Finding counterexamples via reinforcement learning

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Hausdorff School: “Machine Learning and Theorem Proving”

Day 1

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

Reward: $\;_1 + \quad$ (minimize).

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

Conjecture

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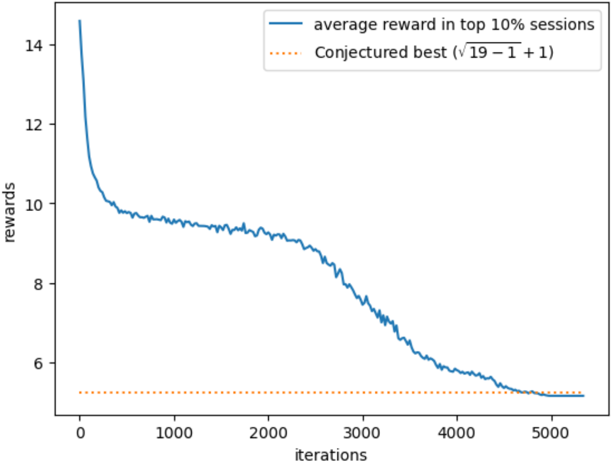

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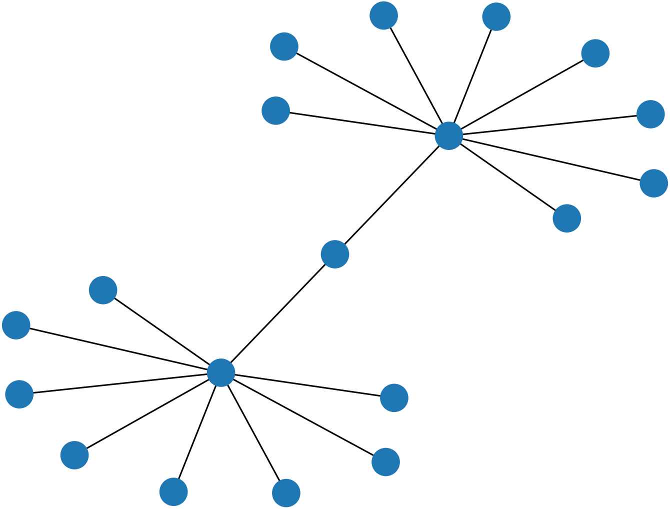

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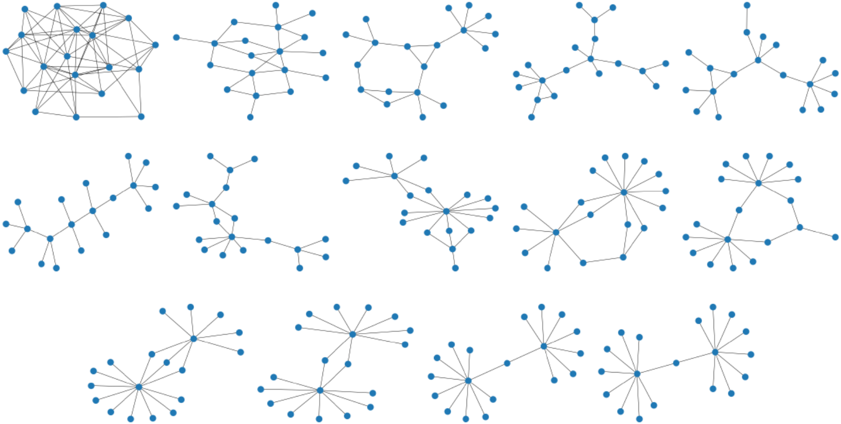

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- When this happens, there is not much to talk about. But often it is not that simple.

- 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.

Conjecture (Auchiche–Hansen, 2016)

Let G be a connected graph with diameter D, proximity and distance spectrum $@_1$ $:::$ $@_n$. Then

$$+ @_{b\frac{2D}{3}c} > 0:$$

Example 2 – What if we don't succeed?

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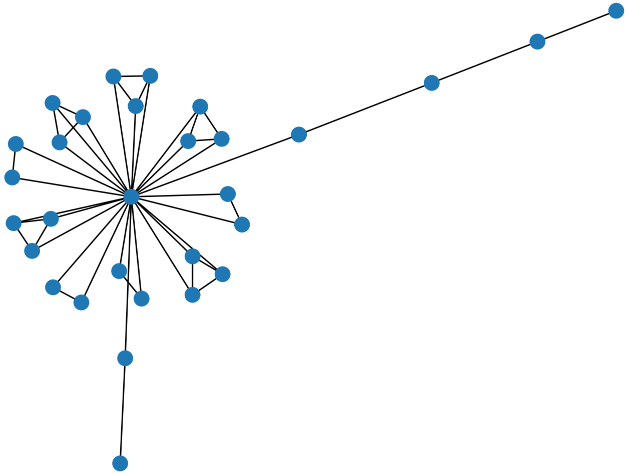
Reward: $+ @_{\lfloor \frac{2D}{3} \rfloor}$ (minimize).

Run it for $n = 30$:

Example 2



This is not quite a counterexample ($+ @_{b\frac{2D}{3}c}$ $0{:}4$), but it tells us very clearly what counterexamples could look like.

Example 2

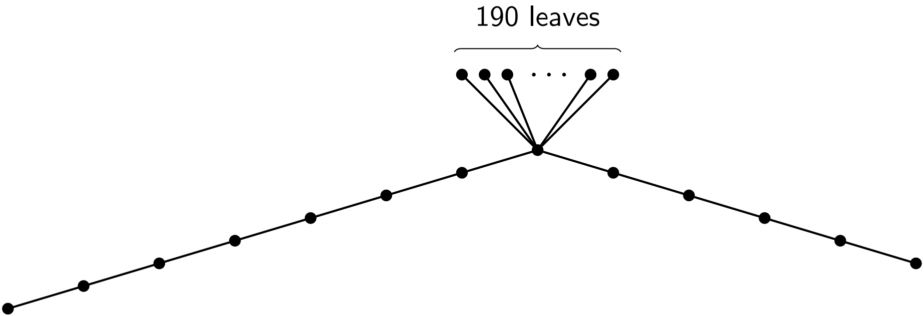


Figure: A counterexample to the conjecture

Example 3 - Not just graphs

Question (Brualdi–Cao)

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

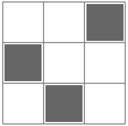


Figure: The pattern 312

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

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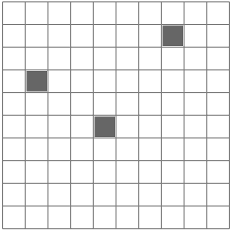

Figure: This is also not allowed

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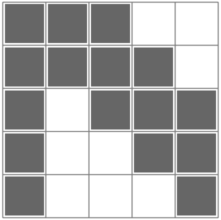
The best you can do is Fib_{n+2} 1.



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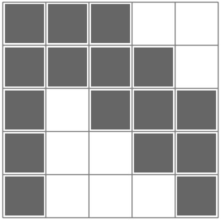

Reward: $\text{per}(A) \quad \text{penalty}(\#\text{ of 312-s})$

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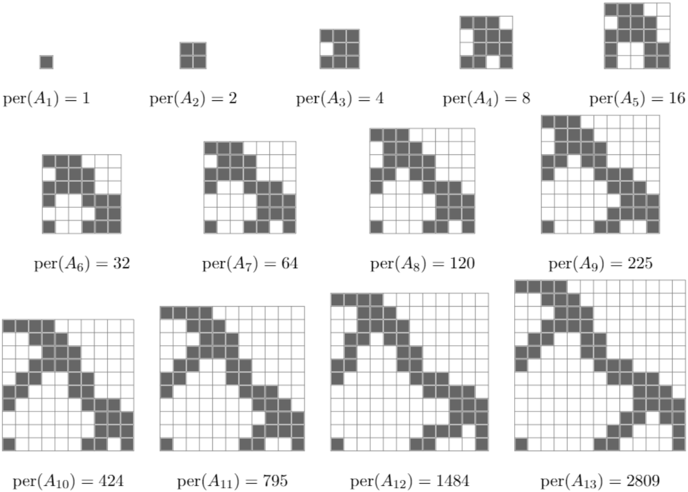

These are best possible for n 8 (computer proof). So the sequence starts with $1; 2; 4; 8; 16; 32; 64;$ **120**.

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 coe cients of p and q are both unimodal, and their peaks are asymptotically at the same place.

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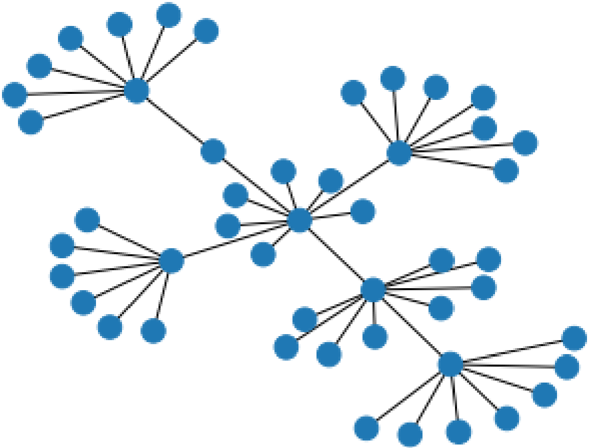

Figure: Best construction found for $n = 48$

Example 5 - non-obvious reward function

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

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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 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.

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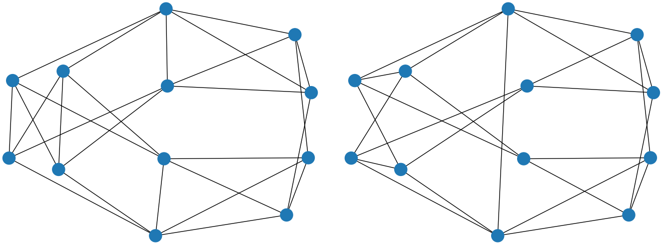

The graph on the left is transmission regular, whereas the graph on the right is not. The characteristic polynomials of their distance Laplacians are the same $\left(x^{12} \quad 216x^{11} + 21188x^{10} \quad 1245904x^{9} + 48797440x^{8} \quad 1336652544x^{7} + 26129121472x^{6} \quad 364516883456x^{5}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

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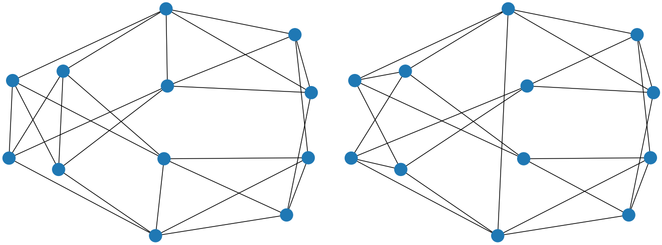

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So transmission regularity is **not** preserved under D^L-cospectrality.

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Many interesting problems can not have nite counterexamples.

[redacted]

The function

$$K_4(G) + K_4(G)$$

is asymptotically minimized by random graphs.

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Figure: Gwenaël Joret

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- Find the best construction for $n = 50$, then generalize \by hand".
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How can we refute such conjectures using RL?

- Find the best construction for $n = 50$, then generalize “by hand”.
- Somehow reduce to a finite conjecture.

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

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

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

Example 6

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

Do not learn a value function: \I have no idea how good this chess position is for black, but I know the best move is c4".

Mixed methods (\Actor-critic methods")

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Task: Find the best algorithm for our problems!

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- Do we o er 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 o er edges in random order? Do we o er multiple edges at a time, is it bene cial to o er an edge again after it was rejected once?
- What neural network architecture to use? Dense layers may not be t
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 $\frac{n(n \quad 1)}{2}$ moves was responsible for getting a bad score?

Bad reward design

Explore-exploit dilemma

What do we conclude if the algorithm produces this output?

Practical problems

What do we conclude if the algorithm produces this output?

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

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Cross-entropy method:

- Simplest possible policy-based method.
- Not sensitive to hyperparameters $\Rightarrow$ 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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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 o 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 ! use it to massively restrict the search space