

# Interpretability, Decision Trees, and Sequential Decision Making

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# Sequential decision making

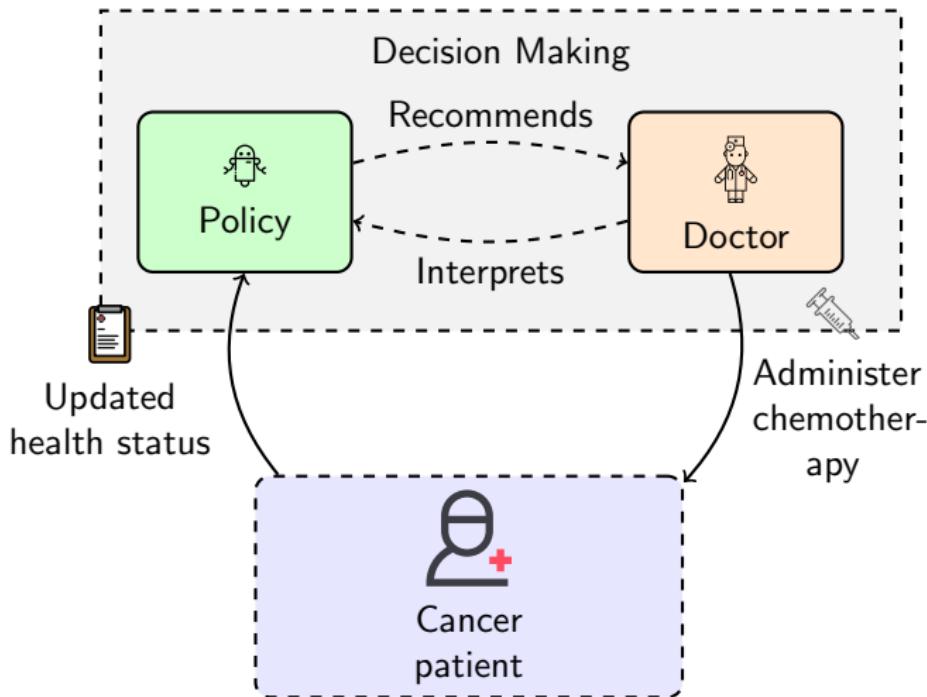
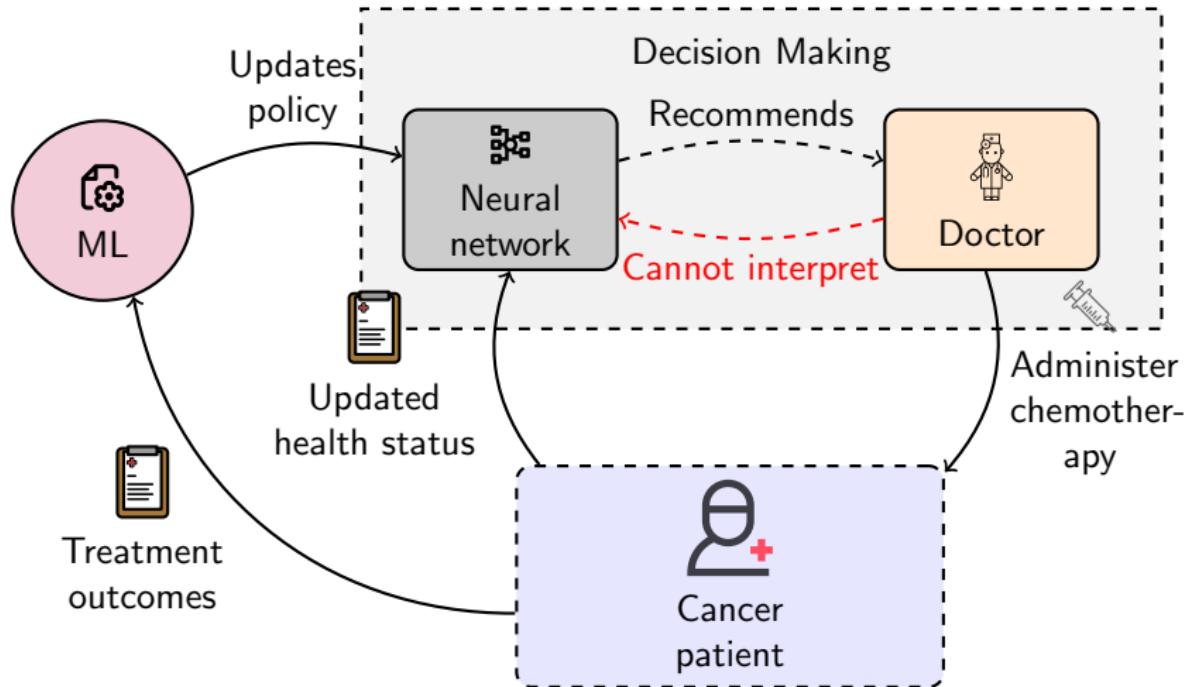


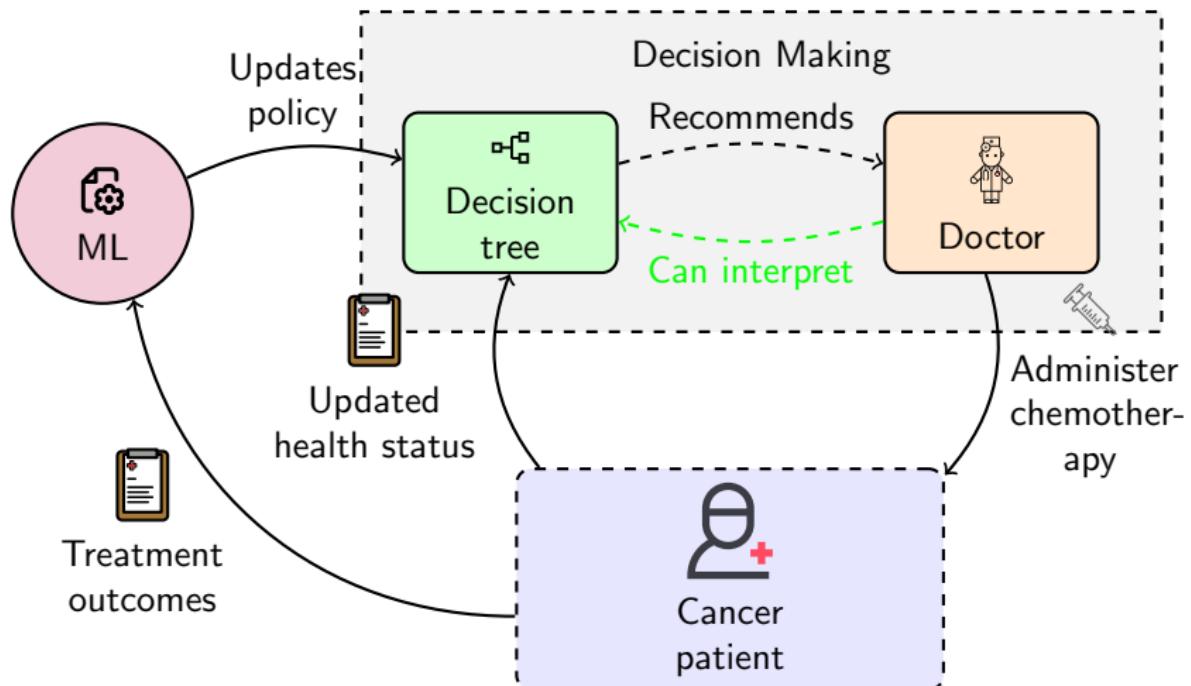
Figure: Sequential decision making in cancer treatment.

# Machine learning of policies for sequential decision making



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

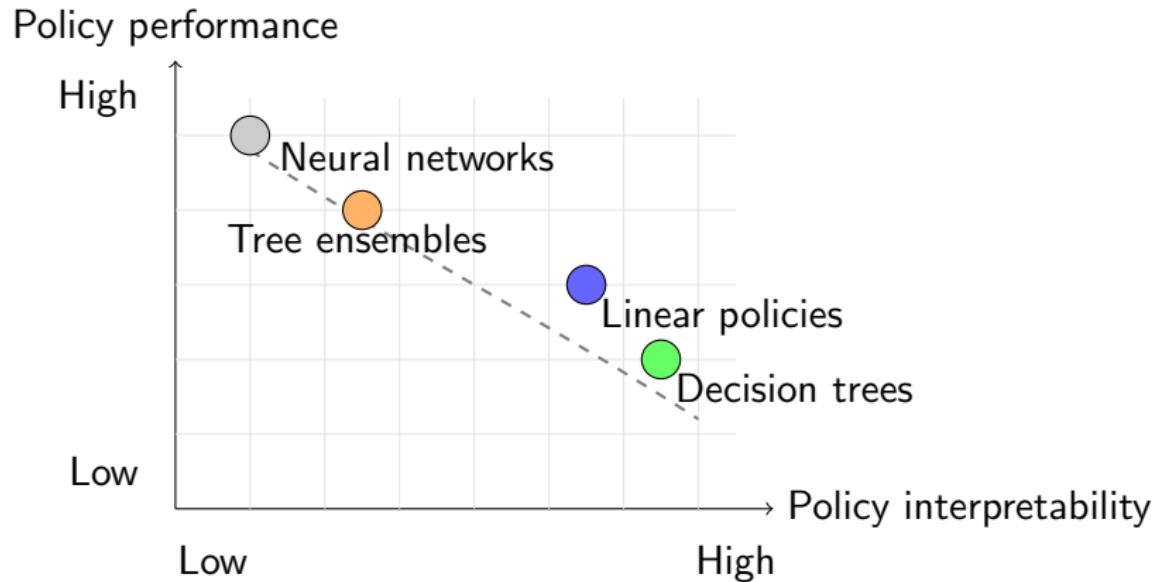
# Interpretable machine learning for sequential decision making



**Figure:** Some machine learning algorithms can learn interpretable policies, e.g. decision trees.

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

# Interpretable policies



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

# Decision trees

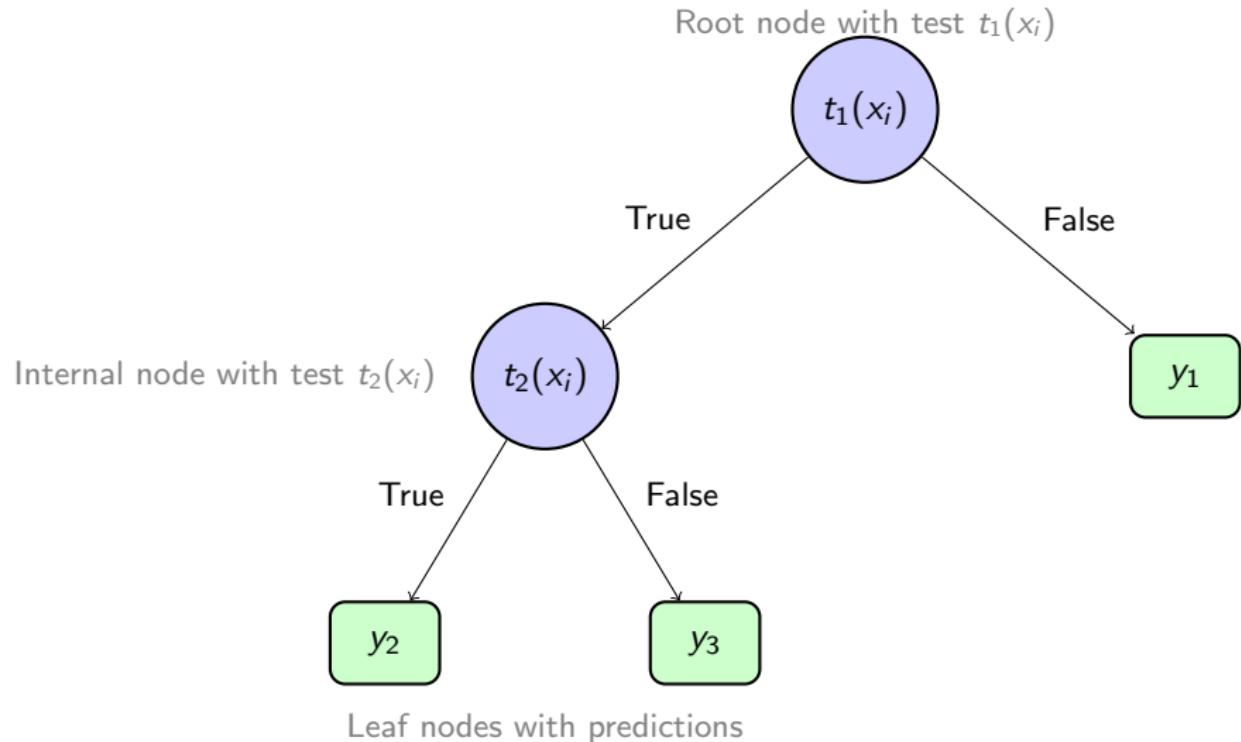


Figure: A generic decision tree of depth  $D = 2$ .

# Markov decision processes

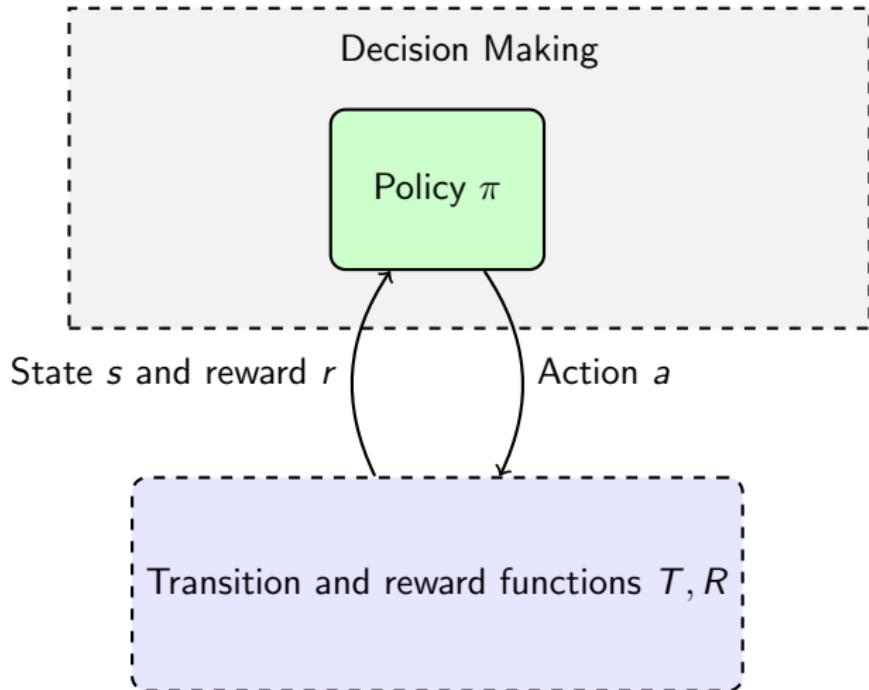


Figure: Markov decision process

# Reinforcement learning objective

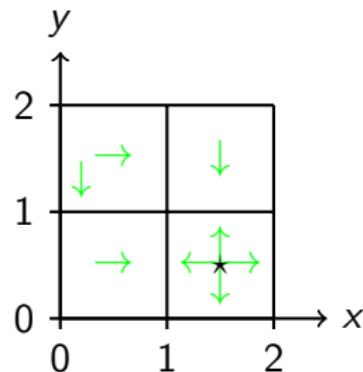
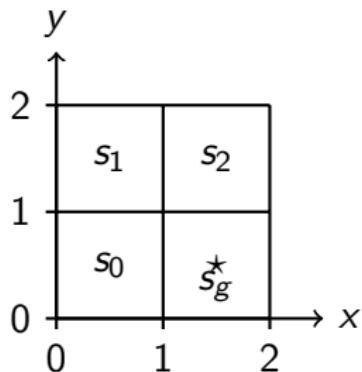
- Given an MDP  $\mathcal{M} = \langle S, A, R, T, T_0 \rangle$  (cf. definition ??), the goal of reinforcement learning for sequential decision making is to find a model, also known as a policy,  $\pi : S \rightarrow A$  that maximizes the expected discounted sum of rewards:

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

where  $0 < \gamma \leq 1$  is the discount factor that controls the trade-off between immediate and future rewards.

- Value iteration, Q-learning, Sarsa, Deep Q Networks, PPO, ...

# Grid world MDP



**Figure:** A grid world MDP (left) and optimal actions w.r.t. the objective (cf. definition ??) (right).

# Machine learning of interpretable models for supervised learning

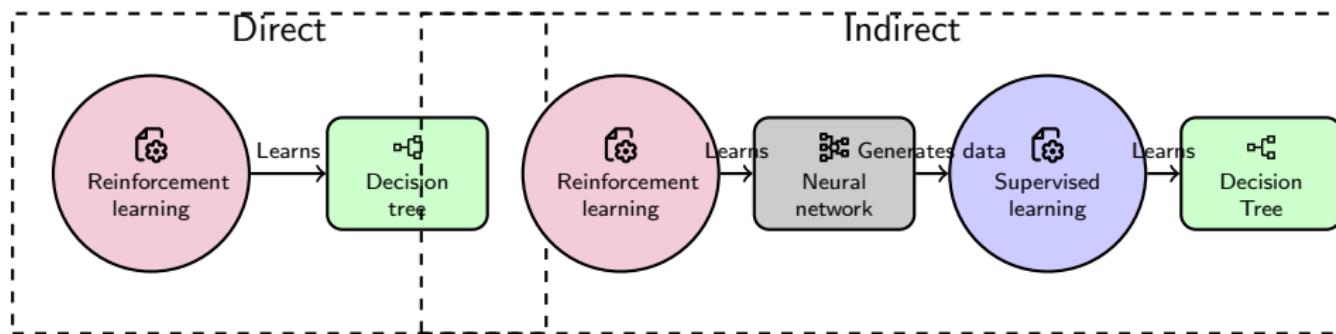
- We assume that we have access to a set of  $N$  examples denoted  $\mathcal{E} = \{(x_i, y_i)\}_{i=1}^N$ . Each datum  $x_i$  is described by a set of  $p$  features.  $y_i \in \mathcal{Y}$  is the label associated with  $x_i$ .

$$f^* = \operatorname{argmin}_{f \in \mathcal{F}} \frac{1}{N} \sum_{i=1}^N \ell(y_i, f(x_i)) + \alpha C(f), \quad (1)$$

where  $C : \mathcal{F} \rightarrow \mathbb{R}$  is a penalty for regularization

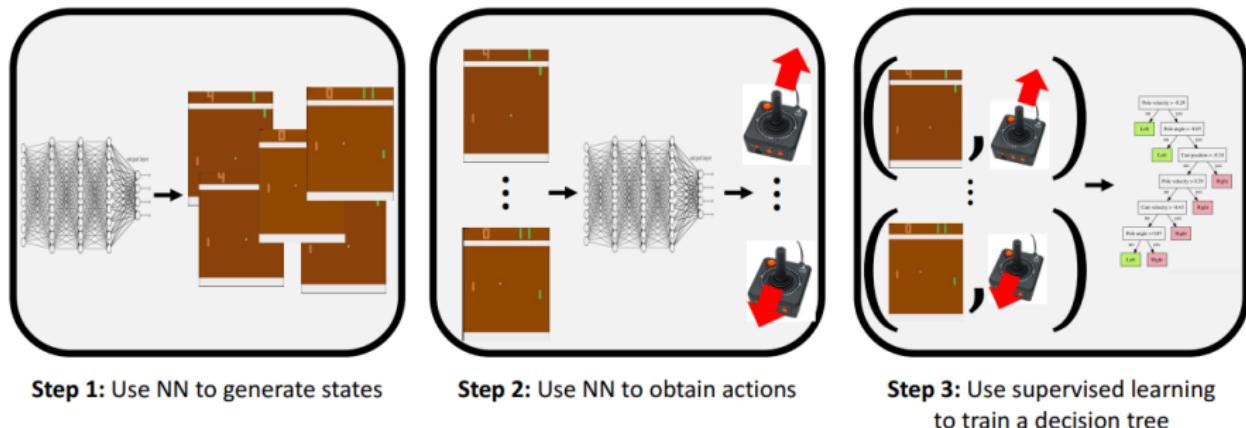
- Classification And Regression Trees (CART, 1984), Optimal Classification Trees (2015)
- What about the RL objective for sequential decision making?

# Two ways to get interpretable policies for sequential decision making



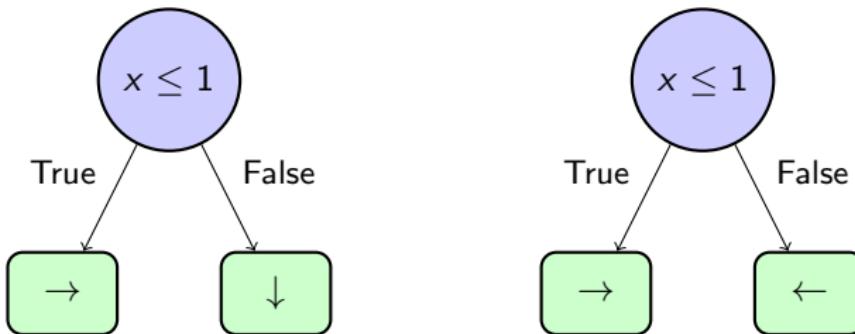
**Figure:** Comparison of direct and indirect approaches for learning interpretable policies in sequential decision making.

# Indirect approach: imitation learning



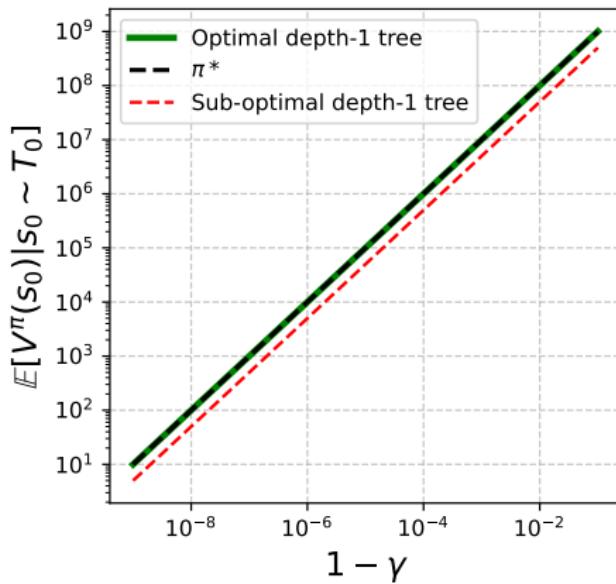
**Figure:** Imitation learning to get interpretable policies (DAgger, VIPER) [**viper**, **dagger**].

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



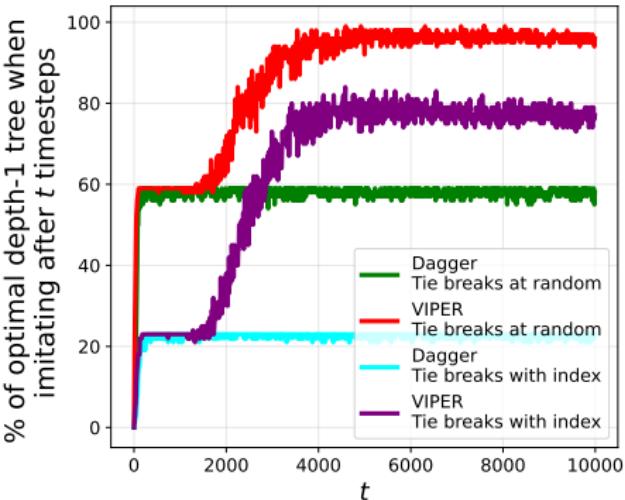
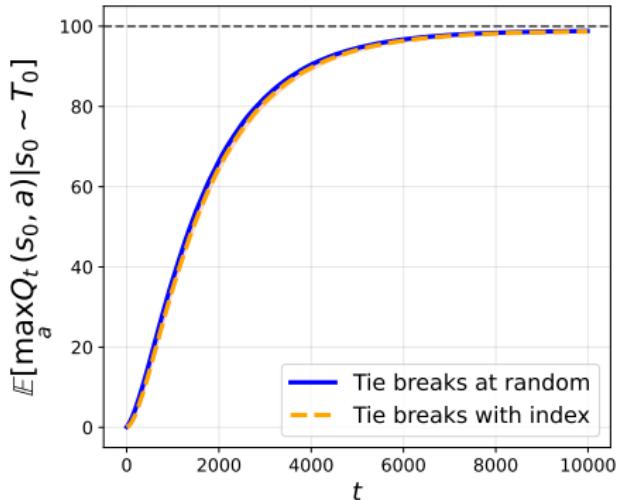
**Figure:** Left, an optimal depth-1 decision tree policy. On the right, a sub-optimal depth-1 decision tree policy.

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



**Figure:** The RL objective values of the optimal policies from figure 7 and of the decision tree policies from figure 10.

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



**Figure:** Left, sample complexity curve of Q-learning with default hyperparameters on the  $2 \times 2$  grid world MDP over 100 random seeds. Right, performance of indirect interpretable methods when imitating the greedy policy with a tree at different Q-learning stages.

# Interpretability, decision trees, and sequential decision making

- How to learn optimal interpretable policies for sequential decision making?
- How to leverage sequential decision making to learn interpretable *classifiers for supervised learning*?
- How to measure policy interpretability in sequential decision making?

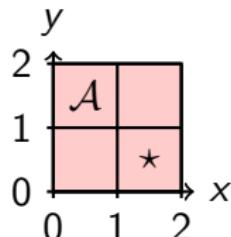
# Thesis results

- ① Direct reinforcement learning of decision tree policies is hard because it involves POMDPs.
- ② One can use dynamic programming in MDPs to induce highly performing decision tree classifiers and regressors.
- ③ In practice, controlling MDPs with interpretable policies does not necessarily decrease performances.

$t = 0$

$s_t = (0.5, 1.5)$

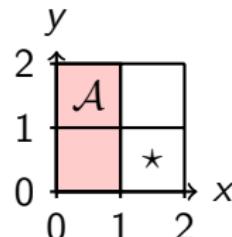
$o_t = (0, 2, 0, 2)$



$t = 1$

$s_t = (0.5, 1.5)$

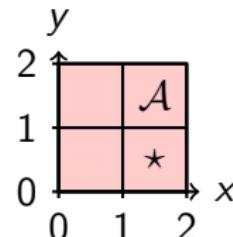
$o_t = (0, 1, 0, 2)$



$t = 2$

$s_t = (1.5, 1.5)$

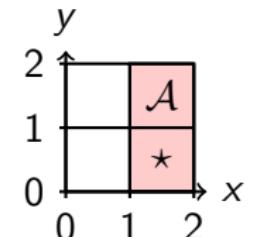
$o_t = (0, 2, 0, 2)$



$t = 4$

$s_t = (1.5, 1.5)$

$o_t = (1, 2, 0, 2)$



$a_t = \langle x, 1 \rangle, r_t = \zeta$

$a_t = \rightarrow, r_t = 0$

$a_t = \langle x, 1 \rangle, r_t = \zeta$

$a_t = \downarrow, r_t =$

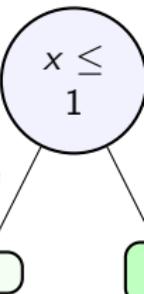
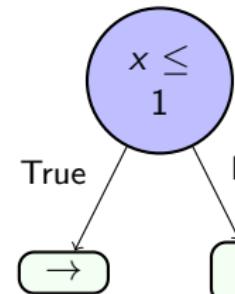
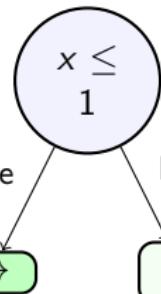
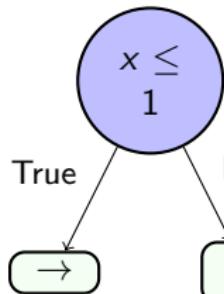
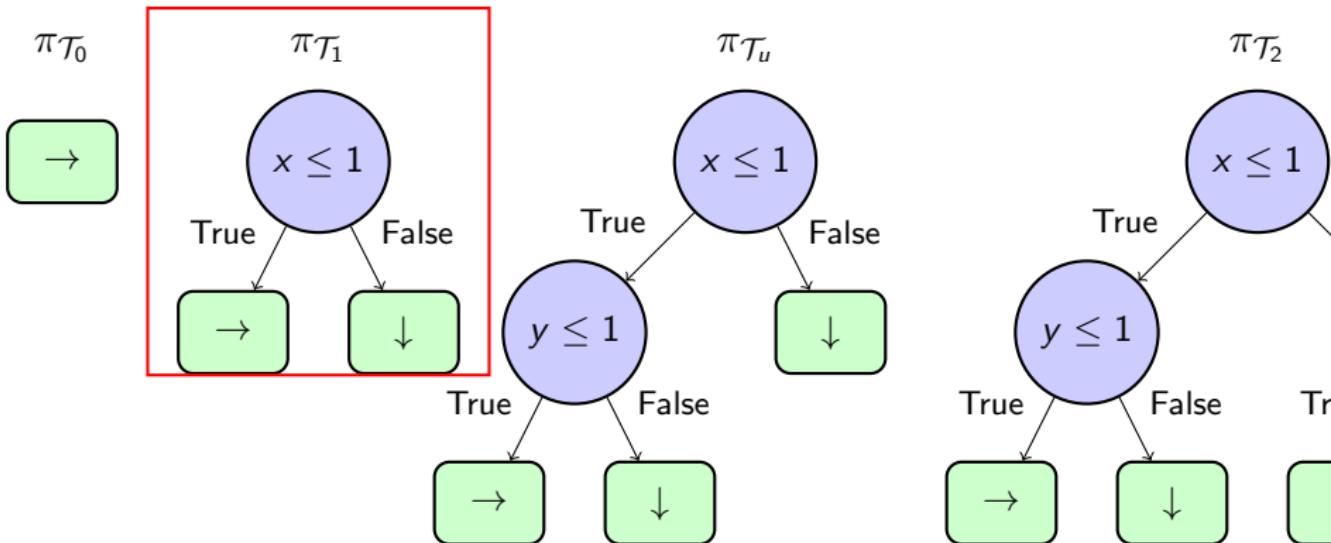
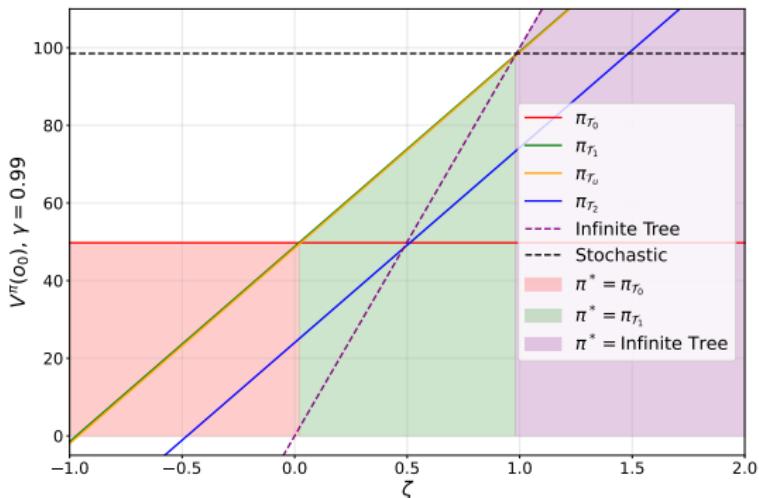


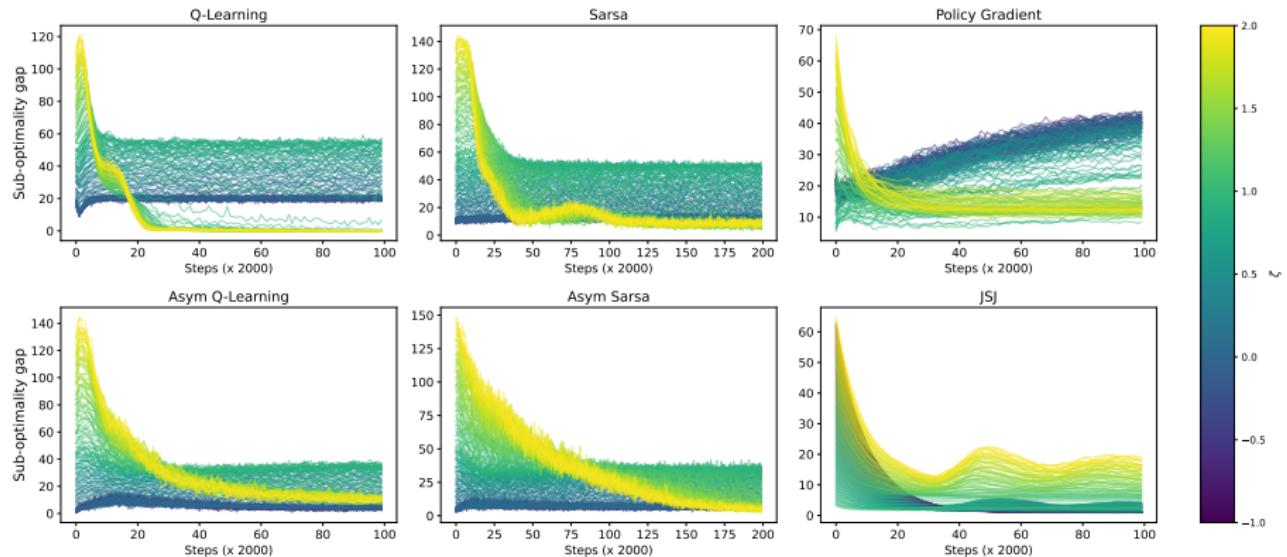
Figure: An IBMMDP trajectory when the base MDP is  $2 \times 2$  grid world.



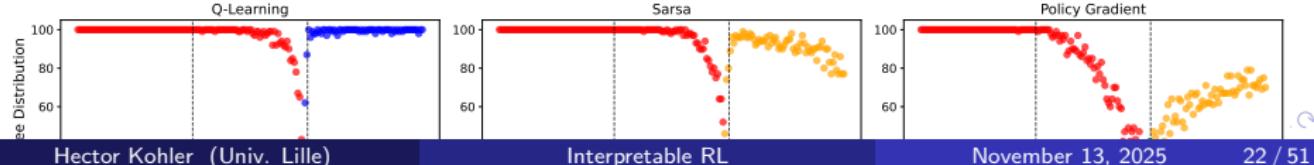
**Figure:** For each decision tree structure, e.g., depth-1 or unbalanced depth-2, we illustrate a decision tree which maximizes the RL objective (cf. definition ??) in the grid world MDP.

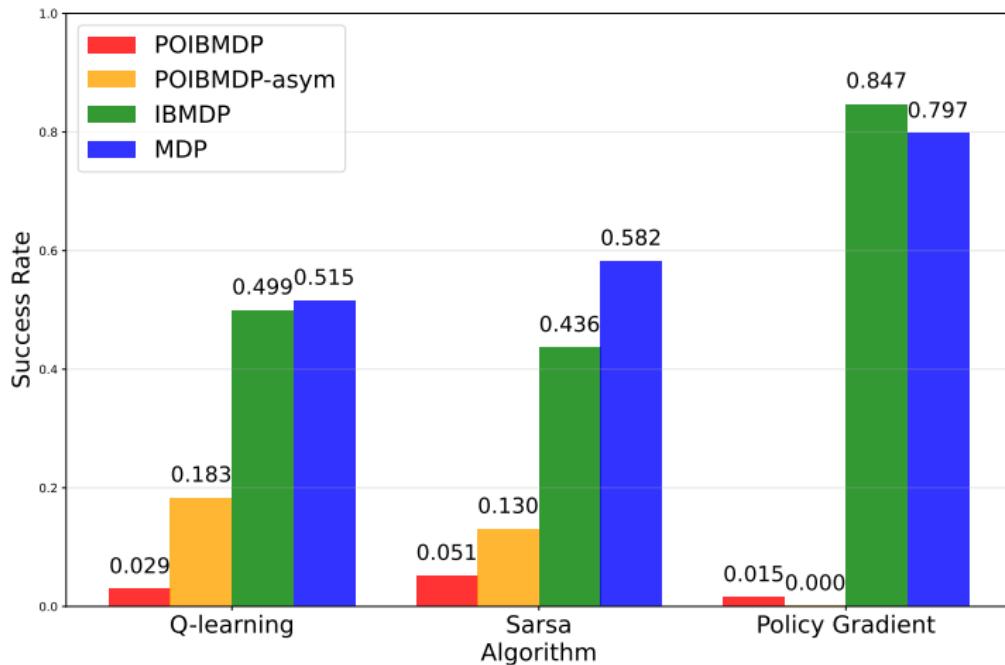


**Figure:** Interpretable RL objective values (cf. definition ??) of different partially observable policies as functions of  $\zeta$ . Shaded areas show the optimal *deterministic* partially observable policies in different ranges of  $\zeta$  values.

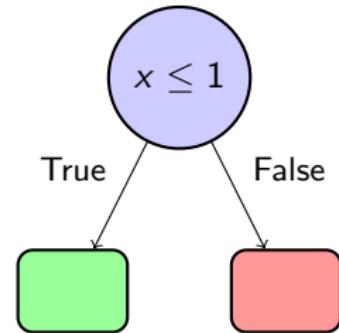
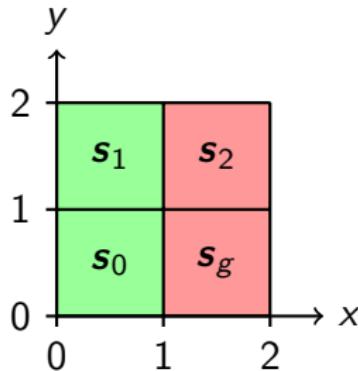


**Figure:** (Asymmetric) reinforcement learning in POIBMDPs. In each subplot, each single line is colored by the value of  $\zeta$  in the corresponding POIBMDP in which learning occurs. Each single learning curve represent the sub-optimality gap averaged over 100 seeds.

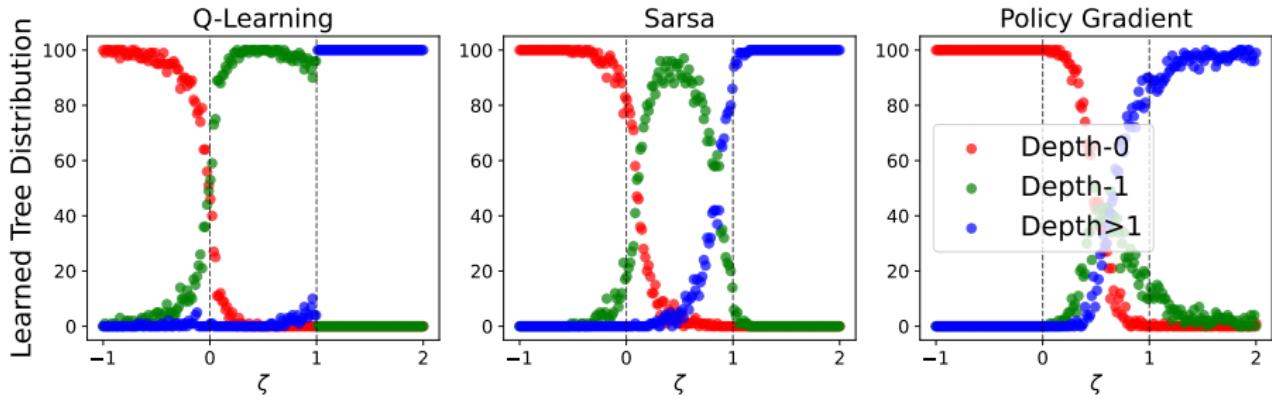




**Figure:** Success rates of different (asymmetric) RL algorithms over thousands of runs when applied to learning deterministic partially observable policies in a POIBMDP or learning deterministic policies in associated MDP and IBMDP.



**Figure:** Classification MDP optimal actions. 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. This depth-1 tree also maximizes the accuracy on the corresponding classification task.



**Figure:** We reproduce the same plot as in figure 17 for classification POIBMDPs. Each colored dot is the number of final learned trees with a specific structure for a given  $\zeta$ .

# Supervised learning

We assume that we have access to a set of  $N$  examples denoted  $\mathcal{E} = \{(x_i, y_i)\}_{i=1}^N$ . Each datum  $x_i$  is described by a set of  $p$  features.  $y_i \in \mathcal{Y}$  is the label associated with  $x_i$ .

$$f^* = \operatorname{argmin}_{f \in \mathcal{F}} \frac{1}{N} \sum_{i=1}^N \ell(y_i, f(x_i)) + \alpha C(f), \quad (2)$$

where  $C : \mathcal{F} \rightarrow \mathbb{R}$  is a penalty for regularization

# Why decision trees ?

- ① Decision trees are **interpretable**.
- ② Tree-based models perform really well on **tabular** data, often **better than deep neural nets** (L. Grinsztajn et. al. 2022).

# Optimal decision tree induction is NP-hard

- Greedy algorithms (C4.5, CART, ID3, ...) **sub-optimal accuracy**, but time complexity in  $O(2^D)$ .
- Optimal algorithms (MurTree, OCT, STreeD, Branches (Jesse Read's work ;)), ...) **optimal accuracy**, but time complexity in  $O((2Np)^D)$ .

# In between?



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

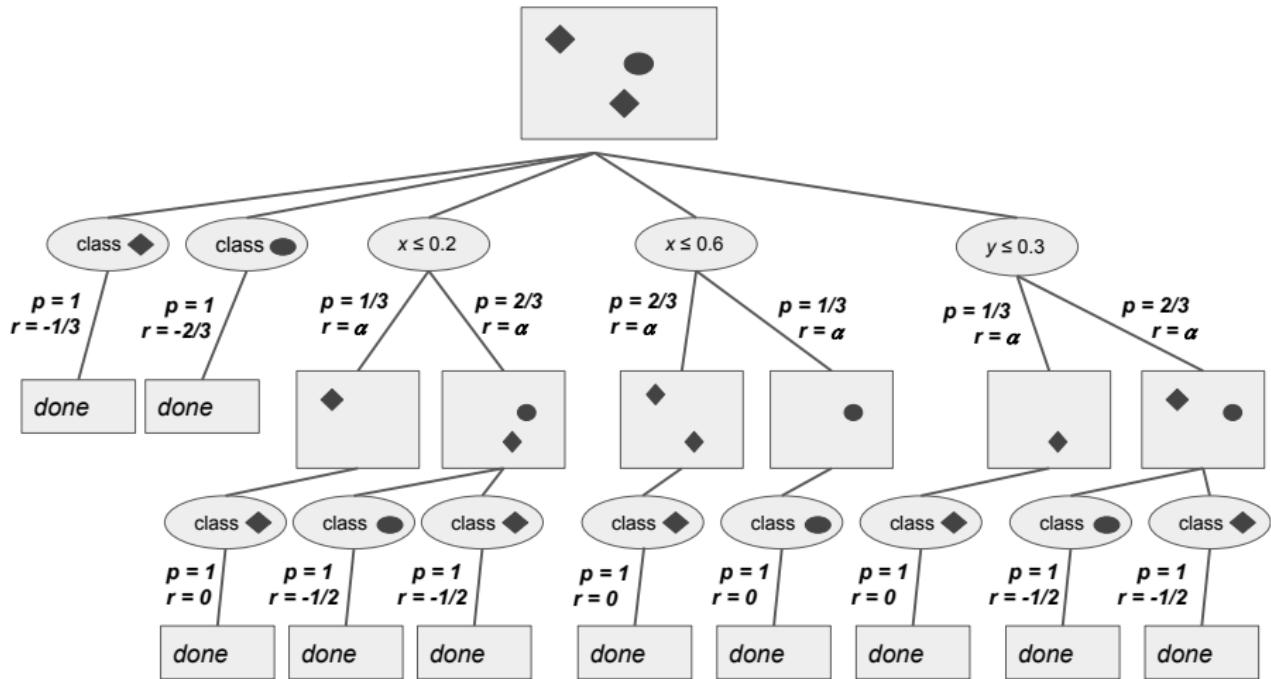
# Decision tree induction as solving MDPs

## Intuition

Given a set of examples  $\mathcal{E}$ , 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.
- Ac: test or leaf nodes that can be added to the tree.
- R: penalty or accuracies.
- T: node traversals.

# Decision tree induction as solving MDPs



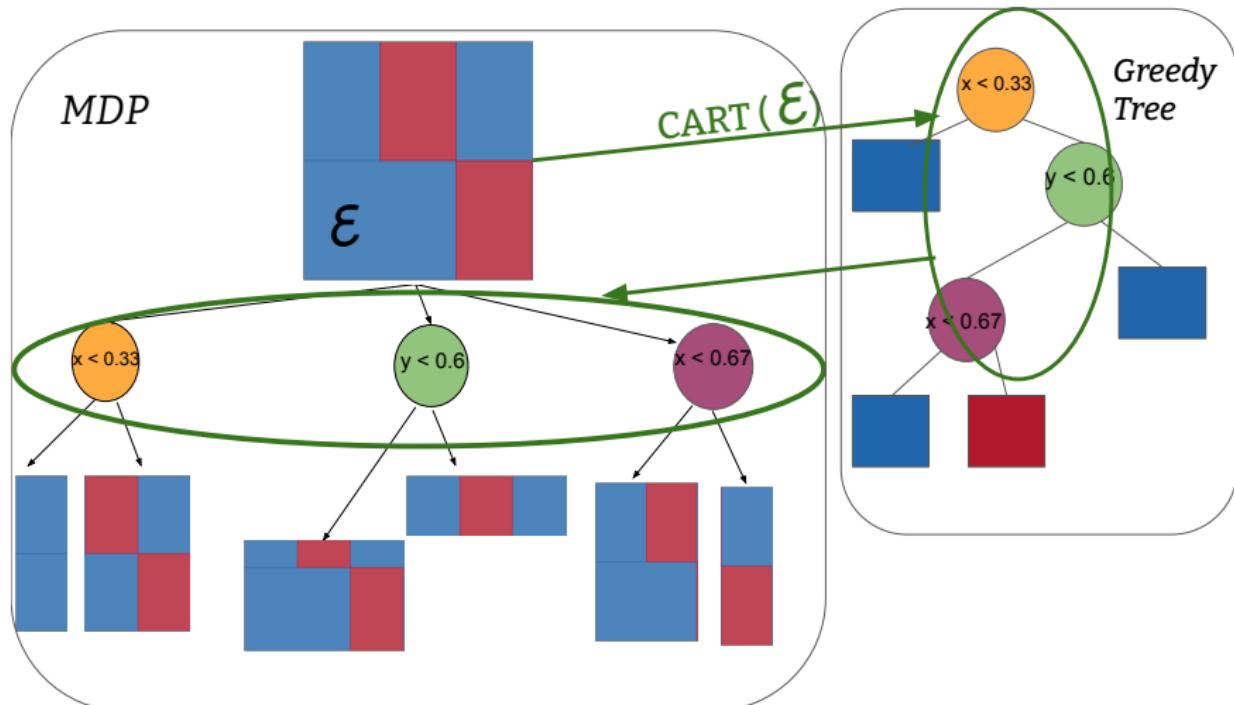
# Controlling the time complexity of decision tree induction

- 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  $O((2Np)^D)$ .

# 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>

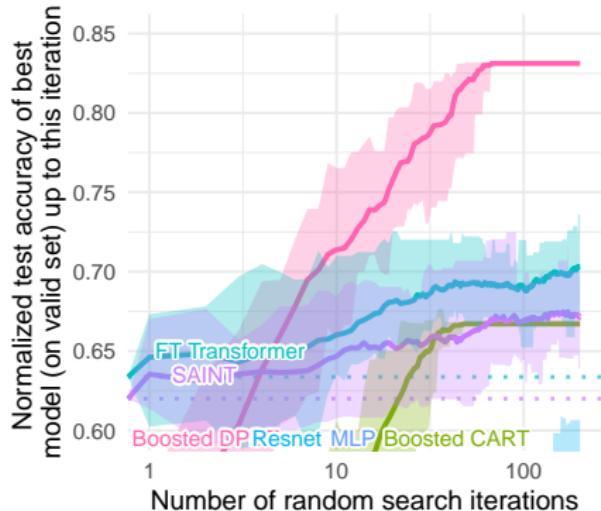
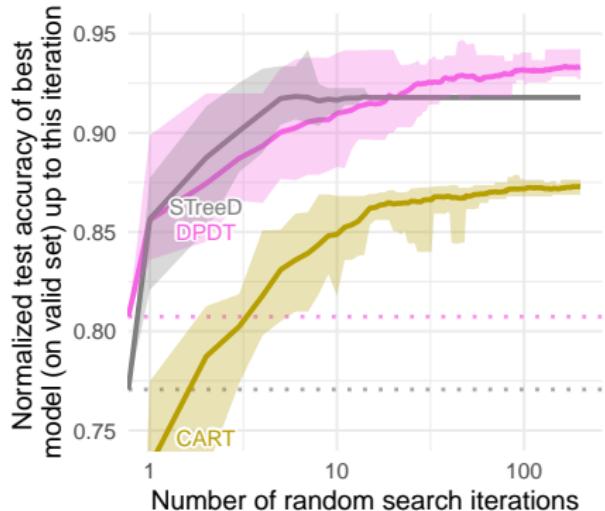


<sup>1</sup>Because states are entire datasets, we implement DPDT with a depth-first search to limit the space complexity.

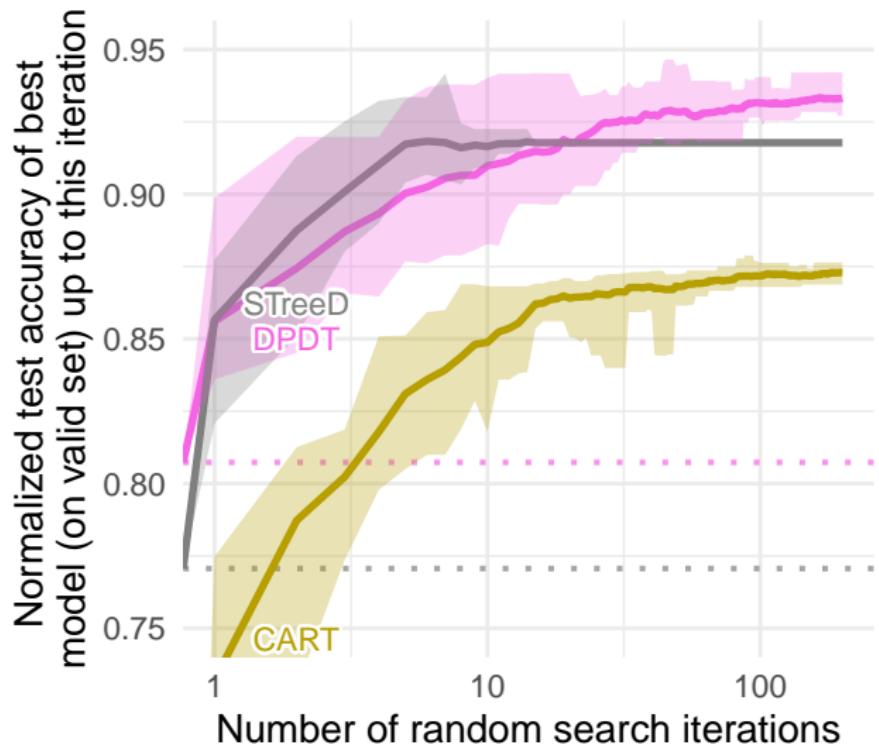
# Comparing trees accuracy versus complexity

Dataset	N	p	Accuracy				Operations			
			Opt Quant-BnB	Greedy CART	DPDT light	DPDT full	Opt Quant-BnB	Greedy CART	DPDT light	DPDT 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

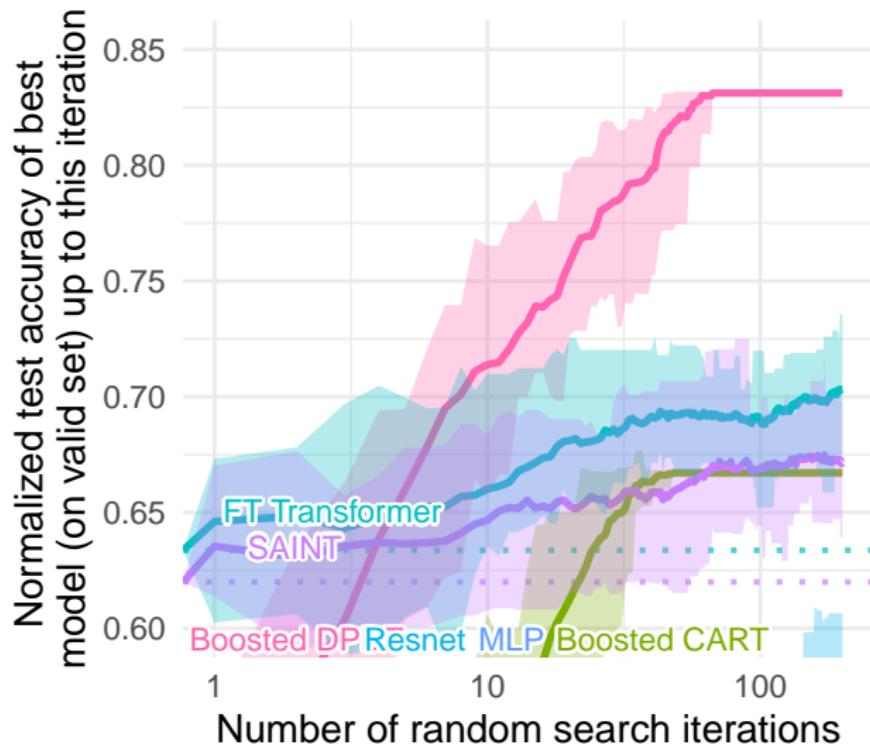
# DPDT trees generalization



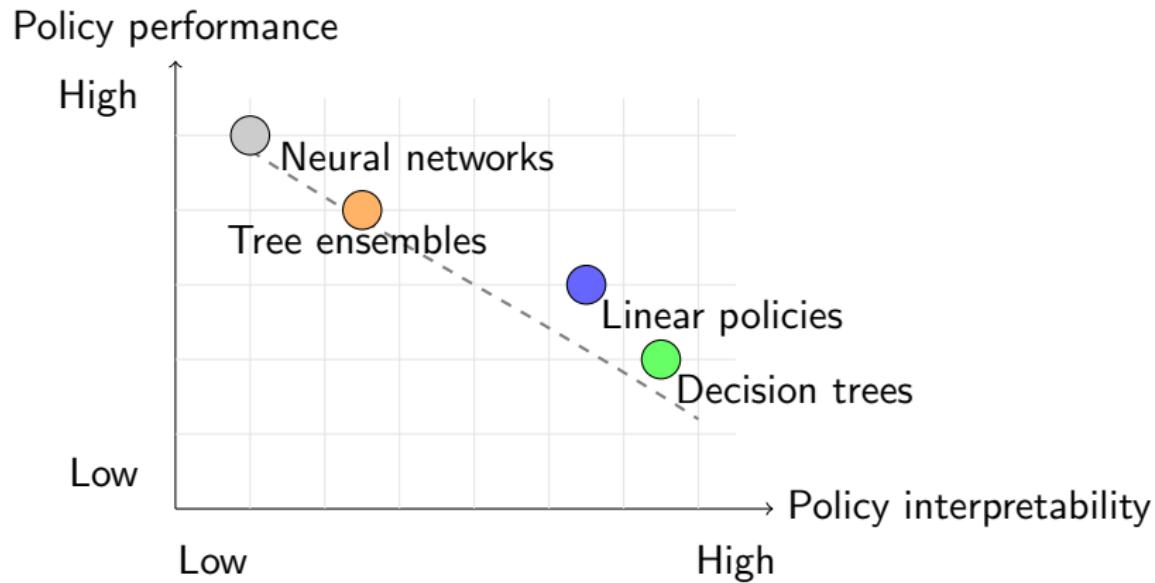
# DPDT generalization



# Boosting DPDT



# How to measure policy interpretability?



**Figure:** **Heuristic** interpretability-performance trade-offs of different policy classes (what-if neural network is very sparsified?). Interpretability is often presented in opposition to performances.

# How to measure policy interpretability?

## Challenges [**gianois-survey**, **lipton**, **rigourous**]

- There is no clear definition of interpretability.
- Measuring interpretability might require humans.

# How to measure policy interpretability?

## Consensus

- The notion of *simulability* [**lipton**]:
  - ① Interpretability  $\simeq$  how long it takes for human to make the same computations given an input.
  - ② Interpretability  $\simeq$  how much effort it would take a human to read through the entire policy once.
- Inside a given policy class, less parameters should mean more interpretability [**study-0**, **study-4**, **study-5**, **study-6**, **study-7**].
- The time required to formally verify a policy should decrease with interpretability [**viper**, **lens-complexity**].

# A methodology to measure policy interpretability without humans

## Simulatability [lipton]

- 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 [insight]

- Different hardwares (tree policies are run on CPUs while neural policies are run on GPUs).
- Different implementations (neural policies compute outputs using matrix operations while tree operate 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]
```

# Empirical validation

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

# Empirical validation: obtaining $\sim 40000$ policies from different classes

Policy Class	Parameters	Training algo.
Linear policies	Determined by state-action dimensions	Linear/logistic Reg.
Decision trees	$\{4, 8, 16, 64, 128\}$ nodes	CART
Oblique decision trees	$\{4, 8, 16, 64, 128\}$ nodes	CART
Relu neural networks	$\{(2, 2), (4, 4), (8, 8), (16, 16)\}$ weights	SGD

**Table:** Summary of policy classes parameters and supervised learning algorithms to fit experts.

# Empirical validation: obtaining $\sim 40000$ policies from different classes

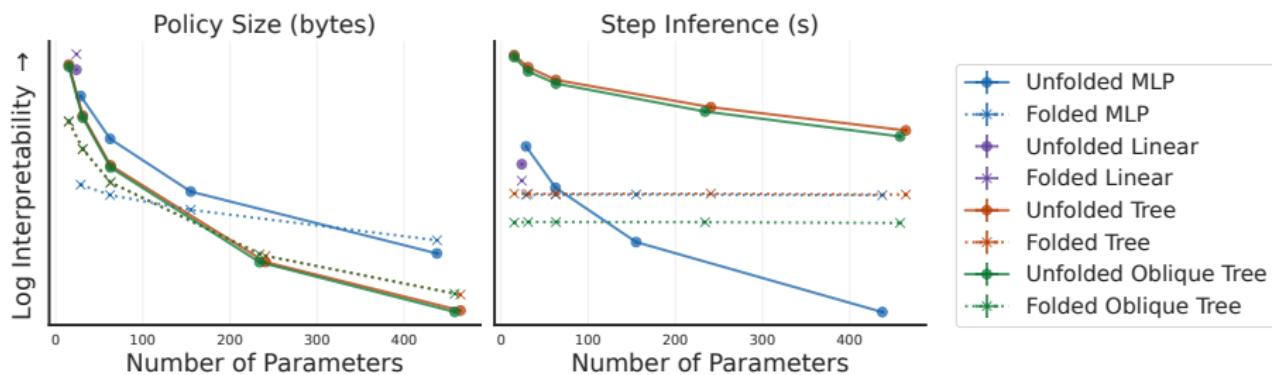
Classic	MuJoCo	OCArcade
CartPole (4, 2, <b>490</b> )	Swimmer (8, 2, <b>300</b> )	Breakout (452, 4, <b>30</b> )
LunarLander (8, 4, <b>200</b> )	Walker2d (17, 6, <b>2000</b> )	Pong (20, 6, <b>14</b> )
// Continuous (8, 2, <b>200</b> )	HalfCheetah (17, 6, <b>3000</b> )	SpaceInvaders (188, 6, <b>680</b> )
BipedalWalker (24, 4, <b>250</b> )	Hopper (11, 3, <b>2000</b> )	Seaquest (180, 18, <b>2000</b> )
MountainCar (2, 3, <b>90</b> )		
// Continuous (2, 1, <b>-110</b> )		
Acrobot (6, 3, <b>-100</b> )		
Pendulum (3, 1, <b>-400</b> )		

**Table:** Summary of considered environments (dimensions of states and number of dimensions of actions, **performance thresholds to solve**). OCArcade is an object-centric version of Arcade.

# Metrics

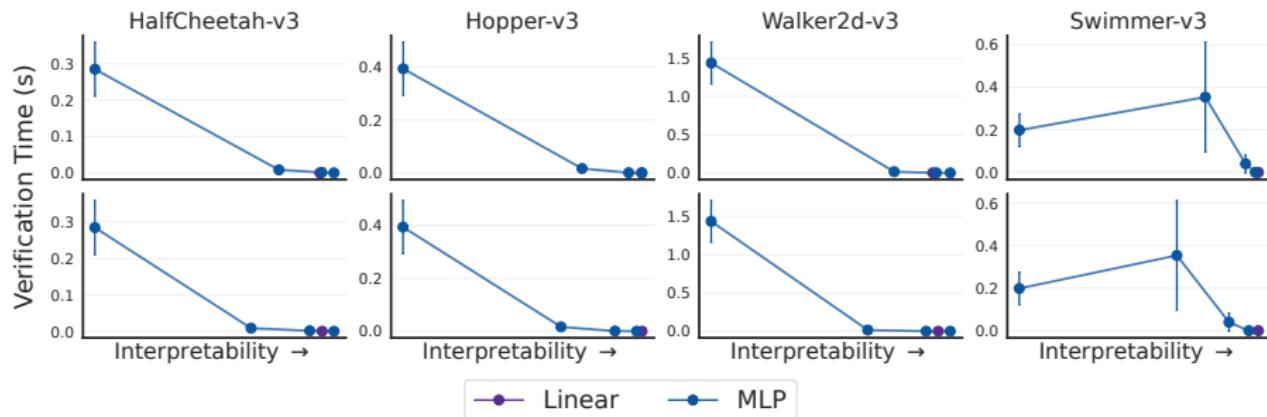
- ① For each policy class and each environment, we keep only the best policy in terms of performance for the task.
- ② We measure the interpretability of each best-in-class policy on dedicated CPUs.
- ③ To measure interpretability, we track two metrics:
  - ① Average inference time in seconds to predict actions given states.
  - ② Space in memory in bytes.

# Result 1: unfolding policies is necessary to respect consensus



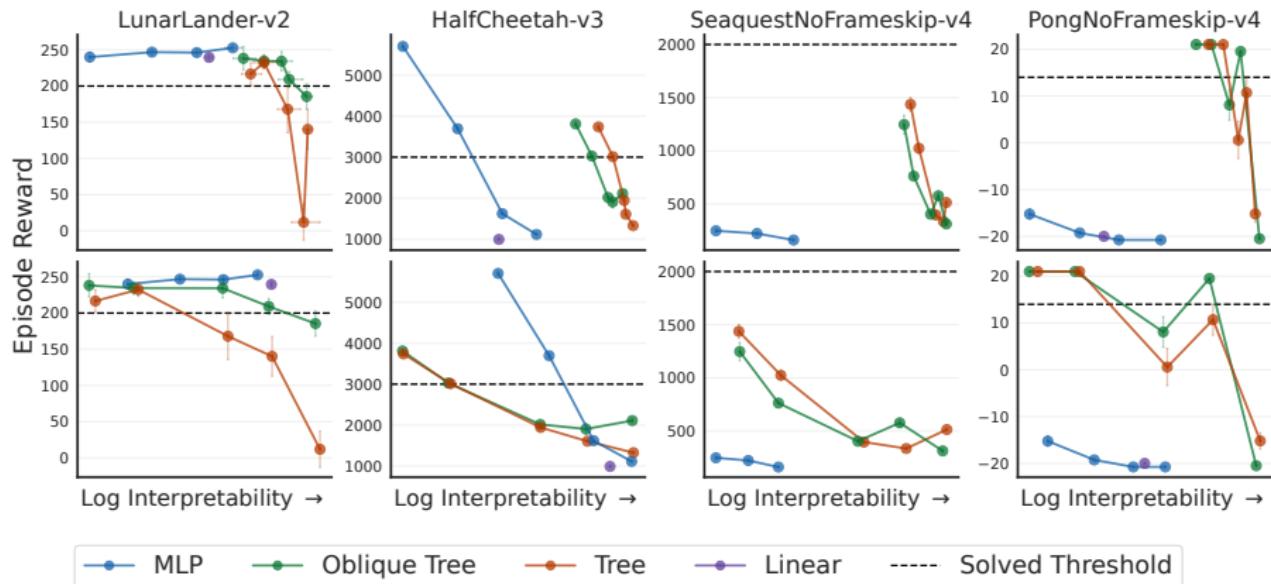
**Figure:** Policies interpretability on classic control environments. We plot 95% stratified bootstrapped confidence intervals around means in both axes. In each sub-plot, interpretability is measured with either bytes or inference speed.

## Result 2: verification time does scale with step inference time



**Figure:** Verification time as a function of policy interpretability. Top row, interpretability is measured with step inference times. Bottom row, the interpretability is measured with policy size.

# Result 3: 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.

# Take home messages

- ① Because there is no dominating class for all problems in terms of interpretability-performance trade-offs, popular beliefs such as "trees are more interpretable than neural networks" should be used with caution.
- ② This further motivates the use of the proposed methodology when comparing policies from different classes.

# Future work

- Can a human study confirm our results?
- Can our methodology be used for evaluating the interpretability of (very) big models?
- Can we use our policy programs as low level skills (hierarchical RL)?

All the policy programs are available on github

<https://github.com/KohlerHECTOR/interpretable-rl-zoo>