Finding counterexamples via reinforcement learning

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IPAM Machine Assisted Proofs Workshop

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I am not an expert in ML.

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- Agent tries to improve his total score (sum of all rewards) through some optimization algorithm.

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Goal: find counterexamples to open conjectures via RL

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- Try to avoid using human insights as much as possible
- Would like a general setup: use the same program for every problem, only change reward function
- Throw this setup at 100 open conjectures and hope for the best.

Example 1

Conjecture

For any graph G, we have $\lambda_1(G) + \mu(G) \geq \sqrt{n-1} + 1.$

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Game: offer edges one by one, agent can accept/reject each. A game lasts $\frac{n(n-1)}{2}$ turns.

Reward: $\lambda_1 + \mu$ (minimize).

Run a reinforcement learning algorithm for $n = 19$:

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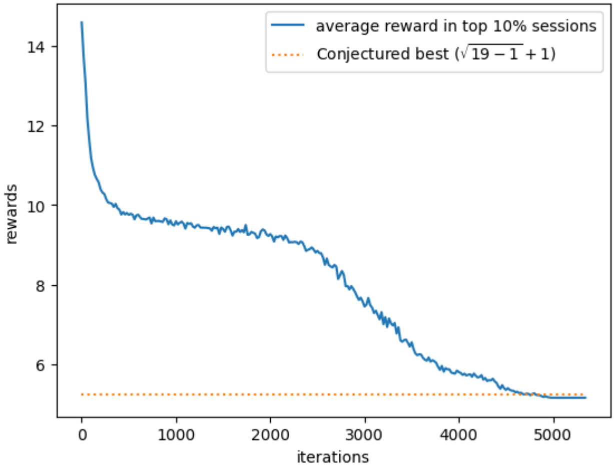

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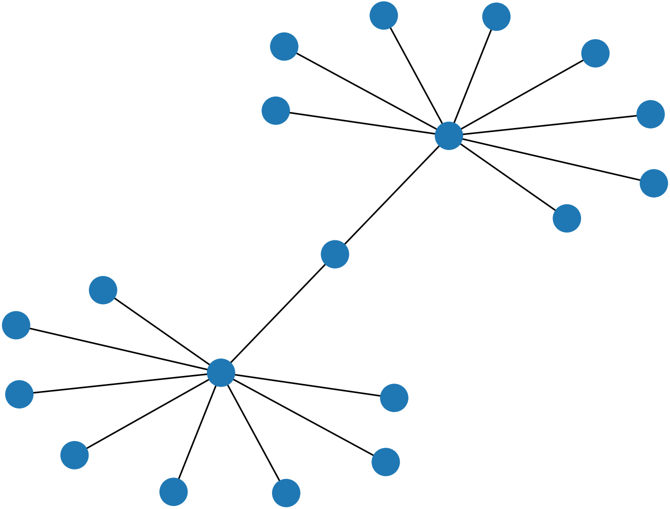

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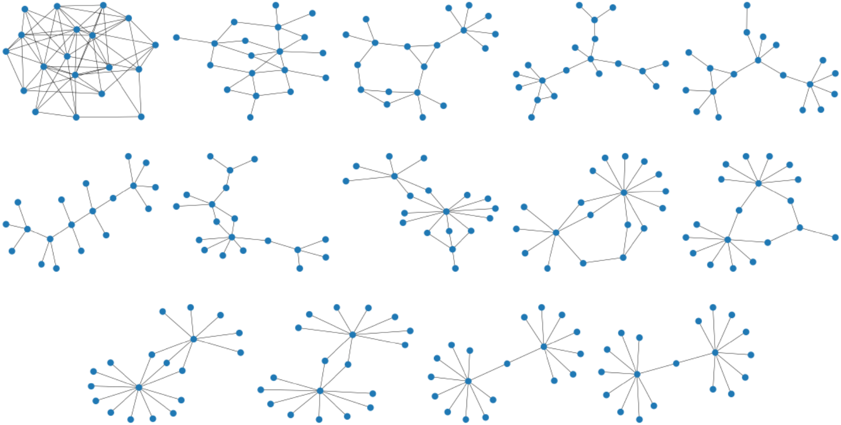

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- This was the dream scenario: there is an obvious way to phrase the conjecture as a game, there is an obvious choice for the score function, we plug these into the RL program and it spits out a counterexample.
- When this happens, there is not much to talk about. But often it is not that simple.
- We will see 5 more examples. In each of them we will succeed in refuting an open conjecture, but each example will illustrate a unique thing that could "go wrong" and how to overcome it.

Example 2 – What if we don't succeed?

Conjecture (Auchiche–Hansen, 2016)

Let G be a connected graph with diameter D, proximity π and distance spectrum $\partial_1 \geq \ldots \geq \partial_n$. Then

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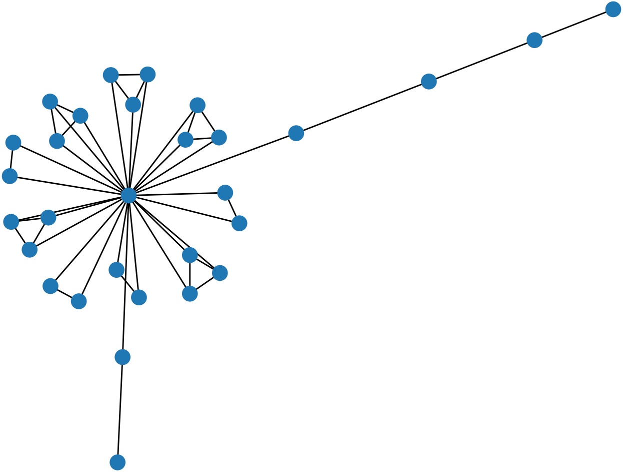
Reward: $\pi + \partial_{\lfloor \frac{2D}{3} \rfloor}$ (minimize).

Run it for $n = 30$:

Example 2



This is not quite a counterexample ($\pi + \partial_{\lfloor \frac{2D}{3} \rfloor} \approx 0.4$), but it tells us very clearly what counterexamples could look like.

Example 2

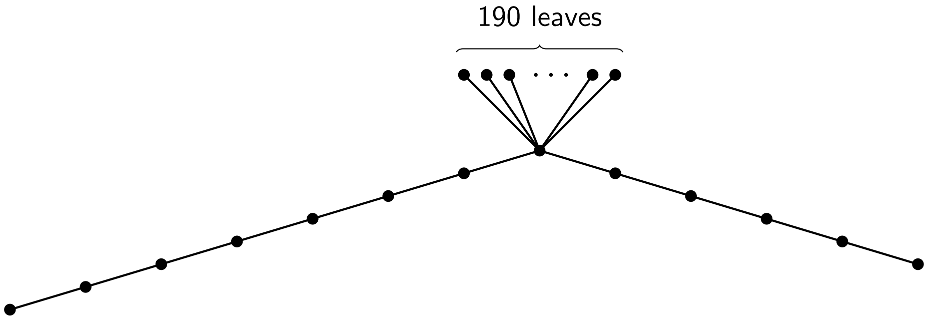


Figure: A counterexample to the conjecture

Example 3 - Not just graphs

Question (Brualdi–Cao)

How large can the permanent of a 312-pattern avoiding 0-1 matrix be?

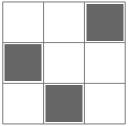


Figure: The pattern 312

$$\mathrm{per}(A) = \sum_{\sigma \in S_n} \prod_{i=1}^{n} A_{i,\sigma(i)}$$

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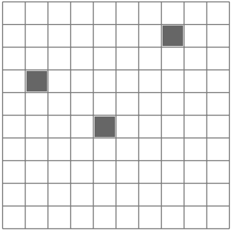

Figure: This is also not allowed

More precisely: we are not allowed to have three ones (dark squares) $(x_i, y_i) : i \in \{1, 2, 3\}$ such that $y_1 < y_2 < y_3$ and $x_2 < x_1 < x_3$.

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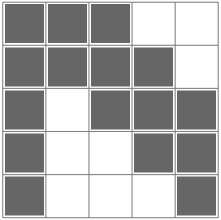
The best you can do is $Fib_{n+2} - 1$.



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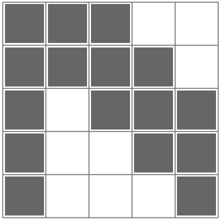

Reward: $\text{per}(A) - \text{penalty}(\#\text{ of 312-s})$

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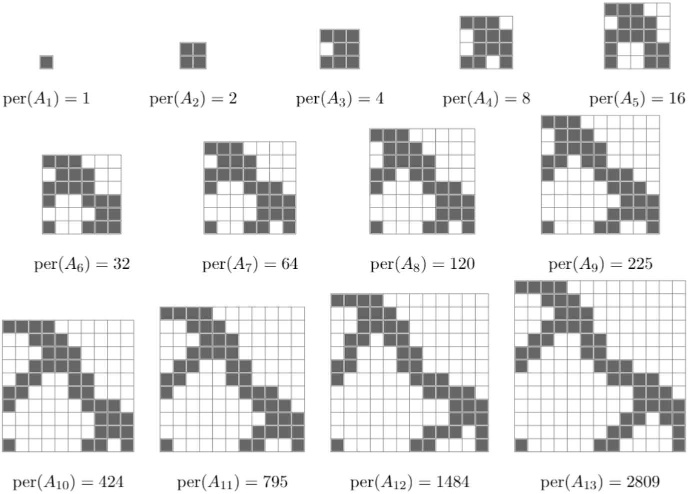

These are best possible for $n \leq 8$ (computer proof). So the sequence starts with $1, 2, 4, 8, 16, 32, 64, \mathbf{120}$.

Example 4 - Problems on trees

Conjecture (Collins, 1989)

Given a tree T, let $p(T)$ and $q(T)$ be the characteristic polynomials of the adjacency and the distance matrices of T, respectively. The coefficients of p and q are both unimodal, and their peaks are asymptotically at the same place.

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Reward: distance of the peaks.

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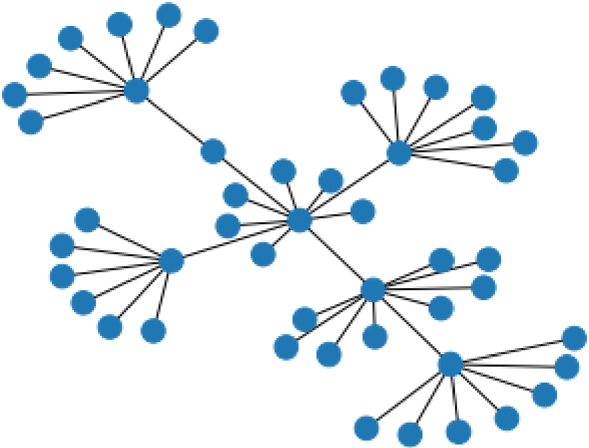

Figure: Best construction found for $n = 48$

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Say that a graph property $\mathcal{P}$ is *preserved under* $\mathcal{D}^L(G)$*-cospectrality* if $\text{spec}_{\mathcal{D}^L}(G) = \text{spec}_{\mathcal{D}^L}(H)$ implies $\mathcal{P}(G) = \mathcal{P}(H)$.

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Property	$\mathcal{D}^L$
# Edges	No
Diameter	No
Girth	No
Planarity	No
Wiener index	Yes
Degree sequence	No
Transmission sequence	No
Transmission regularity	?
# connected components in $\overline{G}$	Yes

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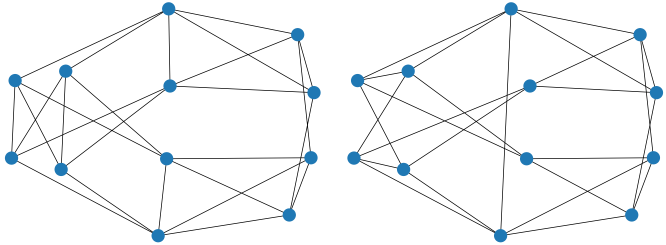
Idea:

$$\text{score}(G,H) = f_1(G,H) + f_2(G) + f_3(H),$$

where

- f_1 measures how close the $\mathcal{D}^L$-spectrum of G and H is,
- f_2 measures how close G is to being transmission regular, and
- f_3 gives a penalty if H is transmission regular.

Example 5



The graph on the left is transmission regular, whereas the graph on the right is not. The characteristic polynomials of their distance Laplacians are the same $(x^{12} - 216x^{11} + 21188x^{10} - 1245904x^9 + 48797440x^8 - 1336652544x^7 + 26129121472x^6 - 364516883456x^5 + 3556516628224x^4 - 23113129559040x^3 + 90045806284800x^2 - 159318669312000x)$, so they are $\mathcal{D}^L$-cospectral.

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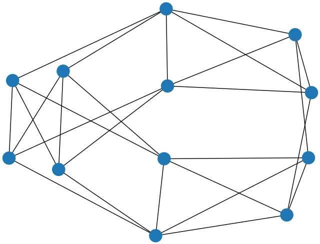

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So transmission regularity is **not** preserved under $\mathcal{D}^L$-cospectrality.

Example 6 - Infinite problems?

Many interesting problems can not have finite counterexamples.

Conjecture (Erdős, 1962)

The function

$$K_4(G) + K_4(\bar{G})$$

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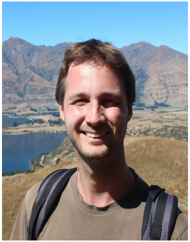

Figure: Gwenaël Joret

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Solution: “blowing up”! Construct a finite graph G, so that $G \times K_m$ is a counterexample as $m \to \infty$.

$\lim_{m\to\infty} \frac{K_4(G\times K_m)+K_4(\overline{G\times K_m})}{m^4}$ depends only on G, and there is an easy formula for it. This will be our reward function.

Run RL for $n = 34 \longrightarrow$ find a counterexample.

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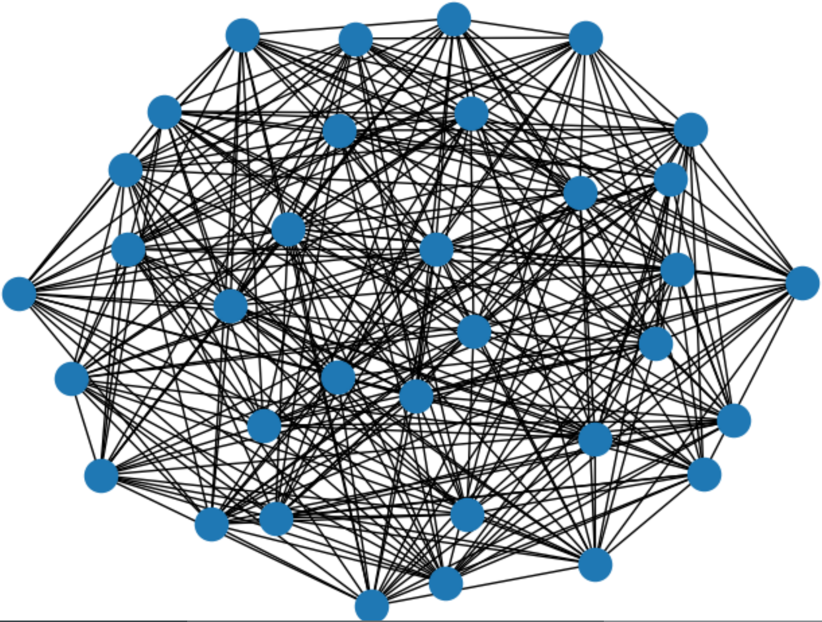

Which RL algorithm to use?

- Value-based methods
  - Learn a value function: “I know how good this chess position is for black”.
- Policy-based methods
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Task: Find the best algorithm for our problems!

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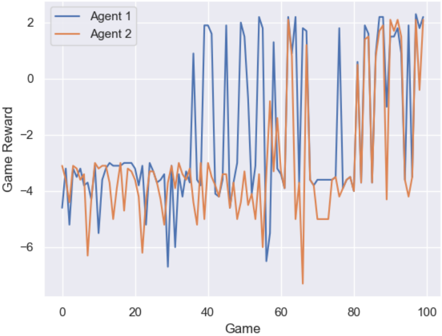
- Do we offer the edges one after the other, starting with $(1, 2), (1, 3)$, $\ldots (n-1, n)$?
- Or do we generate a graph vertex by vertex?
- We could repeatedly ask the neural network to pick one edge to add, out of all remaining edges?
- Do we offer edges in random order? Do we offer multiple edges at a time, is it beneficial to offer an edge again after it was rejected once?
- What neural network architecture to use? Dense layers may not be the best (doesn't understand symmetry).

Reasons an RL algorithm might not work

- Sparse rewards problem: we give rewards only at the end of a game.
- Credit assignment problem: which of my $\frac{n(n-1)}{2}$ moves was responsible for getting a bad score?
- Bad reward design
- Explore-exploit dilemma

Practical problems

What do we conclude if the algorithm produces this output?



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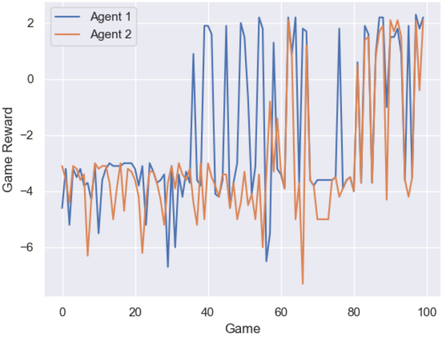

Learning rate too high? Some other hyperparameter is wrong? Not enough training? Coincidence? Maybe this algorithm is unsuited for this specific problem, but good for others?

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Cross-entropy method:

- Simplest possible policy-based method.
- Not sensitive to hyperparameters $\implies$ can use same exact program for every problem.
- Fast convergence, very stable.
- This is the algorithm used in all the examples.

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- For all (state, action) pairs in all top 100 games, adjust neural network weights to make it more likely that for this state we will choose this action.

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Implementation details

- Offer edges one by one: $(1,2)$, then $(1,3)$, $\dots$.
- Input: adjacency matrix we have created so far, and a matrix indicating which edge we consider now.
- Each game lasts $\frac{n(n-1)}{2}$ steps (if we generate a graph).
- The input is two vectors of length $n(n-1)/2$ (or equivalent). The first contains 1-s for each edge we have taken, and 0-s for each edge rejected, or not considered yet. The second is all zeros, except for one place, corresponding to the next edge offered.
- Architecture: dense net, three layers of sizes 128, 64, 4.
- Learn from top 10%, but keep the top 5% for the next iteration.

Improvements to the method

Don't do a generalist approach, focus on one conjecture only, and find the best setup for this one problem!

- Pick an architecture that takes the symmetries of the problem into account (transformers, GNNs, canonicalizing the data)
- We might know that the counterexample must have a specific structure $\rightarrow$ use it to massively restrict the search space

Future goals:

- Improve or find a better RL algorithm for these purposes
- Refute conjectures with a different RL algorithms, or with human + RL collaboration
- Find other ways to use ML in mathematics

Thank you!