Finding counterexamples via reinforcement learning

Adam Zsolt Wagner

Hausdorff School: “Machine Learning and Theorem Proving”

Day 1

September 18, 2023

Lecture series overview

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- Day 1: Reinforcement learning
- Day 2: Saliency analysis
- Day 3: Transformers, Makemore

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Can we teach neural networks to reach superhuman level play in the "game" of constructing graphs without 4-cycles, with as many edges as possible?

Can this same algorithm be used to try to learn to disprove any conjecture, by only inputting the statement and letting the algorithm figure out the rest?

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

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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

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

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

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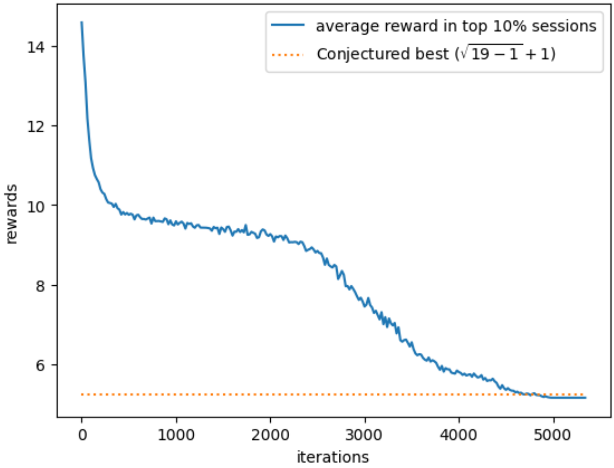

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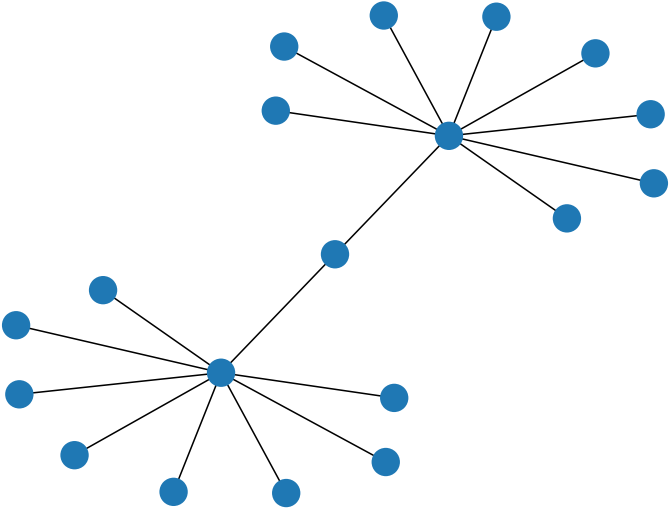

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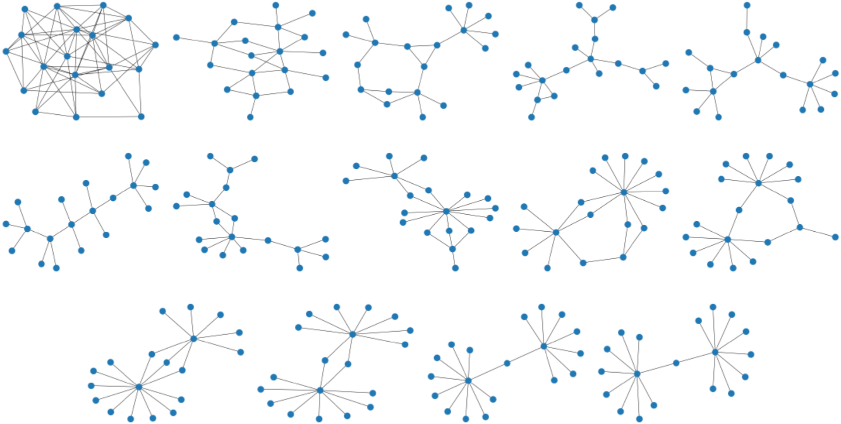

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- This was the dream scenario: there is an obvious way to phrase the conjecture as a game, there is an obvious choice for the score function, we plug these into the RL program and it spits out a counterexample.
- When this happens, there is not much 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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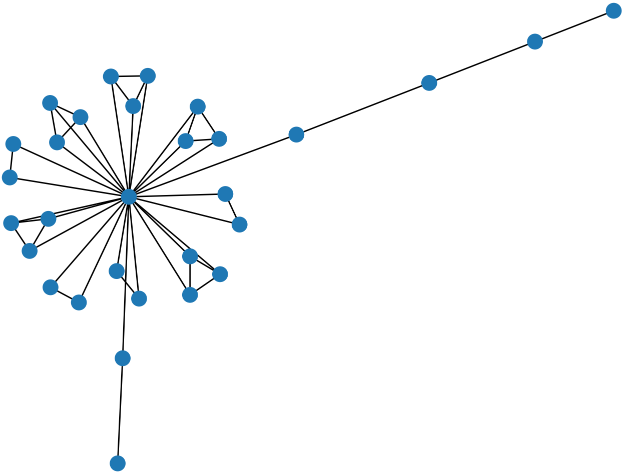
Reward: $\pi + \partial_{\lfloor \frac{2D}{3} \rfloor}$ (minimize).

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

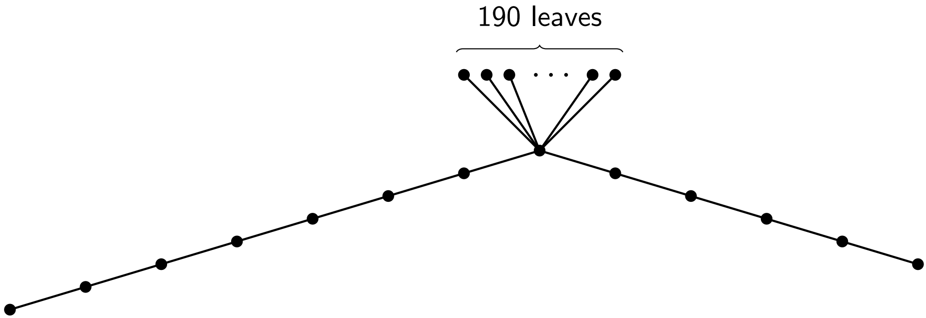


Figure: A counterexample to the conjecture

Question (Brualdi–Cao)

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

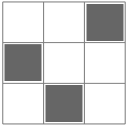


Figure: The pattern 312

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

Example 3 - Not just graphs

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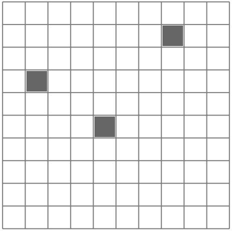

Figure: This is also not allowed

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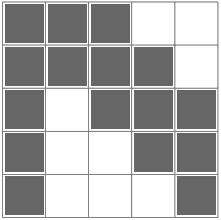
The best you can do is $Fib_{n+2} - 1$.



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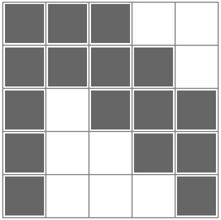
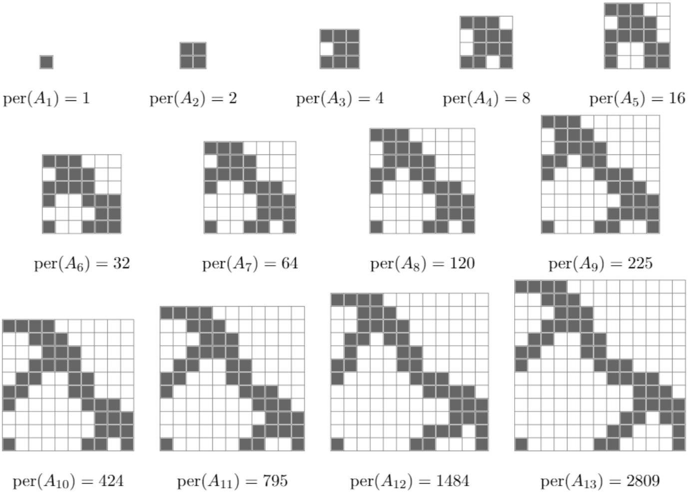


Reward: $\text{per}(A) - \text{penalty}(\# \text{ of } 312\text{-s})$

Example 3



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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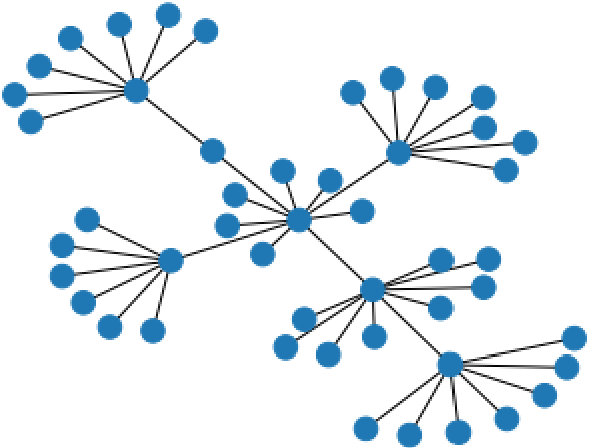

Figure: Best construction found for $n = 48$

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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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A graph is transmission regular, if for each vertex, the sum of distances to all other vertices is the same. So if $\sum_w d(v, w) = \sum_w d(u, w)$ for all vertices u, v.

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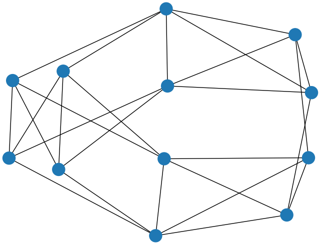
Idea:

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

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 $\left(x^{12} - 216x^{11} + 21188x^{10} - 1245904x^9 + 48797440x^8 - 1336652544x^7 + 26129121472x^6 - 364516883456x^5 + 3556516628224x^4 - 23113129559040x^3 + 90045806284800x^2 - 159318669312000x\right)$, so they are $\mathcal{D}^L$-cospectral.

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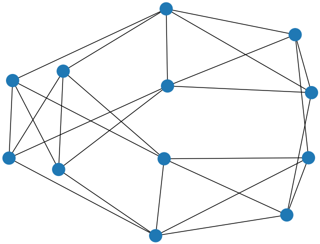
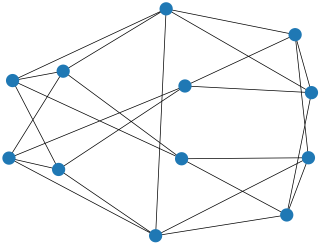

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So transmission regularity is **not** preserved under $\mathcal{D}^L$-cospectrality.

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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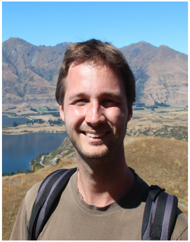

Figure: Gwenaël Joret

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- Somehow reduce to a finite conjecture.

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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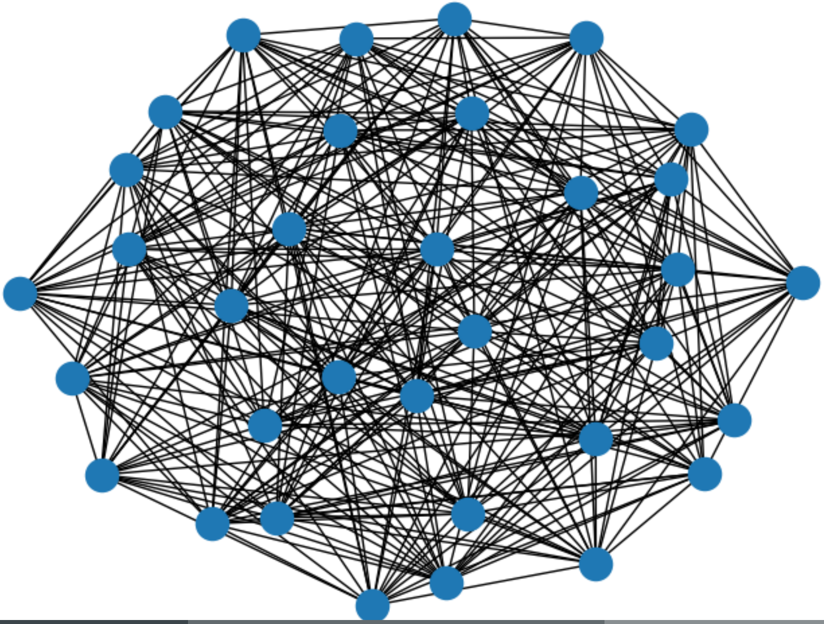

Which RL algorithm to use?

- Value-based methods
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Task: Find the best algorithm for our problems!

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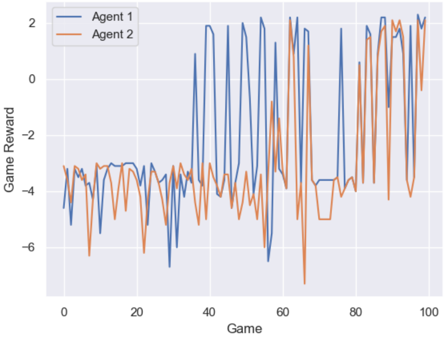
- Do we offer the edges one after the other, starting with $(1,2),(1,3)$, $\ldots(n-1,n)$?
- Or do we generate a graph vertex by vertex?
- We could repeatedly ask the neural network to pick one edge to add, out of all remaining edges?
- Do we offer edges in random order? Do we offer multiple edges at 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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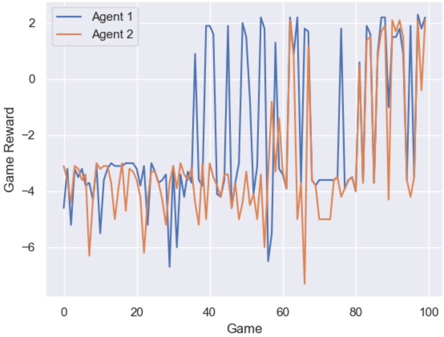

Learning rate too high? Some other hyperparameter is wrong? Not enough training? Coincidence? Maybe this algorithm is unsuited for this specific problem, but good for others?

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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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- Play 1000 games according to neural network
- Keep the top 100 with the highest score, throw away the rest
- 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.

Implementation details

- Offer edges one by one: $(1,2)$, then $(1,3)$, $\ldots$.
- 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