Machine Learning
~~AI~~ in Combinatorics

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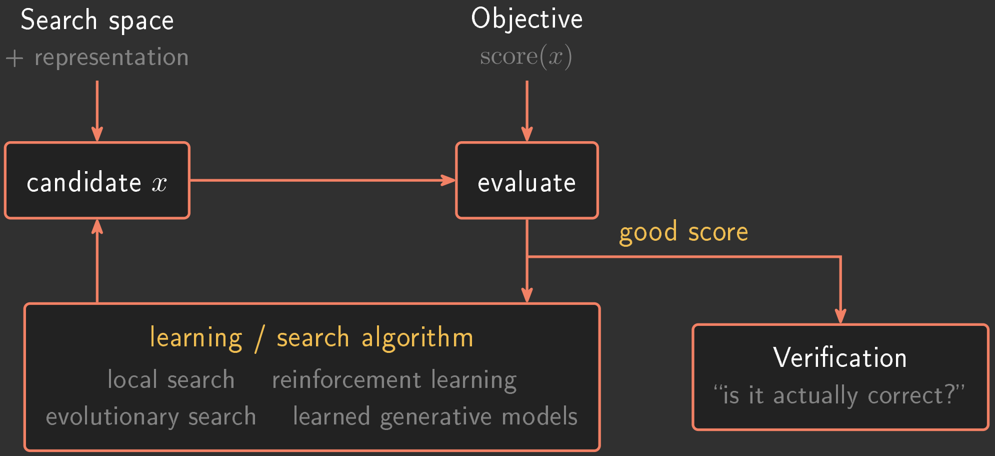
Goal of this talk

- I am looking for an object/map/structure that satisfies certain properties.
- The search space is too large to do an exhaustive search.
- I have some intuition that doesn't work perfectly but is a good starting point for a search.

How can I use machine learning to push this intuition to something concrete?

A typical machine learning workflow



Finding examples and counterexamples

Constructions in combinatorics via neural networks

Adam Zsolt Wagner*

Abstract

We demonstrate how by using a reinforcement learning algorithm, the deep cross-entropy method, one can find explicit constructions and counterexamples to several open conjectures in extremal combinatorics and graph theory. Amongst the conjectures we refute are a question of Brualdi and Cao about maximizing permanents of pattern avoiding matrices, and several problems related to the adjacency and distance eigenvalues of graphs.

TREES AND GRAPHS WITH NON LOG-CONCAVE DOMINATING SET SEQUENCE VIA AI TOOLS

ALINA DU, STEVEN HEILMAN, GRETA PANOVA

Abstract. We give new examples of graphs and trees with dominating set sequences that are not log-concave. These examples were generated by PatternBoost, a transformer-based reinforcement learning software developed by Charton-Ellenberg-Wagner-Williamson. We also show: for any positive integer m, there exists a tree whose dominating set sequence is not log-concave for at least

Advancing Geometry with AI: Multi-agent Generation of Polytopes

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February 11, 2025

Abstract

Polytopes are one of the most primitive concepts underlying geometry. They are defined as

EXAMPLES OF IDP LATTICE POLYTOPES WITH NON-LOG-CONCAVE h^*-VECTOR

JOHANNES HOFSCHEIER, VADYM KURYLENKO, AND BENJAMIN NILL

Abstract. Lattice polytopes are called *IDP polytopes* if they have the integer decomposition property, i.e., any lattice point in a kth dilation is a sum of k lattice points in the polytope. It is a long-standing conjecture whether the numerator of the Ehrhart series of an IDP polytope, called the h^*-polynomial, has a unimodal coefficient vector. In this

Unearthing structure from intuition

Article

Advancing mathematics by guiding human intuition with AI

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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.

One of the central drivers of mathematical progress is the discovery of patterns and formulation of useful conjectures: statements that are suspected to be true but have not been proven to hold in all cases. Mathematicians have always used data to help in this process—from the early hand-calculated prime tables used by Gauss and others that led to the prime number theorem[5], to modern computer-generated data[1,5] in cases such as the Birch and Swinnerton-Dyer conjecture[2]. The introduction of computers to generate data and test conjectures that AI can also be used to assist in the discovery of theorems and conjectures at the forefront of mathematical research. This extends work using supervised learning to find patterns[20–24] by focusing on enabling mathematicians to understand the learned functions and derive useful mathematical insight. We propose a framework for augmenting the standard mathematician's toolkit with powerful pattern recognition and interpretation methods from machine learning and demonstrate its value and generality by showing how it led us to two fundamental

TOWARDS COMBINATORIAL INVARIANCE FOR KAZHDAN-LUSZTIG POLYNOMIALS

CHARLES BLUNDELL, LARS BUESING, ALEX DAVIES, PETAR VELIČKOVIĆ, AND GEORDIE WILLIAMSON

ABSTRACT. Kazhdan-Lusztig polynomials are important and mysterious objects in representation theory. Here we present a new formula for their computation for symmetric groups based on the Bruhat graph. Our approach suggests a solution to the combinatorial invariance conjecture for symmetric groups, a well-known conjecture formulated by Lusztig and Dyer in the 1980s.

1. INTRODUCTION

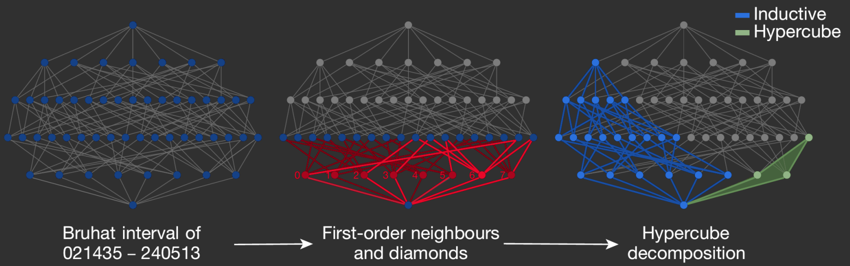
Kazhdan-Lusztig polynomials are important polynomials associated to pairs of elements x, y in Coxeter groups. They appear throughout representation theory and related fields. Lusztig (ca. 1983) and Dyer (1987) independently conjectured that Kazhdan-Lusztig polynomials depend only on the poset of elements between x and y in Bruhat order. This is a fascinating conjecture. For example, it suggests that Kazhdan-Lusztig polynomials are providing subtle invariants of Bruhat order. This conjecture is known in several special cases ([Dye87, Bre04, Inc06, BCM06, Pat21, BLP21], see [Bre04] for an overview).

In this work we prove a new formula Kazhdan-Lusztig polynomials for symmetric groups. Our formula was discovered whilst trying to understand certain machine learning models trained to predict Kazhdan-Lusztig polynomials from Bruhat graphs (see [DVB+]). The new formula suggests an approach to the combinatorial

Unearthing structure from intuition

Conjecture

We can compute the Kazhdan–Lusztig polynomial of (π_1, π_2) by looking at the unlabelled Bruhat interval $[\pi_1, \pi_2]$.



$$\mathrm{KL}(021435, 240513) = 1 + 2q + q^2$$

Theorem

We can compute the Kazhdan–Lusztig polynomial of (π_1, π_2) by looking at the edge-labelled Bruhat interval $[\pi_1, \pi_2]$.

Refining intuition into something concrete

q, t combinatorics: Narayana numbers $\rightsquigarrow$ q, t-Narayana numbers

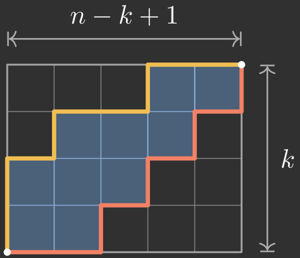
Narayana numbers count parallelogram polyominoes $\mathrm{Polyo}_{m,n}$. Bigrade with two statistics area and bounce:

$$N_{n,k}(q,t) = \sum_{P \in \mathrm{Polyo}_{n-k+1,k}} t^{\mathrm{area}(P)}\, q^{\mathrm{bounce}(P)}.$$

There is an algebraic proof of symmetry:

$$N_{n,k}(q,t) = N_{n,k}(t,q),$$

but no combinatorial proof.



A 5×4 parallelogram polyomino $P \in \mathrm{Polyo}_{5,4}$.

Refining intuition into something concrete

Mapping Uncharted Symmetries: Machine Discovery in Combinatorics

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Abstract

Inspired by long-standing open problems in algebraic combinatorics, we show that modern machine learning can meaningfully contribute to verifiable mathematical discoveries. In particular, we focus on the construction of simple mathematical functions under exact distributional constraints, a setting we formalize as Simple Learning Under Rigid Proportions (SLURP). We tackle this problem by introducing two methods: MapSeek-Functional, which models the desired function alternating pseudo-labeling and supervised training steps; and MapSeek-Symbolic, designed to directly produce symbolic formulas. We successfully apply both methods to a research problem in algebraic combinatorics, discovering a new combinatorial interpretation of the q,t-Narayana polynomials arising from representation theory. To our knowledge, this is the first such interpretation based on noncrossing partitions. Using one discovered statistic, we find a combinatorial proof of the symmetry of these polynomials in a previously unsolved case. To streamline verification and reproducibility, we release all code, including a formalization of all the mathematical discoveries of this paper in Lean 4.

The authors prove $N_{n,3}(q,t) = N_{n,3}(t,q)$ combinatorially.

Strategy. Use a known statistic skip in place of area, so that, summing over $P \in \mathrm{Polyo}_{m,n}$,

$$\sum_P t^{\mathrm{area}(P)} q^{\mathrm{bounce}(P)} = \sum_P t^{\mathrm{skip}(P)} q^{\mathrm{stat}(P)},$$

where stat is a mystery statistic.

Start with a guess for stat that works only for $n \leq 4$, then use machine learning to find a similar statistic that works for all n.

Find more papers in your field that use ML

- `https://seewoo5.github.io/awesome-ai-for-math/`

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Doubly Saturated Ramsey Graphs: A Case Study in Computer-Assisted Mathematical Discovery	Combinatorics, LLM, ATP	arXiv	2026	

How to use these tools

- You do not need to become a machine learning expert
  - Use LLMs! Chat about your problem, see what techniques you can use, ask for code snippets or ask them to make a skeleton folder for your experiment
- The timeline for doing these sorts of experiments has gone down from months to days or even hours!
- Find a well-defined mathematical question and phrase it in a way that gives you a quantity to optimise

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Thank you!