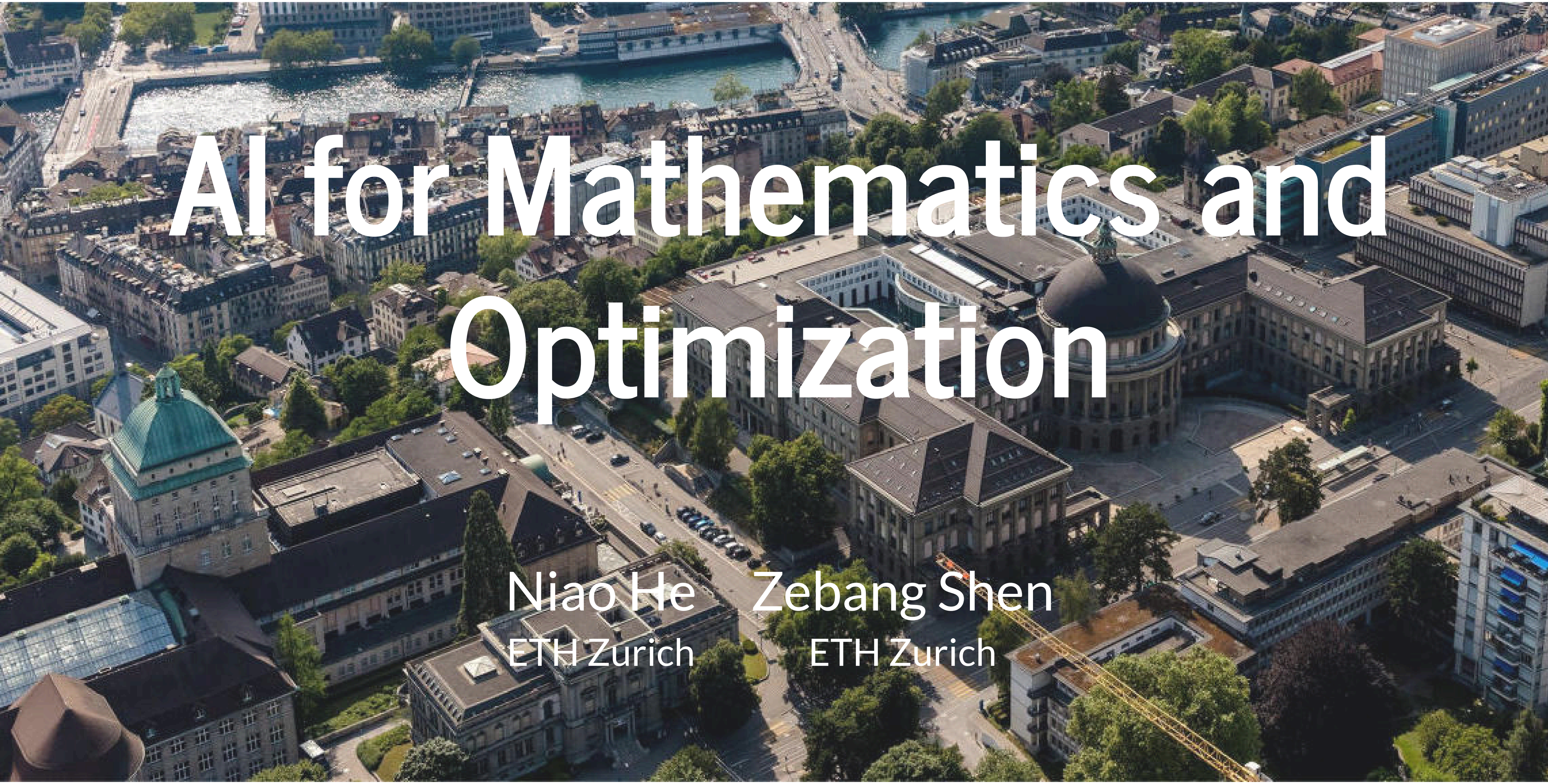


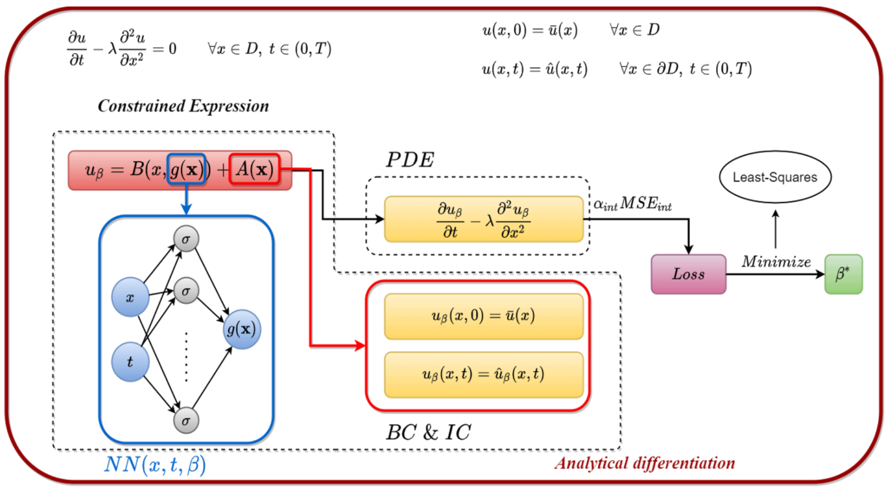
AI for Mathematics and Optimization

Niao He
ETH Zurich

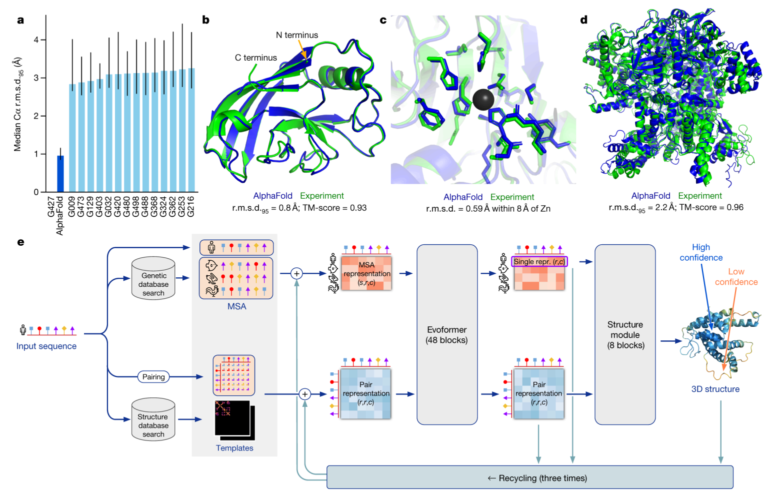
Zebang Shen
ETH Zurich

AI as a tool

- AI accelerates scientific research.
  - Examples in Phyics and Biology: (AI for Science Seminars in the past)



Physics-informed Neural Network



AlphaFold 2

- How does AI help?
  - Function approximation, simulation, routine automation, etc.

AI as a collaborator

- Focus: AI accelerates mathematical research.
  - Core intellecture challenge
    - formulating hypothesis
    - design algorithms
    - proving theorems
    - constructing counterexamples

Article | Open access | Published: 01 December 2021

Advancing mathematics by guiding human intuition with AI

Alex Davies, Petar Veličković, Lars Buesing, Sam Blackwell, Daniel Zheng, Nenad Tomašev, Richard Tanburn, Peter Battaglia, Charles Blundell, András Juhász, Marc Lackenby, Geordie Williamson, Demis Hassabis & Pushmeet Kohli

Nature **600**, 70–74 (2021) | Cite this article

Abstract

The practice of mathematics involves discovering patterns and using these to formulate and prove conjectures, resulting in theorems. Since the 1960s, mathematicians have used computers to assist in the discovery of patterns and formulation of conjectures[1], most famously in the Birch and Swinnerton-Dyer conjecture[2], a Millennium Prize Problem[3]. Here we provide examples of new fundamental results in pure mathematics that have been discovered with the assistance of machine learning—demonstrating a method by which machine learning can aid mathematicians in discovering new conjectures and theorems. We propose a process of using machine learning to discover potential patterns and relations between mathematical objects, understanding them with attribution techniques and using these observations to guide intuition and propose conjectures. We outline this machine-learning-guided framework and demonstrate its successful application to current research questions in distinct areas of pure mathematics, in each case showing how it led to meaningful mathematical contributions on important open problems: a new connection between the algebraic and geometric structure of knots, and a candidate algorithm predicted by the combinatorial invariance conjecture for symmetric groups[4]. Our work may serve as a model for collaboration between the fields of mathematics and artificial intelligence (AI) that can achieve surprising results by leveraging the respective strengths of mathematicians and machine learning.

Example: First Proof

About Questions Get Involved Team FAQ Euler Day

First Proof

A set of ten math questions to evaluate the capabilities of AI systems to autonomously solve problems that arise naturally in the research process.

Example: First Proof (cont.)

Sanjeev Arora @prfsanjeevarora · Feb 15

Surprising indeed, if the claims hold.

> **Lexaaa** @DayShuai · Feb 13
>
> We @AuricSource solved 8/10 problems from the #1stProof benchmark (Abouzaid et al., arXiv:2602.05192) — all with Lean 4 formal verification.
>
> Q4 & Q6: substantial partial QED with precise remaining gaps.
>
> ...
>
> Show more

#	Problem	Field	Answer	Proof	Lean 4
1	Φ^4_3 measure translation	Stochastic Analysis	NO (singular)	QED	✓
2	Rankin–Selberg test vector	Representation Theory	YES	QED	✓
3	Interpolation ASEP ratio	Algebraic Combinatorics	NO (in general)	QED	✓
4	$\boxplus_n$–Φ_n inequality	Polynomial Inequalities	YES ($n \leq 3$, semi-Gauss)	Partial†	✓[a]
5	$\mathcal{O}$-slice filtration	Equivariant Homotopy	YES	QED	✓
6	ε-light vertex sets	Spectral Graph Theory	7 cases; cond. $c = 1/6$	Partial‡	—
7	Lattices with 2-torsion	Lattices / Lie Groups	NO (odd) / YES ($d \geq 5$)	QED	✓
8	Polyhedral Lagrangian	Symplectic Geometry	YES	QED	✓
9	Tensor scale synch.	Multi-view Geometry	YES	QED	✓
10	RKHS-constrained CP	Numerical Linear Algebra	YES (PCG)	QED	✓

7 · 7 · 74 · 22K

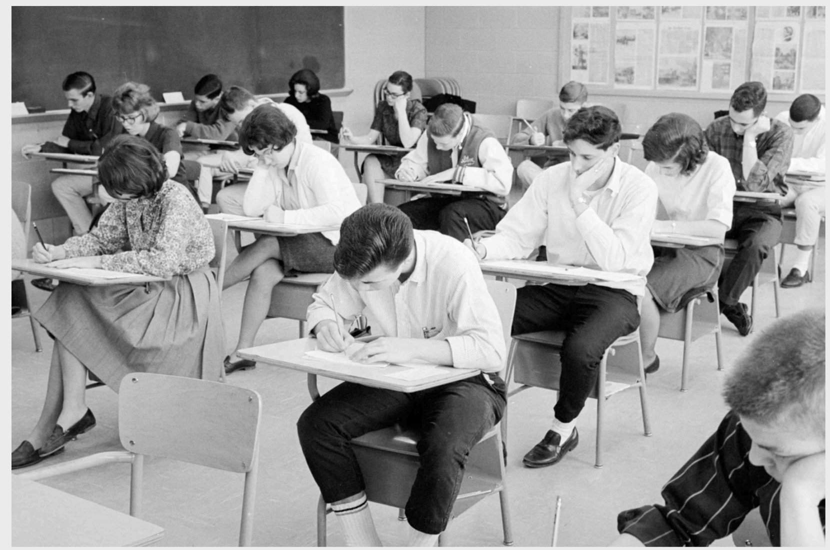
X post

February 14, 2026 | 4 min read | Add Us On Google

AI just got its toughest math test yet. The results are mixed

Experts gave AI 10 math problems to solve in a week. OpenAI, researchers and amateurs all gave it their best shot

BY JOSEPH HOWLETT EDITED BY CLAIRE CAMERON



scientific american

Course organization

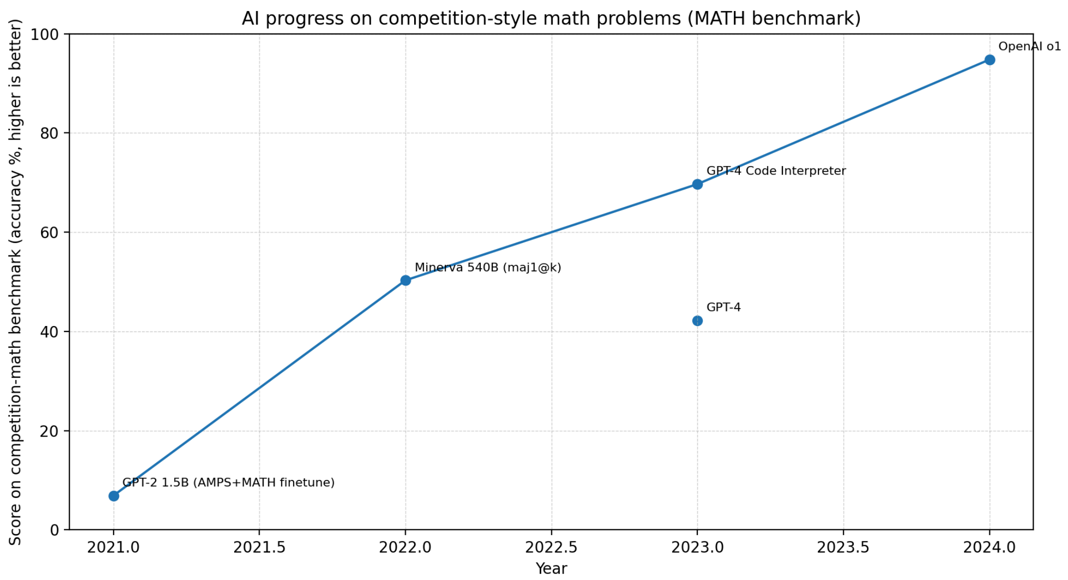
- *Passive* in previous semester:
  - Students are assigned with published papers.
  - Present the existing results in the paper in the end of the semester
- *Active* in this semester:
  - Students are assigned with **open problems** with the ambition to solve it!
  - If succeed, lead to technical report or even **publications**.

Part of a social experiment

- How AI helps students to study new/abstract/challenging materials?
- How AI helps students to solve open problems?

Why can we expect this is achievable?

- Emergence of LLM, success in mathematical competition.



- Many evidentce showing the potential of LLM in mathematical research

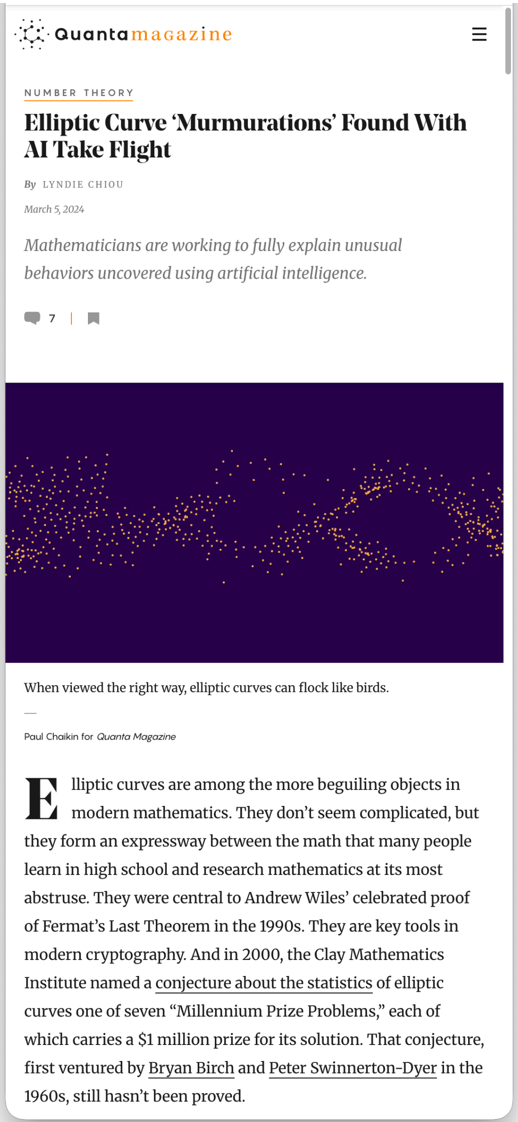
A Long List

awesome-ai-for-math

A curated list of 104 awesome papers exploring the use of artificial intelligence / machine learning / deep learning for mathematical discoveries.

See `CONTRIBUTING.md` for contribution.

Elliptic Curve 'Murmurations' (Hypothesis)



NUMBER THEORY

Elliptic Curve 'Murmurations' Found With AI Take Flight

By LYNDIE CHIOU

March 5, 2024

Mathematicians are working to fully explain unusual behaviors uncovered using artificial intelligence.

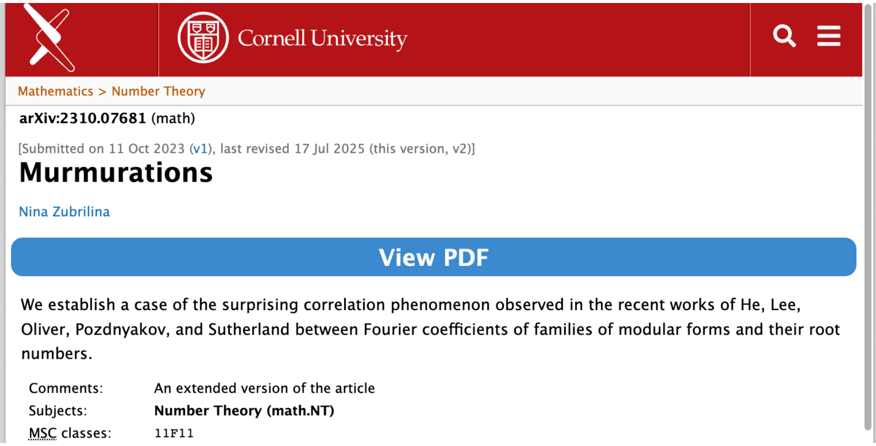
7

When viewed the right way, elliptic curves can flock like birds.

Paul Chaikin for *Quanta Magazine*

Elliptic curves are among the more beguiling objects in modern mathematics. They don't seem complicated, but they form an expressway between the math that many people learn in high school and research mathematics at its most abstruse. They were central to Andrew Wiles' celebrated proof of Fermat's Last Theorem in the 1990s. They are key tools in modern cryptography. And in 2000, the Clay Mathematics Institute named a conjecture about the statistics of elliptic curves one of seven "Millennium Prize Problems," each of which carries a $1 million prize for its solution. That conjecture, first ventured by Bryan Birch and Peter Swinnerton-Dyer in the 1960s, still hasn't been proved.

- Elliptic curves are crucial in number theory
  - A key part of Andrew Wiles' famous proof for Fermat's Last Theorem.
  - Crucial in Cryptography
  - BSD conjecture (a Clay Millennium Prize Problem) is about a curve's `rank`
- AI can (magically) accurately predict the `rank` of the elliptic curve, but why?
  - A wave type relation between prime number and the number of solution to the elliptic curve is observed statistically. Suggest hidden structure.
  - Progress toward "explaining why".



Cornell University

Mathematics > Number Theory

arXiv:2310.07681 (math)

[Submitted on 11 Oct 2023 (v1), last revised 17 Jul 2025 (this version, v2)]

Murmurations

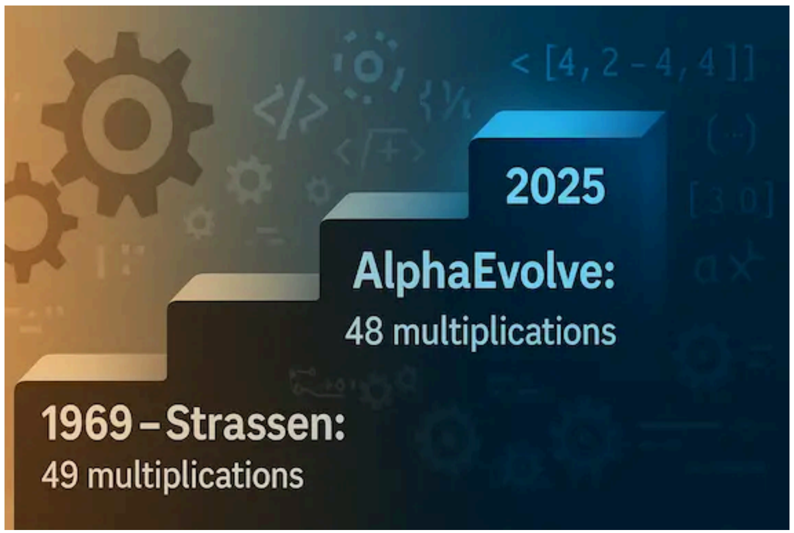
Nina Zubrilina

View PDF

We establish a case of the surprising correlation phenomenon observed in the recent works of He, Lee, Oliver, Pozdnyakov, and Sutherland between Fourier coefficients of families of modular forms and their root numbers.

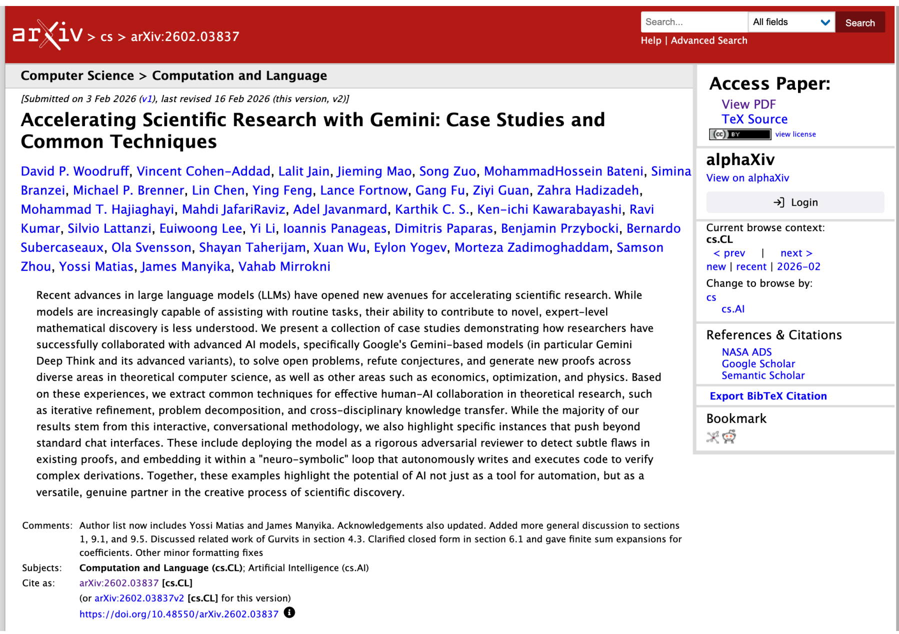
Comments:	An extended version of the article
Subjects:	**Number Theory (math.NT)**
MSC classes:	11F11

Alphaevolve and faster 4×4 matrix multiplication (algorithm)



- Matrix multiplications are building blocks of modern age.
- Key performance metric is (# scalar multiplications).
- AlphaEvolve improves over existing method from 49 to 48, in terms of (# scalar multiplications)
  - sets up matrix multiplication as a searchable optimization problem
  - starts from a known solver, then evolves the solver code
  - loop: propose → run → score → keep best → repeat
- Scales to multiplication in larger sizes if called recursively.

Reports from Big Companies


arXiv > cs > arXiv:2602.03837

Computer Science > Computation and Language

[Submitted on 3 Feb 2026 (v1), last revised 16 Feb 2026 (this version, v2)]

Accelerating Scientific Research with Gemini: Case Studies and Common Techniques

David P. Woodruff, Vincent Cohen-Addad, Lalit Jain, Jieming Mao, Song Zuo, MohammadHossein Bateni, Simina Branzei, Michael P. Brenner, Lin Chen, Ying Feng, Lance Fortnow, Gang Fu, Ziyi Guan, Zahra Hadizadeh, Mohammad T. Hajiaghayi, Mahdi JafariRaviz, Adel Javanmard, Karthik C. S., Ken-ichi Kawarabayashi, Ravi Kumar, Silvio Lattanzi, Euiwoong Lee, Yi Li, Ioannis Panageas, Dimitris Paparas, Benjamin Przybocki, Bernardo Subercaseaux, Ola Svensson, Shayan Taherijam, Xuan Wu, Eylon Yogev, Morteza Zadimoghaddam, Samson Zhou, Yossi Matias, James Manyika, Vahab Mirrokni

Recent advances in large language models (LLMs) have opened new avenues for accelerating scientific research. While models are increasingly capable of assisting with routine tasks, their ability to contribute to novel, expert-level mathematical discovery is less understood. We present a collection of case studies demonstrating how researchers have successfully collaborated with advanced AI models, specifically Google's Gemini-based models (in particular Gemini Deep Think and its advanced variants), to solve open problems, refute conjectures, and generate new proofs across diverse areas in theoretical computer science, as well as other areas such as economics, optimization, and physics. Based on these experiences, we extract common techniques for effective human-AI collaboration in theoretical research, such as iterative refinement, problem decomposition, and cross-disciplinary knowledge transfer. While the majority of our results stem from this interactive, conversational methodology, we also highlight specific instances that push beyond standard chat interfaces. These include deploying the model as a rigorous adversarial reviewer to detect subtle flaws in existing proofs, and embedding it within a "neuro-symbolic" loop that autonomously writes and executes code to verify complex derivations. Together, these examples highlight the potential of AI not just as a tool for automation, but as a versatile, genuine partner in the creative process of scientific discovery.

Comments: Author list now includes Yossi Matias and James Manyika. Acknowledgements also updated. Added more general discussion to sections 1, 9.1, and 9.5. Discussed related work of Gurvits in section 4.3. Clarified closed form in section 6.1 and gave finite sum expansions for coefficients. Other minor formatting fixes
Subjects: **Computation and Language (cs.CL)**; Artificial Intelligence (cs.AI)
Cite as: arXiv:2602.03837 **[cs.CL]**
(or arXiv:2602.03837v2 **[cs.CL]** for this version)
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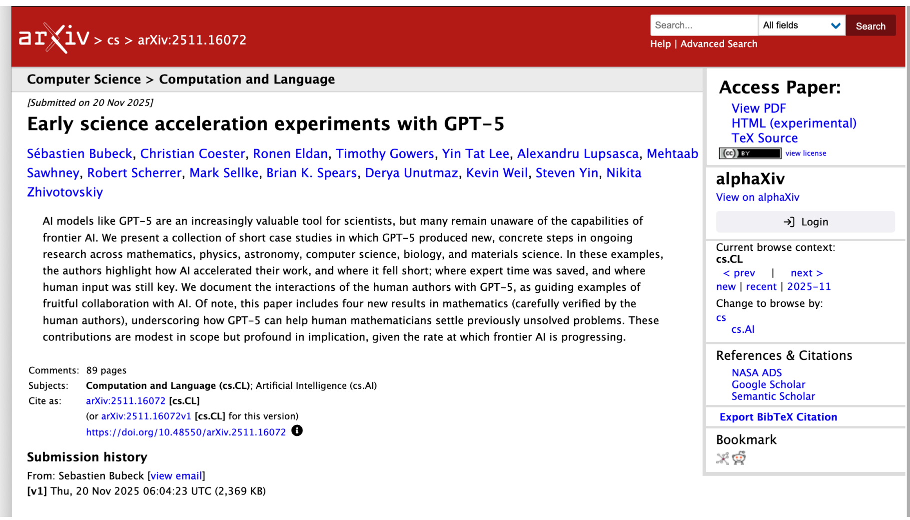
arXiv > cs > arXiv:2511.16072

Computer Science > Computation and Language

[Submitted on 20 Nov 2025]

Early science acceleration experiments with GPT-5

Sébastien Bubeck, Christian Coester, Ronen Eldan, Timothy Gowers, Yin Tat Lee, Alexandru Lupsasca, Mehtaab Sawhney, Robert Scherrer, Mark Sellke, Brian K. Spears, Derya Unutmaz, Kevin Weil, Steven Yin, Nikita Zhivotovskiy

AI models like GPT-5 are an increasingly valuable tool for scientists, but many remain unaware of the capabilities of frontier AI. We present a collection of short case studies in which GPT-5 produced new, concrete steps in ongoing research across mathematics, physics, astronomy, computer science, biology, and materials science. In these examples, the authors highlight how AI accelerated their work, and where it fell short; where expert time was saved, and where human input was still key. We document the interactions of the human authors with GPT-5, as guiding examples of fruitful collaboration with AI. Of note, this paper includes four new results in mathematics (carefully verified by the human authors), underscoring how GPT-5 can help human mathematicians settle previously unsolved problems. These contributions are modest in scope but profound in implication, given the rate at which frontier AI is progressing.

Comments: 89 pages
Subjects: **Computation and Language (cs.CL)**; Artificial Intelligence (cs.AI)
Cite as: arXiv:2511.16072 **[cs.CL]**
(or arXiv:2511.16072v1 **[cs.CL]** for this version)
https://doi.org/10.48550/arXiv.2511.16072

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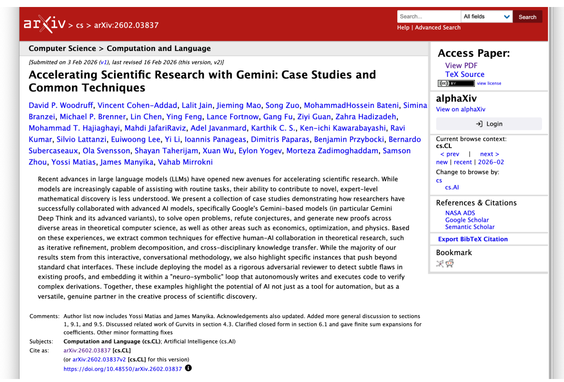
Open AI

Success stories (counterexample)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Computer Science > Computation and Language

[Submitted on 3 Feb 2026 (v1), last revised 16 Feb 2026 (this version, v2)]

Accelerating Scientific Research with Gemini: Case Studies and Common Techniques

David P. Woodruff, Vincent Cohen-Addad, Lalit Jain, Jieming Mao, Song Zuo, MohammadHossein Bateni, Simina Branzei, Michael P. Brenner, Lin Chen, Ying Feng, Lance Fortnow, Gang Fu, Ziyi Guan, Zahra Hadizadeh, Mohammad T. Hajiaghayi, Mahdi JafariRaviz, Adel Javanmard, Karthik C. S., Ken-ichi Kawarabayashi, Ravi Kumar, Silvio Lattanzi, Euiwoong Lee, Yi Li, Ioannis Panageas, Dimitris Paparas, Benjamin Przybocki, Bernardo Subercaseaux, Ola Svensson, Shayan Taherijam, Xuan Wu, Eylon Yogev, Morteza Zadimoghaddam, Samson Zhou, Yossi Matias, James Manyika, Vahab Mirrokni

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Subjects: **Computation and Language (cs.CL)**; Artificial Intelligence (cs.AI)

Cite as: arXiv:2602.03837 **[cs.CL]**

(or arXiv:2602.03837v2 **[cs.CL]** for this version)

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Conjecture 3.2 (Conjecture 15 of [64]). *For any instance of the online submodular welfare maximization problem,*

$$\mathbb{E}_{\pi\sim\mathbb{S}_n}\left[\sum_{i=1}^{n}\mathrm{MG}(n+1,\pi^{Copy,i})\right]\leq\mathbb{E}_{\pi\sim\mathbb{S}_n}\left[\sum_{i=1}^{n}\mathrm{MG}(n,\pi^{Move,i})\right] \tag{1}$$

Theorem 3.3. *Conjecture 3.2 is false. There exists an instance of Online SWM such that:*

$$\mathbb{E}_{\pi\sim\mathbb{S}_n}\left[\sum_{i=1}^{n}\mathrm{MG}(n+1,\pi^{Copy,i})\right]>\mathbb{E}_{\pi\sim\mathbb{S}_n}\left[\sum_{i=1}^{n}\mathrm{MG}(n,\pi^{Move,i})\right]$$

Last iterate convergence (theorem)

- Convex optimization problem

$$\min_{x} f(x)$$

- Gradient Descent, GD (Cauchy, 18th century)

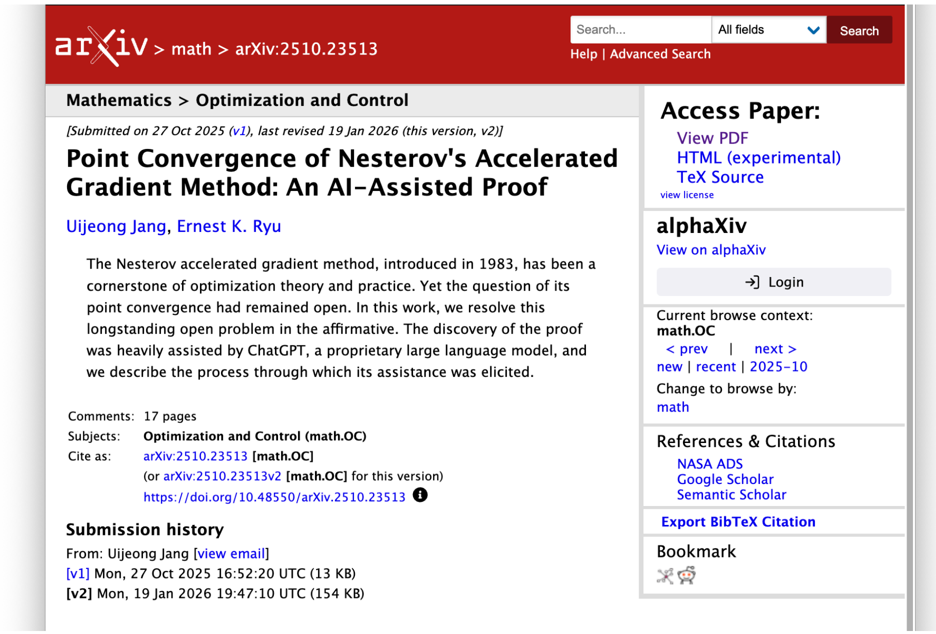
$$z_{k+1} := z_k - \eta \nabla f(z_k)$$

- Nesterov's Accelerated Gradient Descent, NAG (Nesterov, 1983)

$$x_{k+1} := y_k - \eta \nabla f(y_k)$$

$$y_{k+1} := x_{k+1} + \frac{t_k - 1}{t_{k+1}}(x_{k+1} - x_k)$$

- Question: $\lim_{k\to\infty} x_k \in \operatorname{argmin} f$?



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Mathematics > Optimization and Control

[Submitted on 27 Oct 2025 (v1), last revised 19 Jan 2026 (this version, v2)]

Point Convergence of Nesterov's Accelerated Gradient Method: An AI-Assisted Proof

Uijeong Jang, Ernest K. Ryu

The Nesterov accelerated gradient method, introduced in 1983, has been a cornerstone of optimization theory and practice. Yet the question of its point convergence had remained open. In this work, we resolve this longstanding open problem in the affirmative. The discovery of the proof was heavily assisted by ChatGPT, a proprietary large language model, and we describe the process through which its assistance was elicited.

Comments: 17 pages

Subjects: **Optimization and Control (math.OC)**

Cite as: arXiv:2510.23513 **[math.OC]**

(or arXiv:2510.23513v2 **[math.OC]** for this version)

https://doi.org/10.48550/arXiv.2510.23513

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Concrete Example

- Convex optimization problem

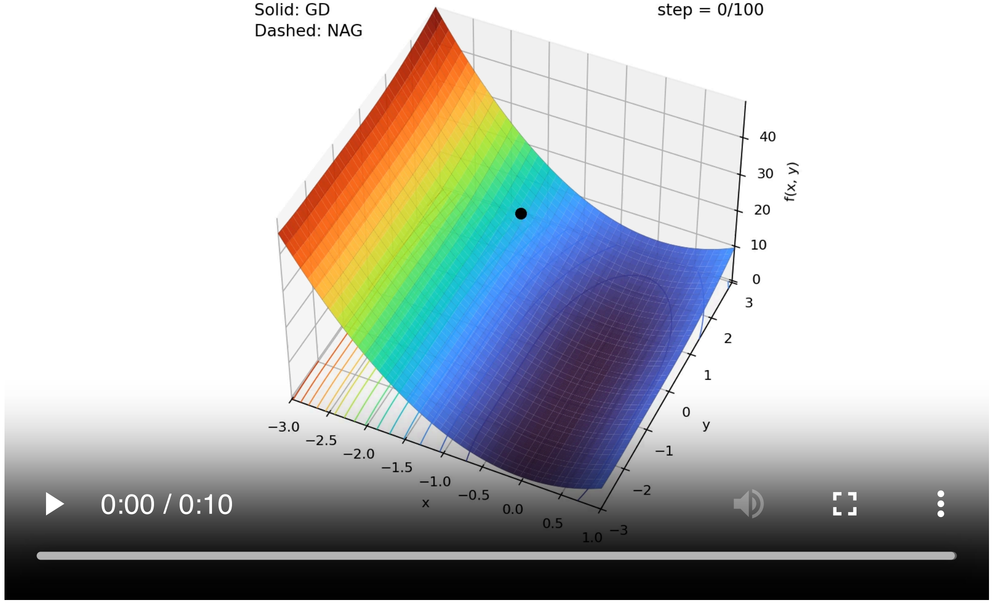
$$f(x_1, x_2) = \frac{x_1^2 + (|x_2 + 1| - 1)_+^2}{2}$$

- GD (slow convergence, convergent)

$$f(z_k) = \mathcal{O}(\frac{1}{k}),$$
$$\lim_{k \to \infty} z_k \in \operatorname{argmin} f$$

- NAG (fast convergence, oscillation)

$$f(x_k) = \mathcal{O}(\frac{1}{k^2}),$$
$$\lim_{k \to \infty} x_k \in \operatorname{argmin} f \ ?$$



Stratgy

- Continuous time model, Nesterov ODE (Su, Boyd, Candès, 2016)

$$\ddot{X}(t) + \frac{\gamma}{t}\dot{X}(t) + \nabla f(X(t)) = 0.$$

- Known results
  - $\gamma > 3$, we have $\lim_{t\to\infty} X(t) = X(\infty) \in \operatorname{argmin} f$.
    - Rely on the integrability of an energy function.
  - $\gamma = 3$ critical case, corresponds to NAG.
    - The integral of the energy function in the $\gamma > 3$ diverges.
- Strategy: Ask query AI to propose a new energy function that is integrable.
  - Once the continous time model converges, same idea applies to the discrete time dynamics.

Interaction with AI

Quote from (Jang and Ryu, 2025):

> The process began by prompting ChatGPT to solve the continuous-time problem. The model did not produce the correct answer in a single attempt; rather, the process was highly interactive. ChatGPT generated numerous arguments, approximately 80% of which were incorrect, but several ideas felt novel and worth further exploring. Whenever a new idea emerged, whether correct or only partially so, we distilled the key insight and prompted ChatGPT to develop it further.
>
> The authors' contribution was to filter out incorrect arguments, consolidate a consistent set of valid facts, identify promising lines of reasoning, and determine when a particular approach had been fully explored. ChatGPT's contribution was to generate candidate arguments, substantially accelerate the exploration of potential avenues, particularly by quickly ruling out unproductive directions, and ultimately produce the final proof argument.