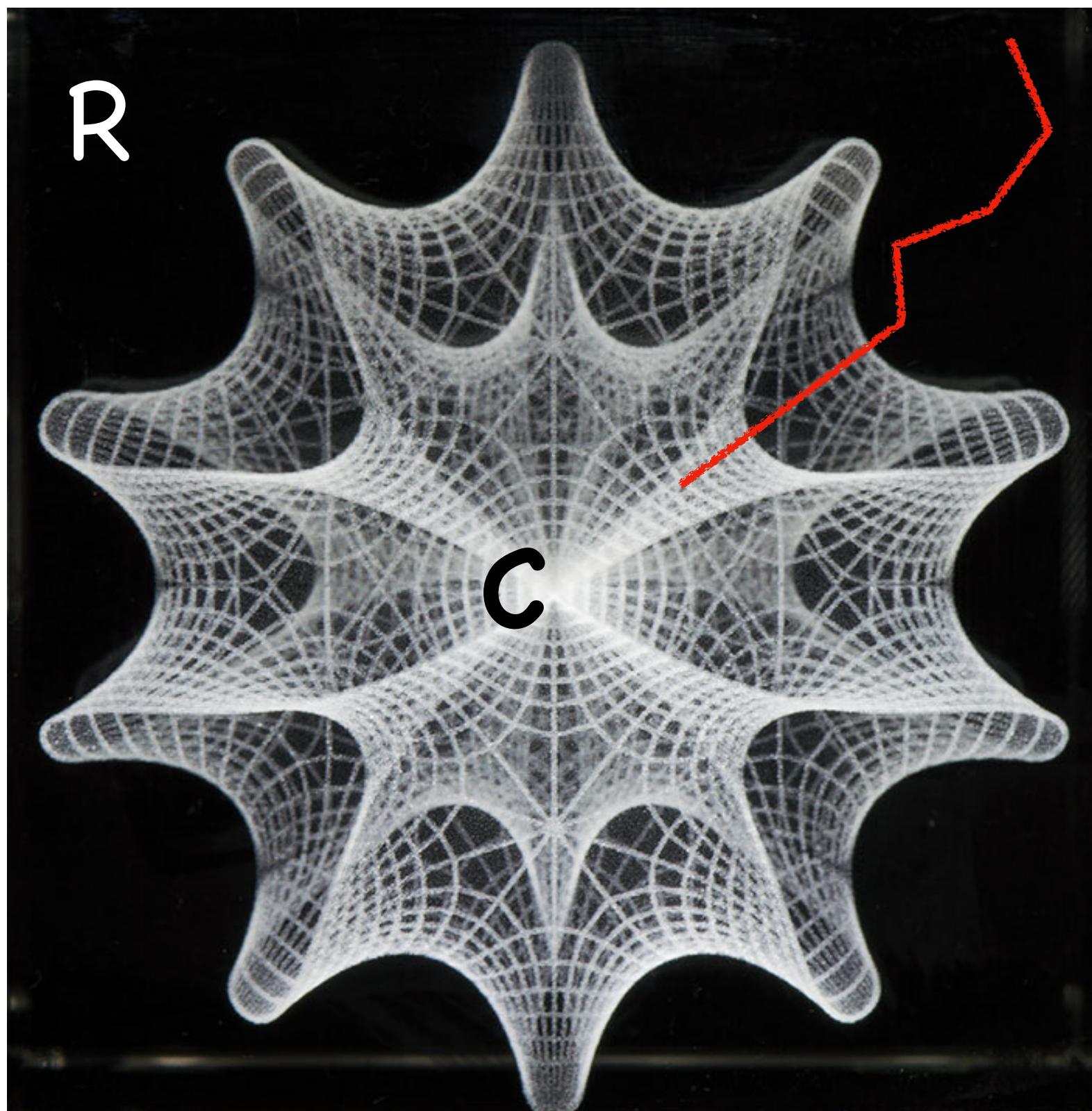
The subgroups \mathcal{J}_1 , \mathcal{J}_2 , and \mathcal{T} act freely on C .

\mathcal{J}_1 , and \mathcal{J}_2 are maximal.

These groups are matrix Lie groups.

These open up a number of questions, but the insights feed into the algorithm that powers the "oracle".

The Oracle



The conjecture space (C) can be seen as a subset of the space of relations (R).

This is a sampling problem! One approach is a naive search ala geometric gradient descent (our space admits a metric). Every point in C and its orbit are conjectures.

Algorithm 1 Oracle

- 1: **Inputs:** Mathematical features $\{x_i\}_{i=1}^N$, function class \mathcal{F}_{d_1, d_2} , and hyperparameters: tolerance (tol), batch-size (b), maximum epochs (emax), learning rate (η).
 - 2: $\theta \leftarrow$ random real vector.
 - 3: **Parameterise:** $c_\theta := (f_\theta, g_\theta) := \mathcal{P}(\theta); f_\theta, g_\theta \in \mathcal{F}(K^T[x])$.
 - 4: **for** $a \leftarrow 1$ to emax **do**
 - 5: **for** $b \leftarrow 1$ to b **do**
 - 6: **if** $\mathcal{L}(c_\theta) \leq \text{tol}$ **then**
 - 7: **return** θ
 - 8: $\theta \leftarrow \theta - \eta \mathcal{J}_\theta^{-1} \nabla \mathcal{L}(\theta)$
 - 9: $\omega(c_\theta) \leftarrow \frac{2}{b} \sum_{i \in \text{rand}} \text{sgn}(f_\theta(x_i) - g_\theta(x_i))$
 - 10: $\mathcal{L}(c_\theta) \leftarrow (1 - \omega(c_\theta))^2$
 - 11: **Output:** $c_\theta = \mathcal{P}(\theta); f_\theta < g_\theta$.
-

Some number theoretic conjectures!

#	Conjecture (c_θ)
1	$\pi(ab) \geq \pi(a) + \pi(b)$
2	$\pi(ab) + \pi(a+b) + \pi(a) + \pi(b) \leq 2ab$
3	$4(\pi(a) + \pi(b)) + \pi(a+b) \leq 4\pi(ab)$
4	$\pi(ab) + 2\pi(a+b) \geq \pi(a) + \pi(b)$
5	$\pi(a+b) \leq \pi(a) + \pi(b)$
6	$\pi(a b c) \geq \pi(a) \pi(b) \pi(c)$
7 [†]	$\pi(a b c \dots) \geq \pi(a) \pi(b) \pi(c) \dots$
8	$\pi(a+b+c) \leq \pi(a) + \pi(b) + \pi(c)$
9 [†]	$\pi(a+b+c+\dots) \leq \pi(a) + \pi(b) + \pi(c) + \dots$

10	$\pi(a)\pi(b)\pi(c) \leq \sqrt{(\pi(a) + \pi(b) + \pi(c))^2 + (\pi(abc))^2}$
11 ^{†*}	$((\sum_i \pi(a_i))^2 + (\pi(\prod_i a_i))^2)^{1/3} \leq \prod_i \pi(a_i) \leq ((\sum_i \pi(a_i))^2 + (\pi(\prod_i a_i))^2)^{1/2}$
12	$\pi(ab+bc+ca)^3 \geq 2\pi(abc)^2 + \pi(abc) + \pi(a+b+c)^2$
13	$\pi(a+b+c)^2 + \pi(abc) \geq \pi(ab+bc+ca)^3 + 2\pi(abc)^2$
14	$\pi(ab+bc+ca)^7 \geq \pi(a+b+c)^7$
15	$\pi(\alpha_1\alpha_2\alpha_3)^2 + \pi(\alpha_1\alpha_2 + \alpha_2\alpha_3 + \alpha_3\alpha_1) \geq \pi(\alpha_1\alpha_2 + \alpha_2\alpha_3 + \alpha_3\alpha_1)^3 + \pi(\alpha_1 + \alpha_2 + \alpha_3)$
16	$\pi(\alpha_1\alpha_2\alpha_3)^3 + 4\pi(\alpha_1\alpha_2\alpha_3)^2 + 4\pi(\alpha_1 + \alpha_2 + \alpha_3)^3 + 3 + \text{dots} \geq \pi(\alpha_1\alpha_2 + \dots)$
17 [°]	$\pi(\chi_2)^3 - \pi(\chi_3)^2 + \pi(\chi_3) \geq \pi(\chi_1)$
18	$\pi(\chi_1)^3 \geq \pi(\chi_2)^3$

19	$5\pi(\chi_2)^3 \geq \pi(\chi_1)$
20	$\pi(\chi_1) + \pi(\chi_3) < \pi(\chi_2)$
21	$5\pi(\pi(\chi_1)) + 2\pi(\pi(\chi_3)) \geq \pi(\pi(\chi_2))$
22	$\pi(\pi(\chi_2)) \geq 2\pi(\pi(\chi_3)) + 3\pi(\pi(\chi_1))$
22	$11 \left(\pi(ab) + \frac{ab}{\log(ab)} \right) > 9\pi(a+b) + \frac{9(a+b)}{\log(a+b)}$
23	$\pi(x + \sqrt{x}) \leq 3\pi(x) + 1$
24 ^{††}	$\pi(x)^2 > x^3 + 2x + 2$
25	$\pi(x + \sqrt{x}) < 3\pi(x)$
26	$\pi(x + \sqrt{x}) < \frac{12}{5}\pi(x) + 1$

A theorem for the prime counting function

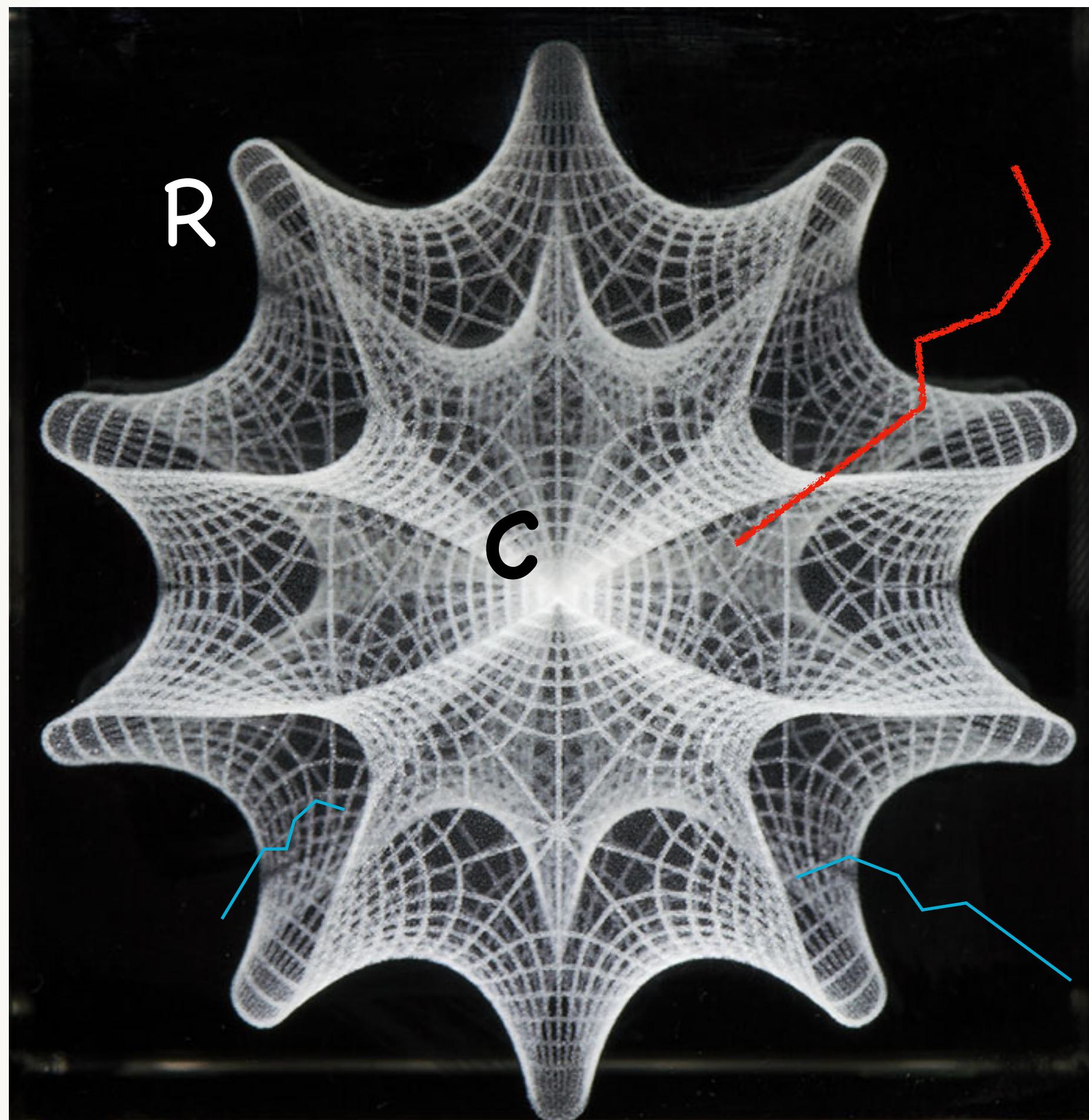
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Theorem: $\pi(ab) \geq \pi(a) + \pi(b)$, $\forall a, b \geq 17$

CM, RS, SRM (2023)

Second Hardy-Littlewood conjecture
(1923)

Outlook



1. Representations: symbolic, HOL, NLP
 2. Coupling with proof assistants
 3. Quantum processor
 4. Brining in machine architectures
 5. Applications: Physical systems, Machine Learning, Number theory, Group theory, Random Matrix models, ...
 6. Conjectures beget conjectures?
 7. Rethinking mathematics education.
- Limitations:
1. Curse of dimensionality!
 2. Needs easily computable functions.
 3. Human readability.

[Submitted on 12 Jun 2023]

Mathematical conjecture generation using machine intelligence

Challenger Mishra, Subhayan Roy Moulik, Rahul Sarkar

Mathematical conjecture generation using machine intelligence

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Abstract

Conjectures have historically played an important role in the development of pure mathematics. We propose a systematic approach to finding abstract patterns in mathematical data, in order to generate conjectures about mathematical inequalities, using machine intelligence. We focus on strict inequalities of type $f < g$ and associate them with a vector space. By geometrising this space, which we refer to as a *conjecture space*, we prove that this space is isomorphic to a Banach manifold. We develop a structural understanding of this *conjecture space* by studying linear automorphisms of this manifold and show that this space admits several free group actions. Based on these insights, we propose an algorithmic pipeline to generate novel conjectures using geometric gradient descent, where the metric is informed by the invariances of the *conjecture space*. As proof of concept, we give a toy algorithm to generate novel conjectures about the prime counting function and diameters of Cayley graphs of non-abelian simple groups. We also report private communications with colleagues in which some conjectures were proved, and highlight that some conjectures generated using this procedure are still unproven. Finally, we propose a pipeline of mathematical discovery in this space and highlight the importance of domain expertise in this pipeline.



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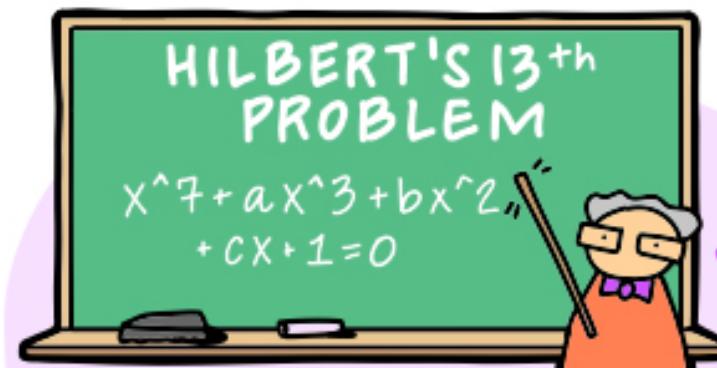


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Stanford



Being humbled in Chess
@Berkeley, 2023

MATHEMATICAL CONJECTURE GENERATION USING MACHINE INTELLIGENCE



HILBERT'S 13th PROBLEM
RELATES to the IMPORTANCE
of GOOD CONJECTURES
in MATHS

... a CATALYST for IMPORTANT
MATH DEVELOPMENTS... like
★ FUNCTIONAL ANALYSIS
★ GEOMETRY
★ ML!

CHALLENGER MISHRA

WHAT MAKES a
GOOD CONJECTURE?

ROBERT DIJKGRAAF'S LIST...

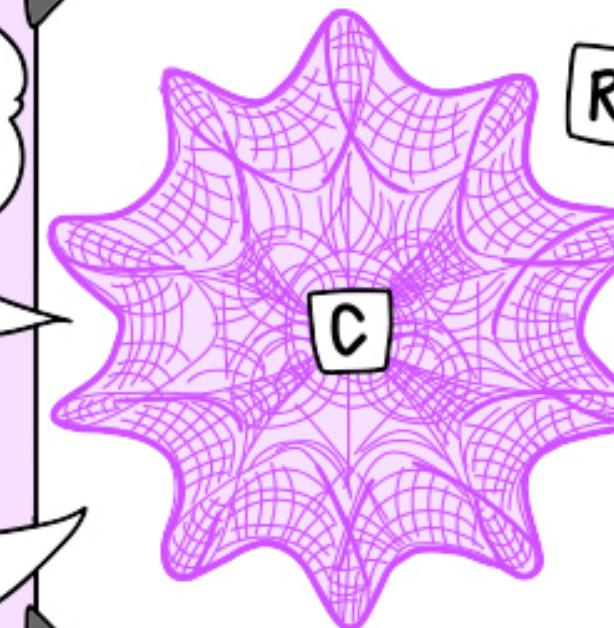
- MILESTONE in MATHEMATICS
- NON-TRIVIAL
- COME w/ EVIDENCE in its FAVOUR
- TERSE
- COULD UNLOCK NEW THEOREMS
- are 'OUTRAGEDOUS'

WHAT do we DO with THIS?

- ✓ EXPLOIT OTHER REPRESENTATIONS
- ✓ COUPLING w/ PROOF ASSISTANTS
- ✓ QUANTUM PROCESSOR
- ✓ BRING in MACHINE ARCHITECTURES

EMILY NOETHER
SUGGESTED SYMMETRY
as an ORGANISING PRINCIPLE

HOW do we CONSIDER
the SPACE of RELATIONS
& CONJECTURES?

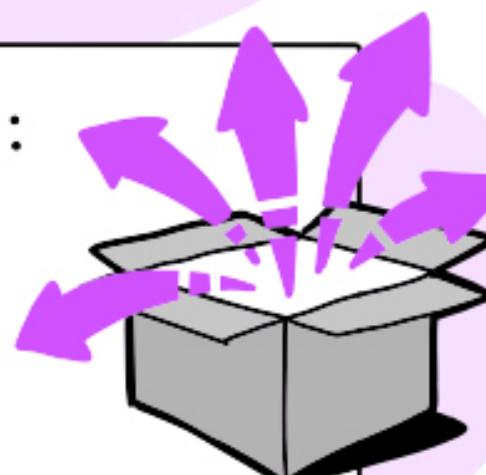


LARGEST
GROUP
ACTING
on "C"?

to HUNT for
CONJECTURES in a
SYSTEMATIC WAY,
SOLVE the SAMPLING
PROBLEM.

for HIGH DIMENSIONAL
PROBLEMS, TAKE ACCOUNT
of SYMMETRIES

- ✓ POTENTIAL APPLICATIONS:
 - ... PHYSICAL SYSTEMS
 - ... MACHINE LEARNING
 - ... NUMBER THEORY
 - ... GROUP THEORY
 - ... RANDOM MATRIX MODELS



Let's make some conjectures?