

# Interpretability, Decision Trees, and Sequential Decision Making

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# Sequential decision making (SDM)

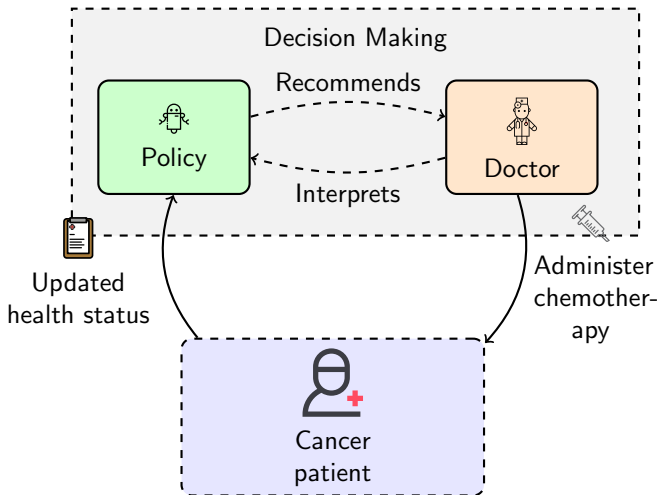
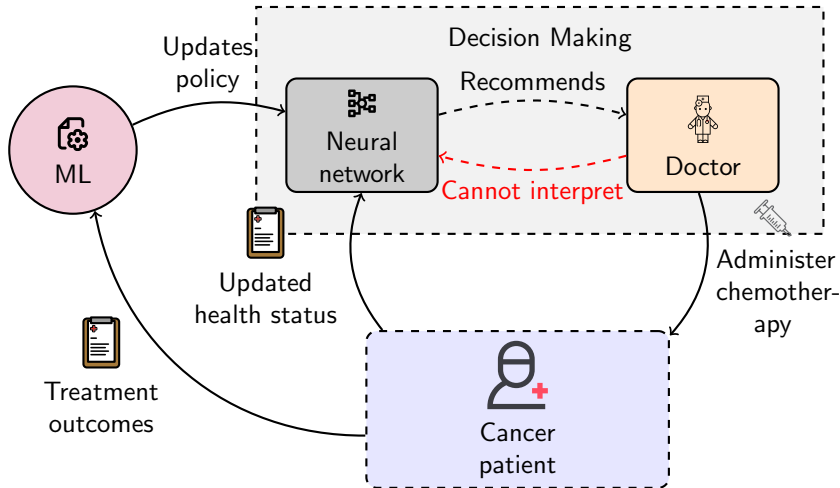


Figure: Sequential decision making in cancer treatment.

# Machine learning (ML) of policies for SDM



**Figure:** Machine learning of neural networks has many recent successes but neural networks are black-box.

How to **learn interpretable** policies for **sequential decision making**?

# Decision trees

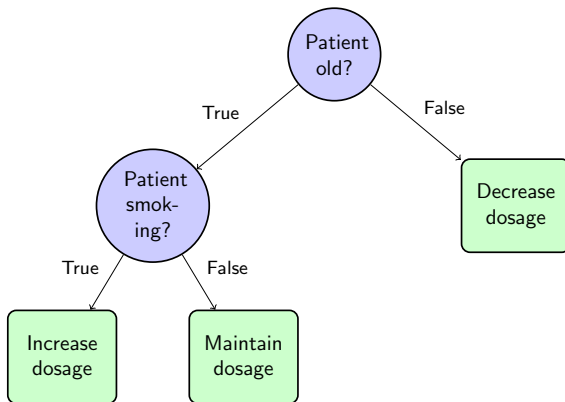


Figure: A generic decision tree of depth  $D = 2$ .

Algorithms are well understood for non-sequential learning: CART, OCT [7, 6, 9, 40, 26] .... What about SDM?

# Markov decision processes

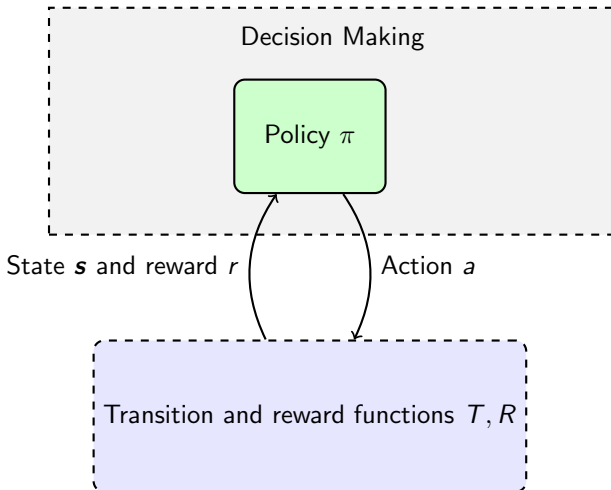


Figure: Markov decision process ([30]).

# Reinforcement learning (RL) objective

- The goal of RL ([38]) for SDM is to find a policy,  $\pi : S \rightarrow A$  that maximizes:

$$J(\pi) = \mathbb{E} \left[ \sum_{t=0}^{\infty} \gamma^t R(s_t, a_t) \mid s_0 \sim T_0, a_t = \pi(s_t), s_{t+1} \sim T(s_t, a_t) \right]$$

- Value iteration, Q-learning, Sarsa, Deep Q Networks, Proximal Policy Optimization, ... ([5, 38, 28, 35])

# Grid world MDP

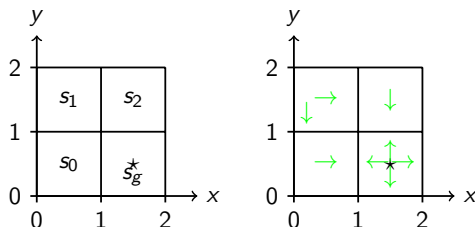


Figure: A grid world MDP and optimal actions.

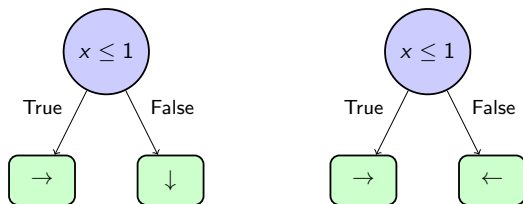
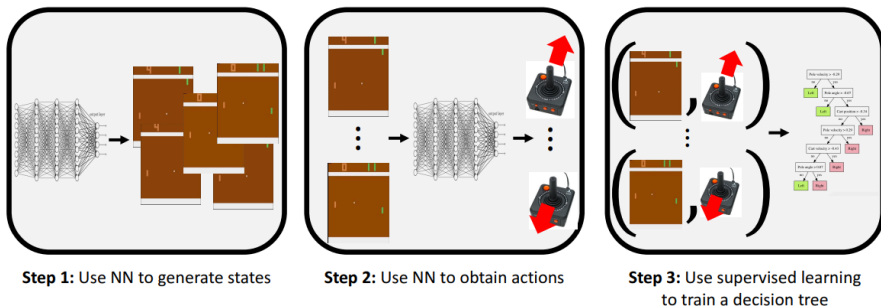


Figure: An optimal depth-1 decision tree policy and a sub-optimal depth-1 decision tree policy.

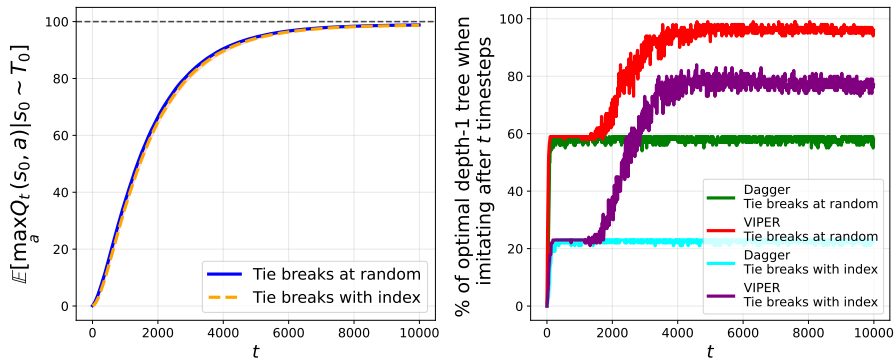


# Indirect approach: imitation learning



**Figure:** Imitation learning works well in practice to get interpretable policies ([27, 4, 34]) but no optimality guarantees.

# Example: a decision tree policy for the grid world MDP

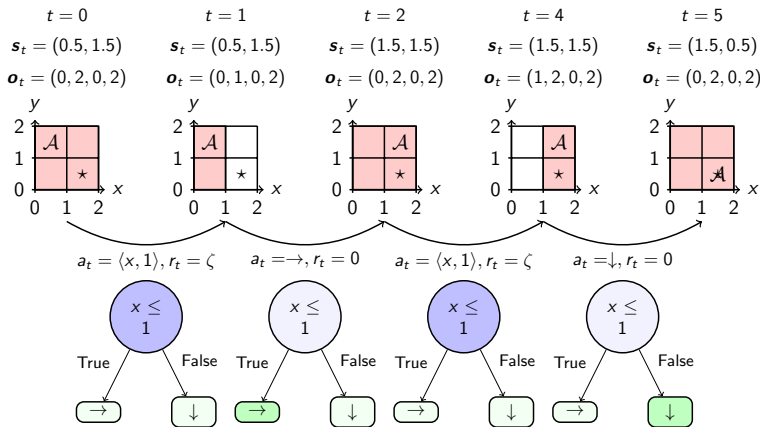


**Figure:** Sample complexity curve of Q-learning over 100 random seeds and performance of indirect interpretable methods when imitating the greedy policy with a tree at different Q-learning stages.

*Q: Can we use reinforcement learning to directly optimize trade-offs of performance and interpretability in SDM?*

**A: direct reinforcement learning is hard because it involves partial observability.**

# Iterative bounding Markov decision processes (IBMDP)



**Figure:** Trajectory in an IBMDP of the grid world MDP ([39]). Actions build a decision tree policy and rewards control the interpretability-performance trade-off.

# Pros and cons of IBMDPs

## Pros

- No need to design new algorithm: we can use deep RL.
- IBMDP rewards trade-off naturally interpretability and performances.

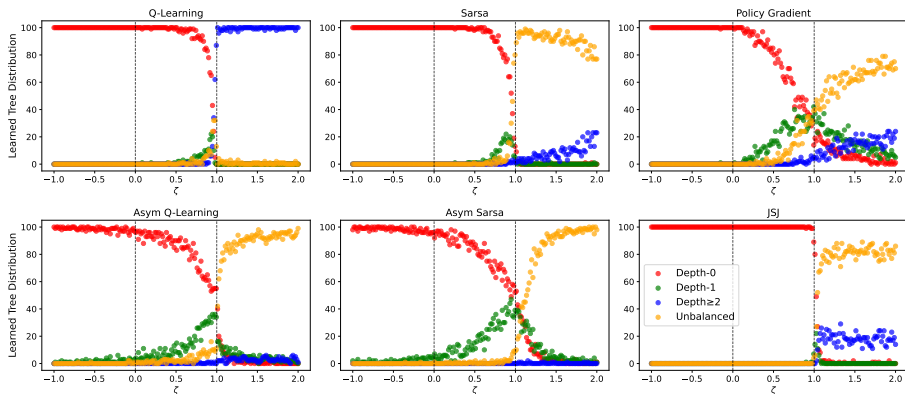
## Cons

- Only **deterministic** and **partially observable** (a.k.a. memoryless or reactive) policies are equivalent to decision tree policies.
- Finding the best **deterministic** and **partially observable** policy is NP-hard ([22])!

*Q: Can we use reinforcement learning to directly optimize trade-offs of performance and interpretability in SDM?  $\Leftrightarrow$*

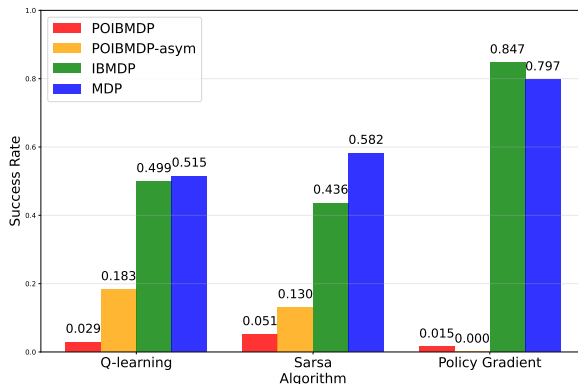
*Q: How does RL perform for optimizing **deterministic** and **partially observable** policies in IBMDPs?*

# Result: RL cannot retrieve optimal depth-1 trees for the grid world MDP



**Figure:** Distributions of final tree policies learned with various (asymmetric) RL algorithms ([38, 36, 23, 1, 2]) across 100 seeds. For each different performance-interpretability trade-off value  $\zeta$ , each point represent the share of different trees.

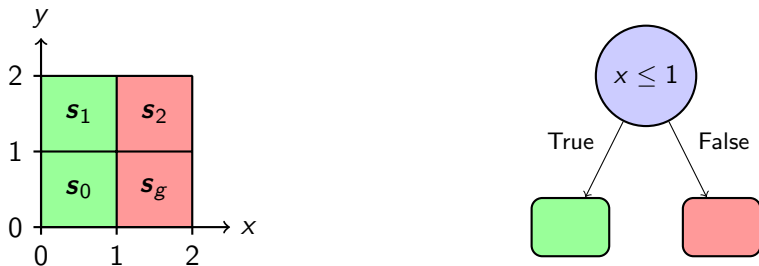
Result: for similar problems, RL struggles when there is partial observability (not surprising)



**Figure:** Success rates of different (asymmetric) RL algorithms over thousands of runs when applied to learning either deterministic partially observable policies in an IBMDP deterministic Markovian policies in the same IBMDP.



# Interesting sub-class of MDPs: classification MDPs



**Figure:** In this classification MDP, there are four data to which to assign either a green or red label. On the right, there is the unique optimal depth-1 tree for this particular classification MDP.

**We show that in theory, deterministic partially observable policies for classification IBMDPs ( $\Leftrightarrow$  decision tree policies) are in fact Markovian.**

# Perspectives for direct RL of decision tree policies.

- Interpretability for SDM problems is difficult because for most problems there is **partial observability**.
- Should we focus on indirect approach? Hybrid approaches ([33])?
- Fixing the policy tree structure a priori (parametric trees, [25])?
- Design algorithms that learn deterministic partially observable policies ([17, 18])?

## RL works in classification MDPs

*Q: Can we leverage SDM in classification MDPs to design new decision tree induction algorithms for the supervised learning (no sequentiality) setting? A: Yes!*

# Decision trees in supervised learning

- $N$  data points. Each  $x_i$  is described by  $p$  features and has a label  $y_i \in \mathcal{Y}$ .

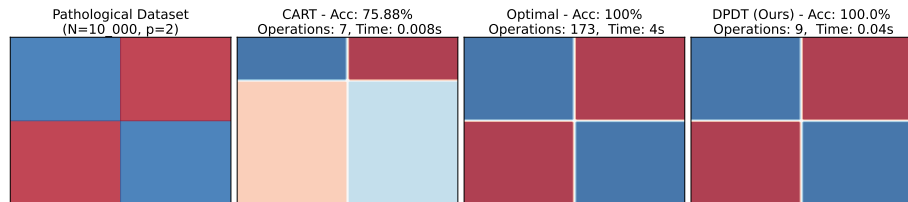
$$\mathcal{L}(T) = \frac{1}{N} \sum_{i=1}^N \ell(y_i, f(x_i)) + \alpha C(T)$$

- Tree-based models are **interpretable** and perform really well on **tabular** data, often **better than deep neural nets** ([13]).

# Optimal decision tree induction is NP-hard

- Greedy algorithms ([7, 32, 31]) **sub-optimal accuracy**, but time complexity in  $O(2^D)$ .
- Optimal algorithms ([6, 9, 20, 8] ...) **optimal accuracy**, but time complexity in  $O((2Np)^D)$  (NP-hard [15]).

# In between?



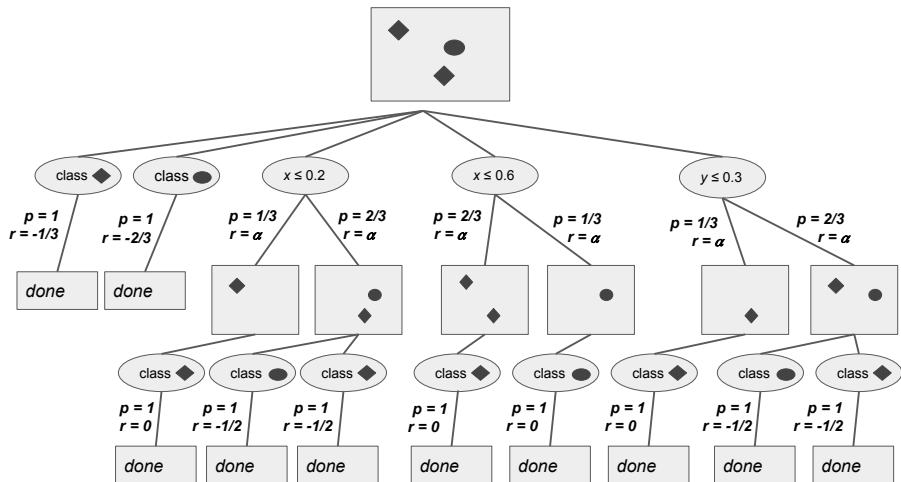
**Figure:** A checkers board data set highlights the limitations of existing works.

## Intuition

The induction of a decision tree is made of a sequence of decisions: at each node, we must decide whether it is better to split (a subset of)  $\mathcal{E}$ , or to create a leaf node.

- S: data subsets.
- A: test or leaf nodes that can be added to the tree.
- R: penalty or accuracies.
- T: node traversals.

# Decision tree induction as solving MDPs



**Figure:** MDP formulation of a generic decision tree induction for a supervised learning task.

# Controlling the time complexity of decision tree induction

- Greedy algorithms consider only one candidate action in each state which is the test that minimizes some impurity criterion → **MDP state space size is  $O(2^D)$** .
- Optimal algorithms consider all possible actions in each state → **MDP state space size is  $O((2Np)^D)$** .
- Let's choose candidate actions adaptively → for each MDP state consider  $B$  actions: **state space size is  $O((2B)^D)$** .



# Dynamic Programming Decision Trees (DPDT)<sup>1</sup>

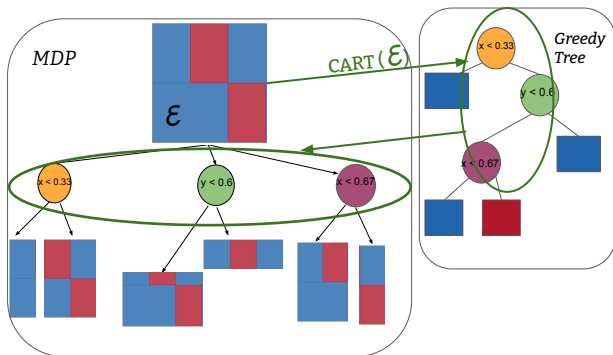


Figure: Overview of our algorithm DPDT presented at the 31st ACM SIGKDD conference.

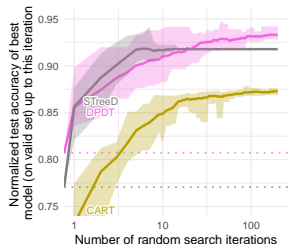
<sup>1</sup>Because states are entire datasets, we implement DPDT with a depth-first search to limit the space complexity.

# Comparing tree accuracy to complexity

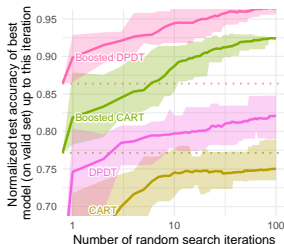
**Table:** Train accuracy and operation count when learning depth-3 decision trees.

Dataset			Accuracy				Operations			
	N	p	Opt Quant-BnB	Greedy CART	DPDT		Opt Quant-BnB	Greedy CART	DPDT	
					light	full			light	full
room	8103	16	<b>0.992</b>	0.968	<b>0.991</b>	<b>0.992</b>	$10^6$	15	286	16100
bean	10888	16	<b>0.871</b>	0.777	0.812	<b>0.853</b>	$5 \cdot 10^6$	15	295	25900
eeg	11984	14	<b>0.708</b>	0.666	0.689	<b>0.706</b>	$2 \cdot 10^6$	13	289	26000
avila	10430	10	<b>0.585</b>	0.532	<b>0.574</b>	<b>0.585</b>	$3 \cdot 10^7$	9	268	24700
magic	15216	10	<b>0.831</b>	0.801	0.822	<b>0.828</b>	$6 \cdot 10^6$	15	298	28000
htru	14318	8	<b>0.981</b>	0.979	0.979	<b>0.980</b>	$6 \cdot 10^7$	15	295	25300
occup.	8143	5	<b>0.994</b>	0.989	0.991	<b>0.994</b>	$7 \cdot 10^5$	13	280	16300
skin	196045	3	<b>0.969</b>	<b>0.966</b>	<b>0.966</b>	<b>0.966</b>	$7 \cdot 10^4$	15	301	23300
fault	1552	27	<b>0.682</b>	0.553	0.672	<b>0.674</b>	$9 \cdot 10^8$	13	295	24200
segment	1848	18	<b>0.887</b>	0.574	0.812	<b>0.879</b>	$2 \cdot 10^6$	7	220	16300
page	4378	10	<b>0.971</b>	0.964	<b>0.970</b>	<b>0.970</b>	$10^7$	15	298	22400
bidding	5056	9	<b>0.993</b>	0.981	<b>0.985</b>	<b>0.993</b>	$3 \cdot 10^5$	13	256	9360
raisin	720	7	<b>0.894</b>	0.869	0.879	<b>0.886</b>	$4 \cdot 10^6$	15	295	20900
rice	3048	7	<b>0.938</b>	0.933	0.934	<b>0.937</b>	$2 \cdot 10^7$	15	298	25500
wilt	4339	5	<b>0.996</b>	0.993	0.994	<b>0.995</b>	$3 \cdot 10^5$	13	274	11300
bank	1097	4	<b>0.983</b>	0.933	0.971	<b>0.980</b>	$6 \cdot 10^4$	13	271	7990

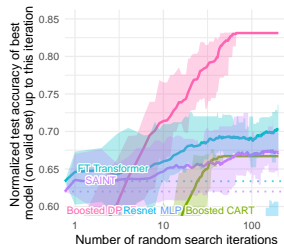
# DPDT trees generalization



(a) DPDT depth-5 trees vs. other depth-5 trees



(b) Boosted DPDT vs. Boosted CART



(c) Boosted DPDT vs. other classifiers

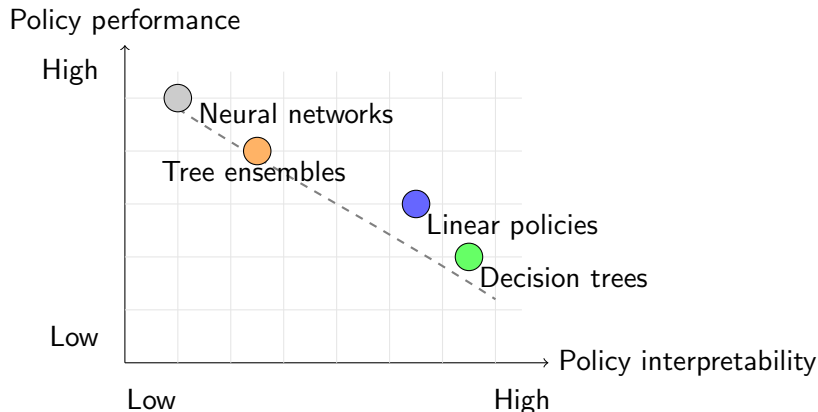
- New SOTA decision tree induction with dynamic programming in MDPs.
- What about using DPDT for indirect decision tree policy learning for SDM?
- What performances could we reach with an industry-grade implementation of XGboost+DPDT?

Let us take a step back

*Q: Are decision trees really the most interpretable model?*

**A: It depends.**

# Policy interpretability



**Figure:** **Heuristic** interpretability-performance trade-offs of different policy classes. Interpretability is often presented in opposition to performances.

# How to measure policy interpretability?

## Challenges ([12, 21, 10])

- No definition of interpretability.
- Measuring might require humans.

## The notion of *simulatability* ([21])

- Interpretability  $\simeq$  how long for human to make the same computations.
- Interpretability  $\simeq$  how much effort for a human to read through the entire policy.
- Less parameters mean more interpretability ([11, 19, 16, 37, 14]).
- Time to formally verify a policy decreases with interpretability ([4, 3]).

# A methodology to measure policy interpretability without humans

## Simulatability ([21])

- 1 How long it takes for human to make the same computations given an input  $\simeq$  policy inference time.
- 2 How much effort it would take a human to read through the entire policy once  $\simeq$  policy size in memory.

## Not that simple in practice ([24])

- Different hardwares (CPUs vs GPUs).
- Different implementations (matrix operations vs fully sequentially) ...

# We propose policy unfolding

```
# Decision tree for Mountain Car
def play(x):
    if x[1] <= -0.2597:
        if x[1] <= -0.6378:
            return 0
        else:
            if x[0] <= -1.0021:
                return 2
            else:
                return 0
    else:
        if x[1] <= -0.0508:
            if x[0] <= 0.2979:
                if x[0] <= 0.0453:
                    return 2
                else:
                    if x[1] <=
-0.2156:
                        return 0
                    else:
                        return 2
            else:
                return 0
        else:
            return 2
```

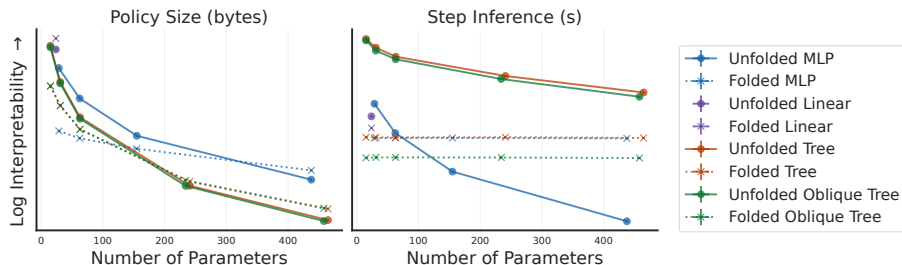
```
# Small ReLU MLP for Pendulum
def play(x):
    h_layer_0_0 = 1.238*x[0]+0.971*x[1]
                +0.430*x[2]+0.933
    h_layer_0_0 = max(0, h_layer_0_0)
    h_layer_0_1 = -1.221*x[0]+1.001
                *x[1]-0.423*x[2]
                +0.475
    h_layer_0_1 = max(0, h_layer_0_1)
    h_layer_1_0 = -0.109*h_layer_0_0
                -0.377*h_layer_0_1
                +1.694
    h_layer_1_0 = max(0, h_layer_1_0)
    h_layer_1_1 = -3.024*h_layer_0_0
                -1.421*h_layer_0_1
                +1.530
    h_layer_1_1 = max(0, h_layer_1_1)
    h_layer_2_0 = -1.790*h_layer_1_0
                +2.840*h_layer_1_1
                +0.658
    y_0 = h_layer_2_0
    return [y_0]
```



- ① Does our methodology respect consensus on policy interpretability?
- ② Is policy unfolding necessary?
- ③ What kind of results we can obtain using our proposed methodology?

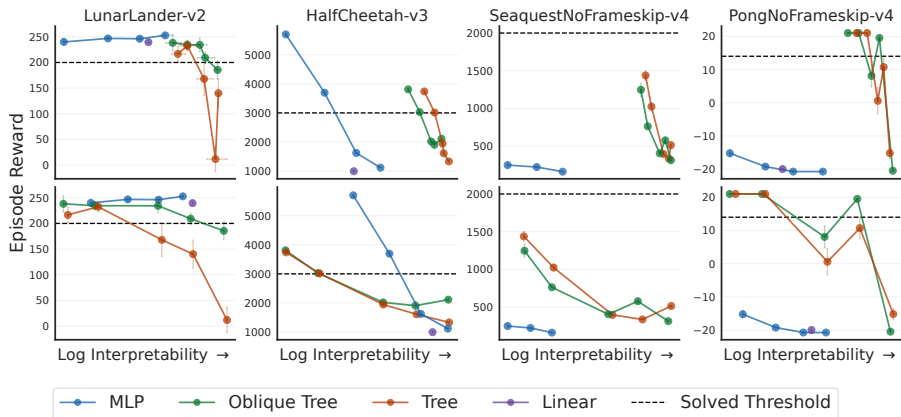
We imitate  $\sim 40000$  expert policies from `stable-baselines3` using various policy classes/nb parameters on various environments.

# Result: unfolding policies is necessary to respect consensus



**Figure:** Policies interpretability on classic control environments. We plot 95% stratified bootstrapped confidence intervals around means in both axes. In each sub-plot, interpretability is measured with either bytes or inference speed.

# Result: there is no dominating policy class for all environments



**Figure:** Interpretability-Performance trade-offs for representative environments. Top row, interpretability is measured with step inference times. Bottom row, the interpretability is measured with policy size.

- Beliefs such as "trees are more interpretable than neural networks" should be used with caution.
- Tree-like policy classes can have good inductive bias (e.g. Atari).
- Can a human study confirm our results?
- What about (very) big models?
- Can we use our policy programs as low level skills (hierarchical RL)?

# Conclusion: interpretable machine learning is a difficult research topic

- Technical challenges: **partial observability** in SDM, NP-hardness.  
→ Focus on indirect approaches and/or on POMDP research first.
- Fundamental challenges: **no definition**.  
→ Discuss with the community (InterpPol workshop).
- **Decision trees offer good inductive bias for SDM in games or tabular data.**

## My hope

Motivate interpretability by finding a real-world problem where interpretability is *really* necessary ([29]).

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