Graph Networks for Graph Theory

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Plan

- AI for Pure Mathematics
- Reinforcement Learning
- Counterexamples in graph theory
- Graph Neural Networks
- GNNs for graph constructions

This is work in progress joint with Fanglan Feng

AI for Mathematics

Different flavours

- For **conjecture generation**: in knot theory and representation theory (Davies et al 2021), in number theory (He et al 2024), algebraic geometry (Coates et al 2023).

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In this talk we focus on using reinforcement learning to find counterexamples to conjectures.

Some questions

Key Problems

Sampling bias
What is a random variety or a random knot?

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Let's think about model choice and data representation today

RL for Counterexamples

AI to disprove conjectures

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Which conjectures?

“over all combinatorial structures X
an associated numerical quantity Z is bounded by B.”

Example conjecture

Conjecture from AutoGraphiX

Given any connected graph G on $n \geq 3$ vertices, with largest eigenvalue λ and matching number μ we have

$$\lambda + \mu - \sqrt{n-1} - 1 \geq 0$$

[The conjecture had already been disproved by Stevanović, who provided an example with 600 vertices.]

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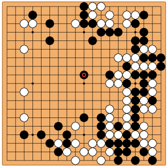
Agent

Environment



Wagner uses a simple reinforcement learning algorithm called **(deep) cross entropy method**.

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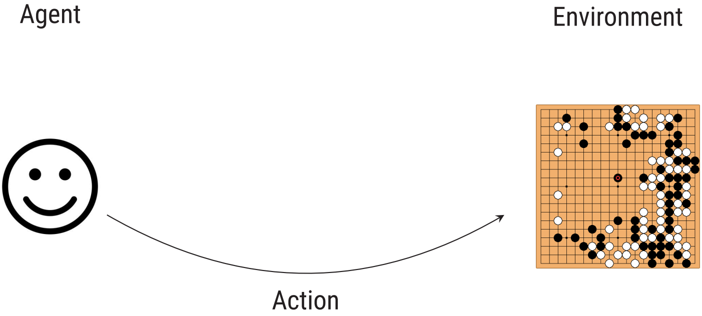

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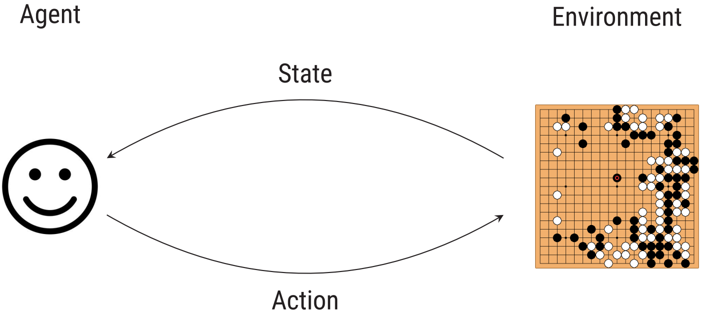

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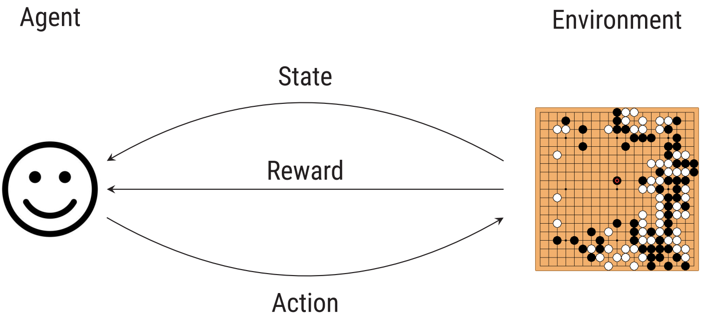

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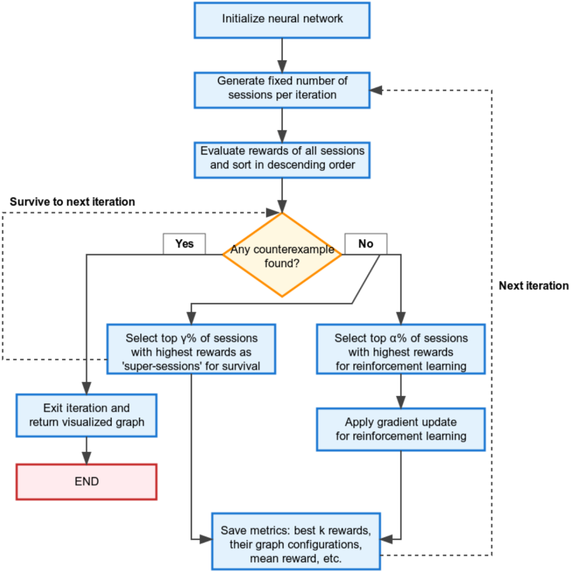
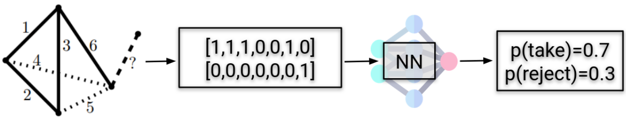
Cross entropy



Method

For us, the game is *Do I keep this edge?*



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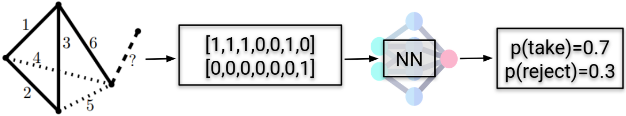
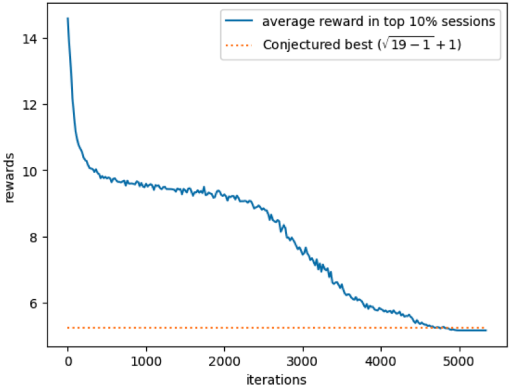


- Reward function: $\lambda + \mu$, the aim is to minimise it [Of course the reward depends on the conjecture you are disproving]
- Input: two vectors, one keeping track of the edges that have been taken so far, and one indicating the edge that is under consideration.
- The action are sampled according to an MLP.

Results

Wagner finds a counterexample to the above conjecture with $n = 19$.



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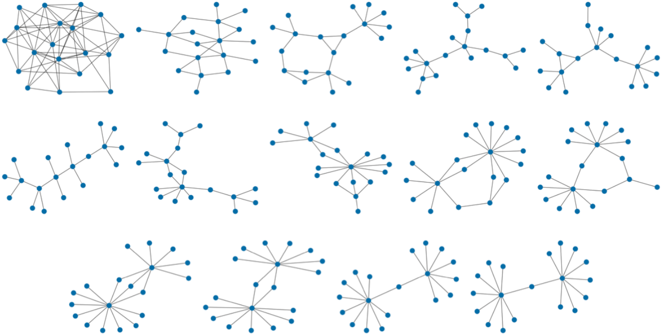

Further work

Limitations

- It is quite slow (it needs 5 000 iterations to find a counterexamples).
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- Roucairol et al. 2022
- Angileri et al. 2024
- Ghebleh et al. 2024

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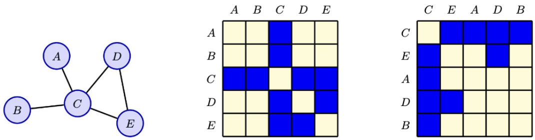
How can we learn on graphs?

Consider a graph $\mathcal{G} = (\mathcal{V}, \mathcal{E})$. A convenient way to represent it is using an *adjacency matrix*, and use it as the input to a sequential or convolutional network. For this we have to choose a node ordering.



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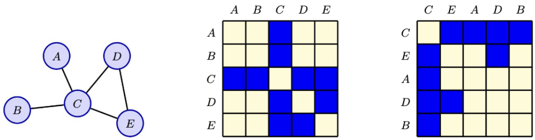
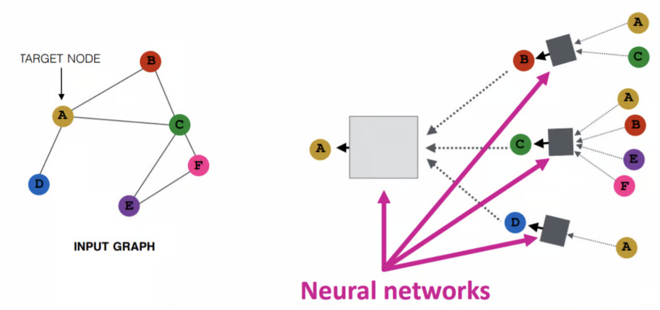


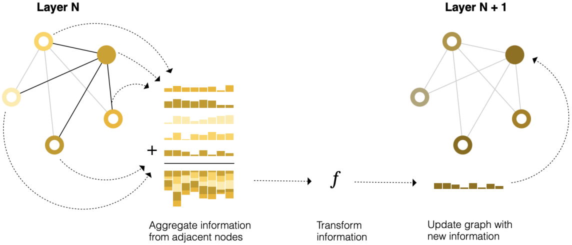
Problem: Most questions about graphs do not depend on the choice of node ordering.

Graph Neural Networks

Answer: Graph Neural Networks. They learn a meaningful embedding of the nodes by a series of layers that perform an operation called *message passing*.



Graph Neural Networks



Let h_i^k be the embedding of the ith node at layer k,

$$h_i^{k+1} = f\left(\sum_{j \in \mathcal{N}(i) \cup \{i\}} \frac{1}{\sqrt{\deg i}\sqrt{\deg j}} (\mathbf{W}_k^T \cdot h_j^k) + \mathbf{b_k}\right)$$

the weight matrix $\mathbf{W}_{k-1}$ (and the bias vector $\mathbf{b}_{k-1}$) is shared by all nodes and depends on the layer. Here f could be something like ReLU.

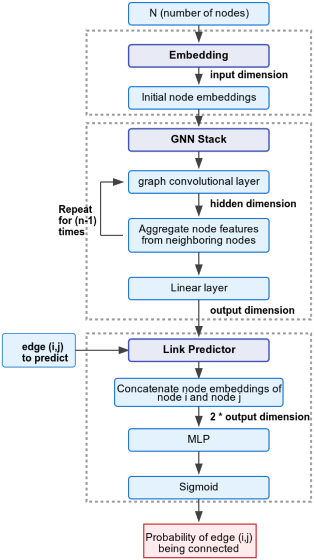
Graph Neural Networks

- **Node task**: e.g., use the final node embeddings for classification/regression.
- **Edge task**: e.g., get the probability of an edge between nodes *i* and *j* by

$$p(i,j) = \sigma((h_i^N)^T \cdot h_j^N)$$

  where σ is just the sigmoid function.
- **Graph task**: e.g., aggregate node embeddings to a unique graph embedding and use that for classification/regression.

Our model



N (number of nodes)
Embedding
input dimension
Initial node embeddings
GNN Stack
graph convolutional layer
hidden dimension
Aggregate node features from neighboring nodes
Repeat for (n-1) times
Linear layer
output dimension
edge (i,j) to predict
Link Predictor
Concatenate node embeddings of node i and node j
2 * output dimension
MLP
Sigmoid
Probability of edge (i,j) being connected

Comparison

We replace the MLP by our GNN model, to approximate the policy function, leaving the cross entropy method unchanged.

Preliminary results

Our method

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- converges much more quickly (20–30 iterations vs 5 000–10 000 iterations) and with fewer sessions per iteration (250–300 vs 1 000)
- it will hopefully be much more flexible (e.g. node colouring problems, working with graphs with different number of nodes etc).

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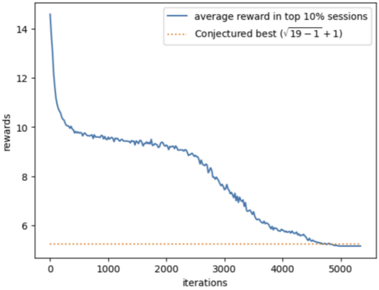
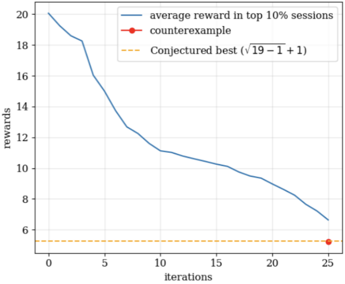


average reward in top 10% sessions
Conjectured best ($\sqrt{19-1}+1$)
rewards
iterations



average reward in top 10% sessions
counterexample
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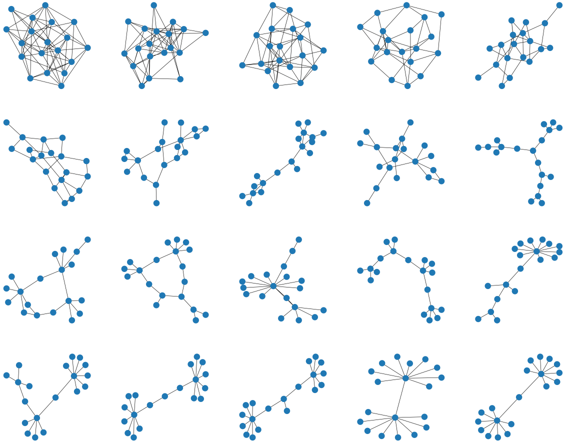

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Advertisement: We are organising an AI for Maths conference this summer at Imperial. Details: