Interpretability, Decision Trees, and Sequential Decision Making

Hector Kohler

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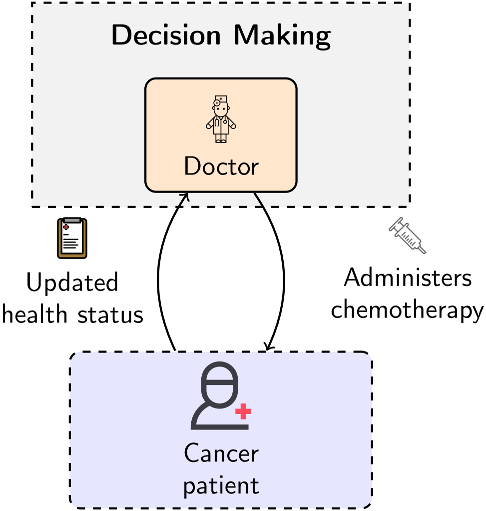
Sequential decision making (SDM)



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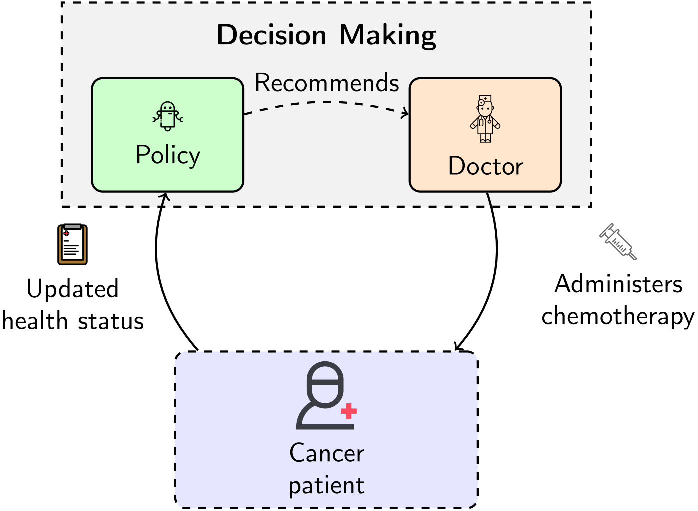
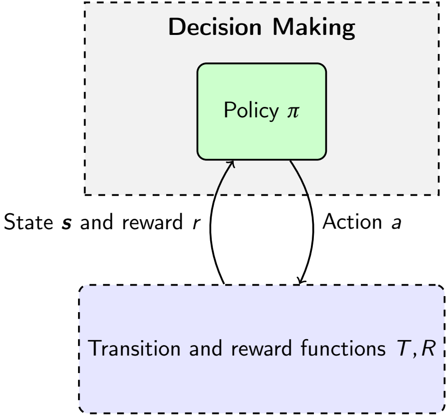


Markov decision processes (MDPs) and reinforcement learning (RL)



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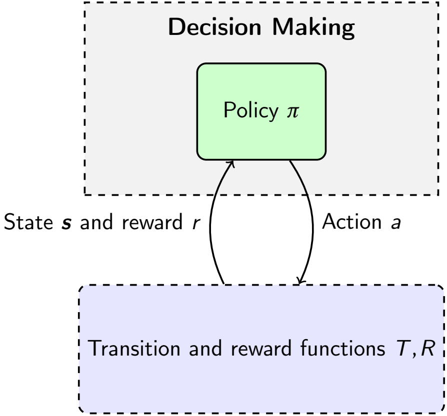

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- RL (Sutton and Barto 1998) aims to find a policy, $\pi : S \rightarrow A$ that maximizes:

$$J(\pi) = \underset{s_t \sim T}{\mathbb{E}} \left[\sum_{t=0}^{\infty} \gamma^t R(s_t, \pi(s_t)) \right]$$

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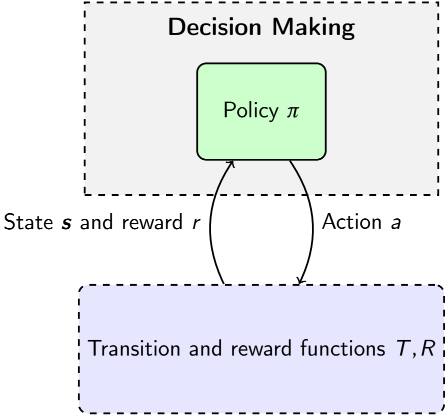

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- Lots of succesful (deep) RL algorithms (Schulman et al. 2017).

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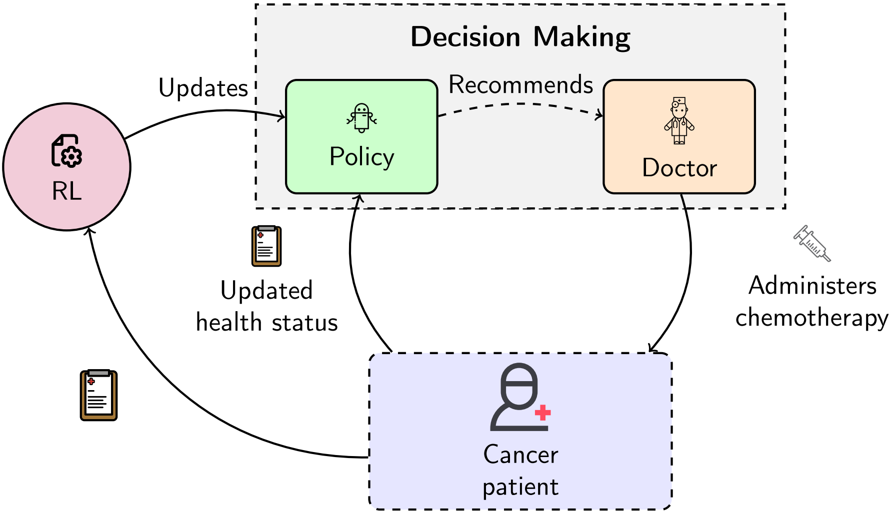

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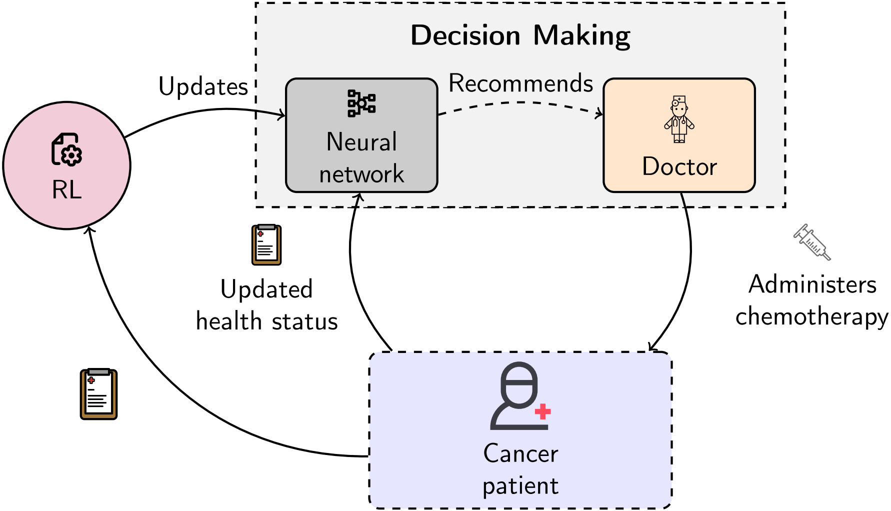

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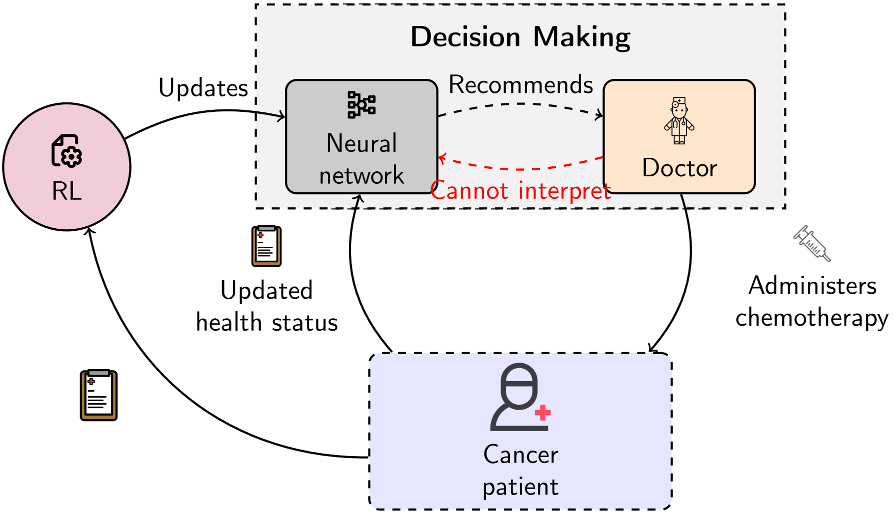

What is interpretability?

⚠ **No concensus on what interpretability is.**

- Different evaluations (e.g. with or without humans?) (Doshi-Velez and Kim 2017).
- Set of properties (e.g. transparency) (Lipton 2018).
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Local interpretation (a.k.a. explainability) requires additional computations (Greydanus et al. 2018).

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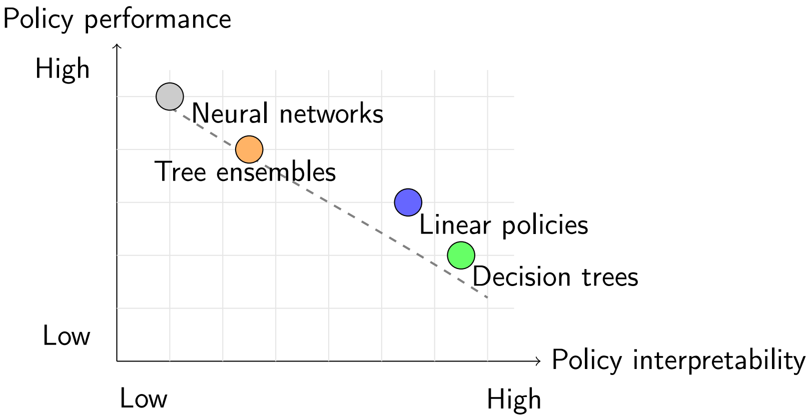
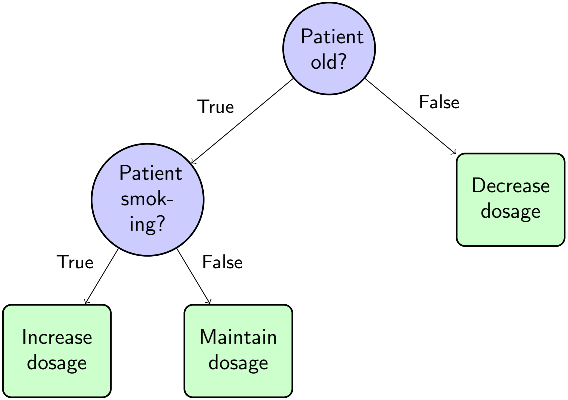


Interpretable policy classes do not require additional computations[1].

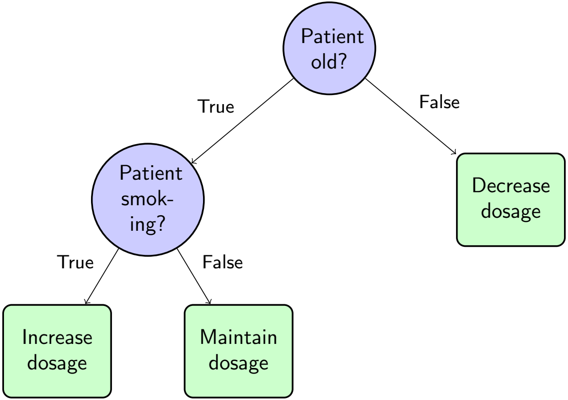
[1] Google image result for *interpretable machine learning models*
https://fr.mathworks.com/discovery/interpretability.html

Decision trees



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

Decision trees



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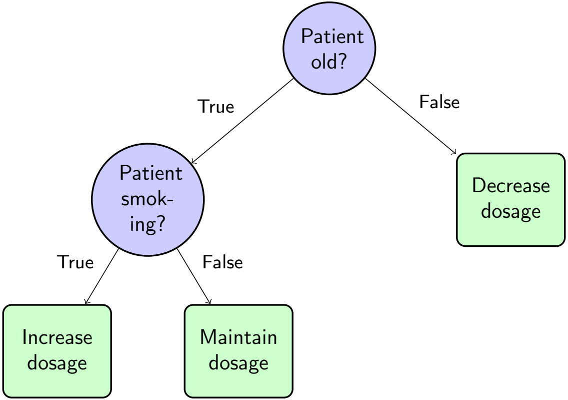

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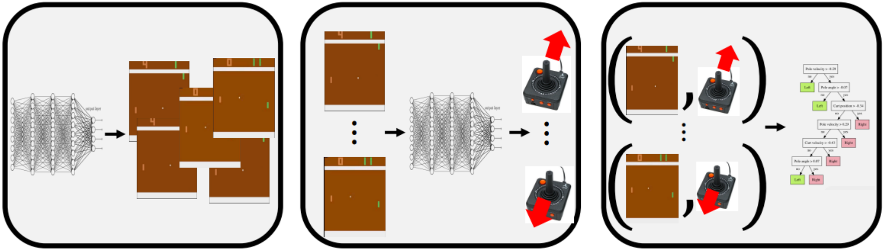
What about SDM?

Imitation learning



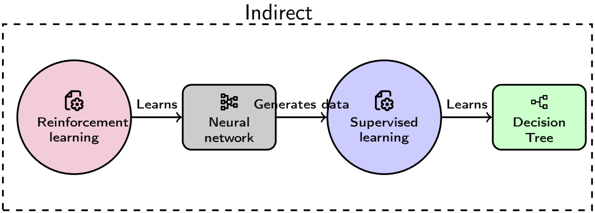
Step 1: Use NN to generate states

Step 2: Use NN to obtain actions

Step 3: Use supervised learning to train a decision tree

Most research focuses on imitation learning of interpretable policies (Bastani, Pu, and Solar-Lezama 2018; Milani et al. 2024).

Two ways to get interpretable policies for SDM (Glanois et al. 2024)



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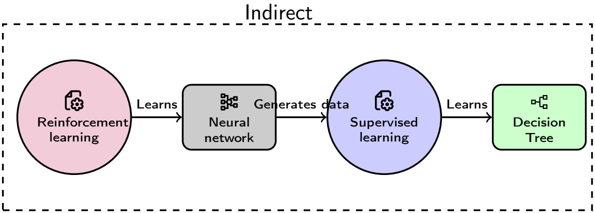

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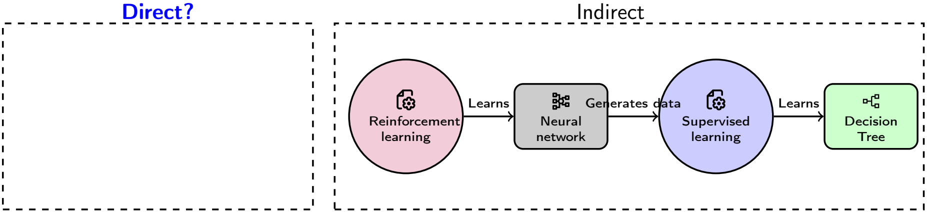

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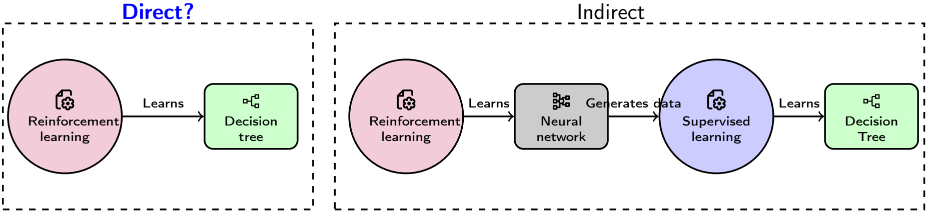

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3. How to measure policy interpretability in SDM?

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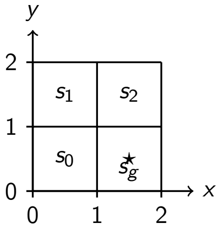

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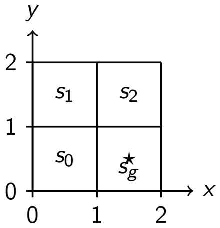

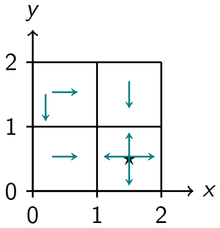

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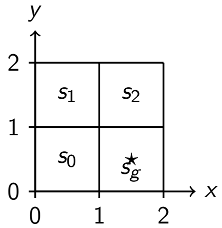

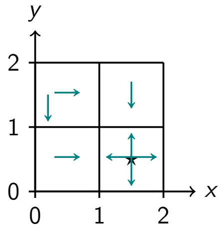

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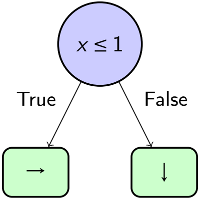

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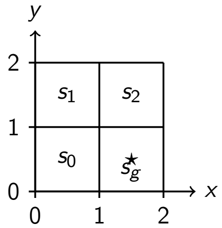

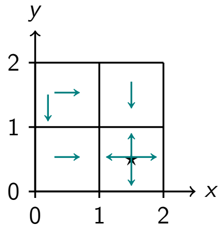

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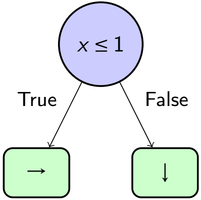

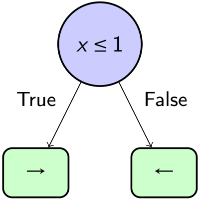

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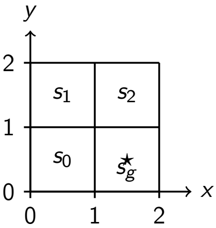

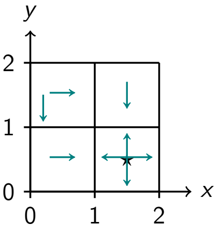

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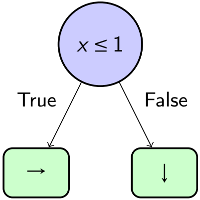

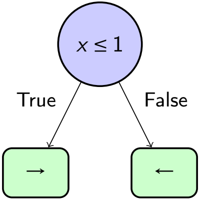

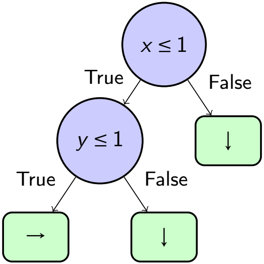

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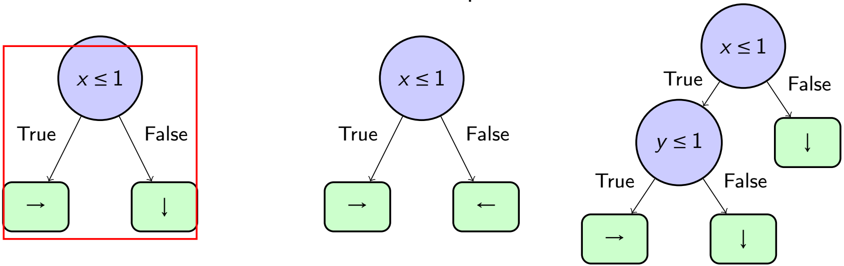
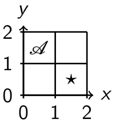


Decision tree policies with different interpretability-performance trade-offs.

Iterative bounding Markov decision processes (Topin et al. 2021)

$t = 0$



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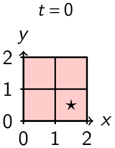

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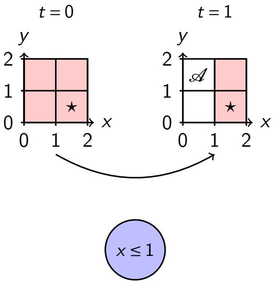

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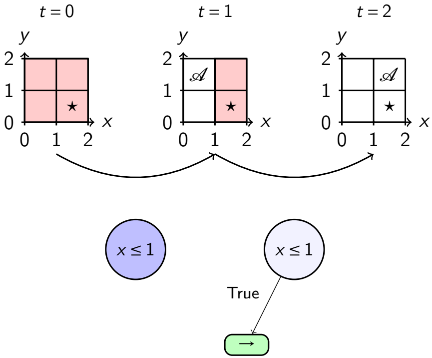

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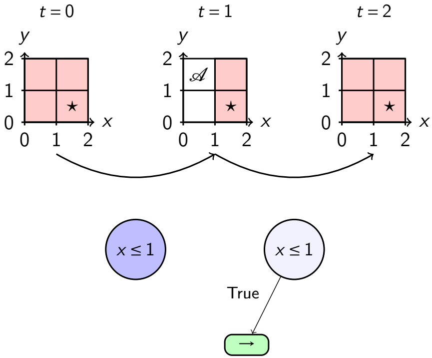

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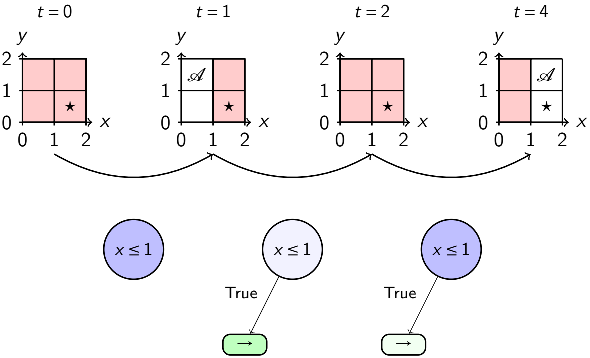

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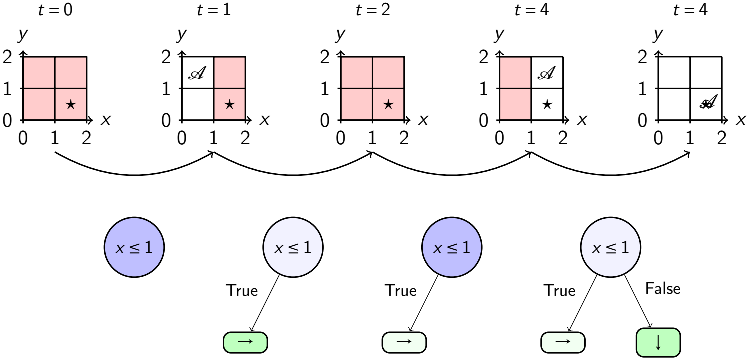

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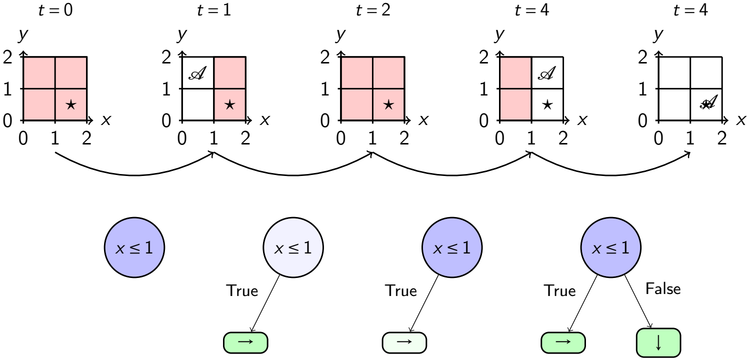

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$$\langle S \times O, A \cup A_{info}, (R, \zeta), (T_{info}, T) \rangle$$

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- O: observations of some state features.

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- ⚠**Topin et al. 2021: deterministic memoryless policies $\pi_{po} : O \rightarrow A \cup A_{info}$ in an IBDMP for $\mathscr{M}$ are decision trees for $\mathscr{M}$.**

RL for memoryless policies in POMDPs

RL for memoryless policies

- Finding the best deterministic and memoryless policy in a POMDP is NP-hard (Littman 1994)!
- The best memoryless policy can be stochastic (Singh, Jaakkola, and Jordan 1994).
- No optimality guarantees for value-based RL (Singh, Jaakkola, and Jordan 1994).

Asymmetric RL (Pinto et al. 2017)

- Value-based → learns $Q(o, a)$ with TD targets $U(s, a)$ (Baisero, Daley, and Amato 2022).
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- Topin et al. 2021 uses asymmetric RL (not knowing it) for their experiments.

RL for memoryless policies in POMDPs

RL for memoryless policies

- Finding the best deterministic and memoryless policy in a POMDP is NP-hard (Littman 1994)!
- The best memoryless policy can be stochastic (Singh, Jaakkola, and Jordan 1994).
- No optimality guarantees for value-based RL (Singh, Jaakkola, and Jordan 1994).

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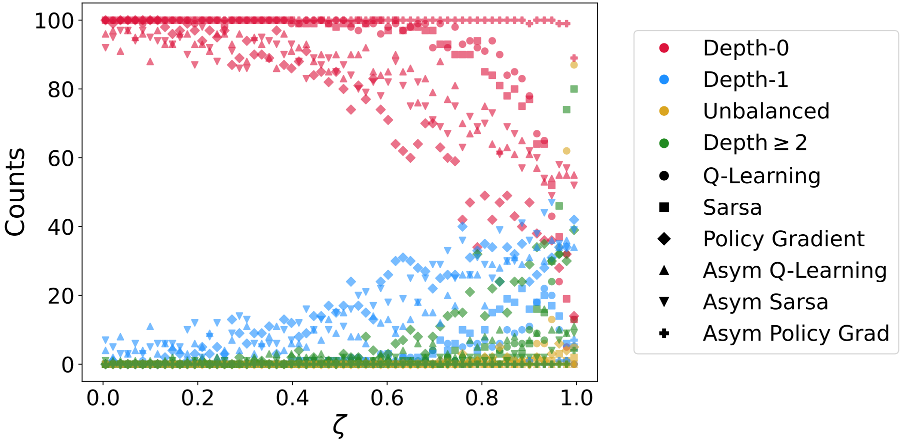
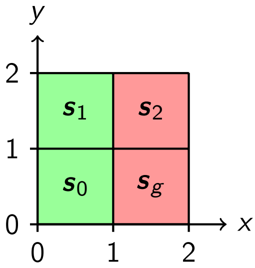
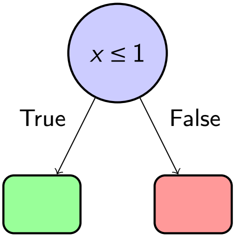
Result: RL cannot retrieve optimal depth-1 trees for the grid world MDP



Distributions of tree policies learned with (asymmetric) RL algorithms as a function of the interpretability reward ζ.

Direct RL of decision trees for classification tasks does not involve partial observability





Classification MDP and the unique optimal depth-1 tree.

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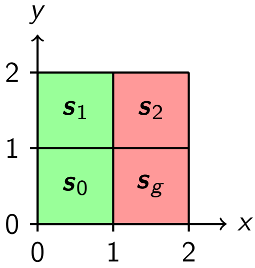

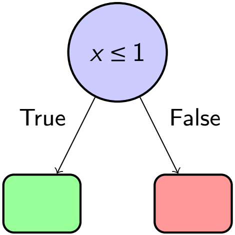

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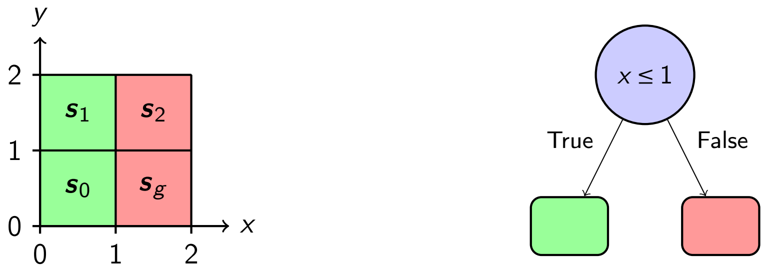

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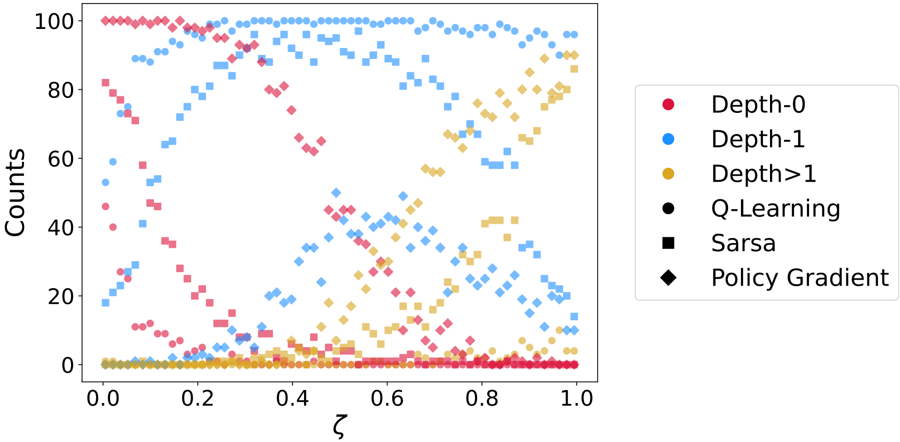
Result: RL can retrieve optimal depth-1 trees for the toy classification MDP



Distributions of tree policies learned with various RL algorithms.

Perspectives for direct RL of decision tree policies.

- It seems that directly learning decision tree trading off interpretability and performances in MDPs can be difficult to achieve because of **partial observability**.
- Should we focus on indirect approaches? Hybrid approaches (Wu et al. 2020)?
- Fixing the policy tree structure a priori (parametric trees, (Marton et al. 2025))?

RL can train good decision trees for classification MDPs

Q: Can we leverage SDM to design new decision tree induction algorithms for classification/regression?

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Decision trees in supervised learning

- N data points $\{\boldsymbol{x}_i, y_i\}$. Each $\boldsymbol{x}_i$ is described by p features and has a label $y_i \in \mathscr{Y}$. We want to find a tree of depth at most D, $T \in \mathscr{T}_D$ that minimizes:

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

- Trees **interpretable** and **competitive with neural nets** (Grinsztajn, Oyallon, and Varoquaux 2022).
- Greedy algorithms **sub-optimal accuracy**, but $\boldsymbol{O(2^D)}$ operations (Breiman et al. 1984) .
- Optimal algorithms, **optimal accuracy**, but $\boldsymbol{O((2Np)^D)}$ operations (NP-hard) (Bertsimas and Dunn 2017).
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Decision tree induction as solving MDPs

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) the training data, or to create a leaf node.

- S: data subsets.
- A: test or leaf nodes that can be added to the tree.
- R: interpretability term $-\alpha$ and misclassifications.
- T: node traversals.

Proposition (Objective Equivalence)

Let π be a deterministic policy of the MDP. Then $J_\alpha(\pi) = -\mathscr{L}_\alpha(E(\pi, s_0))$ where E is an algorithm that extracts a decision tree from π (Topin et al. 2021).

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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 $O(2^D)$**.
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Top-B greedy splits (Blanc et al. 2023), quantiles, random...

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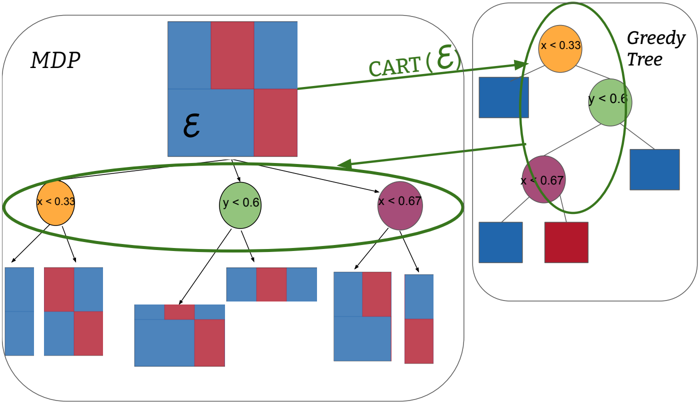

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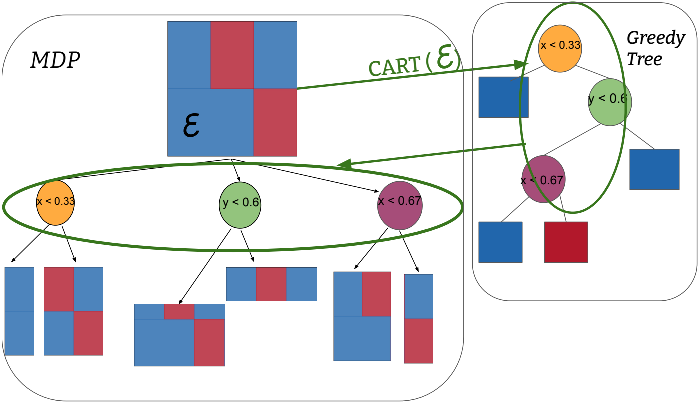

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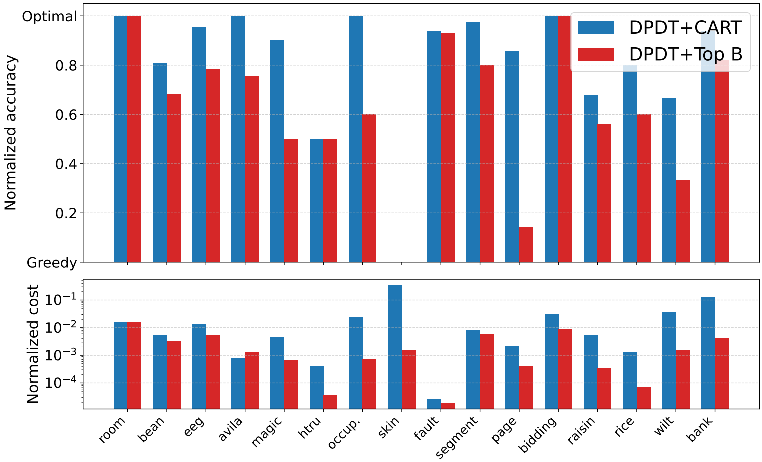
Fast like greedy trees, accurate like optimal trees



Train accuracies against cost for detph-3 trees.

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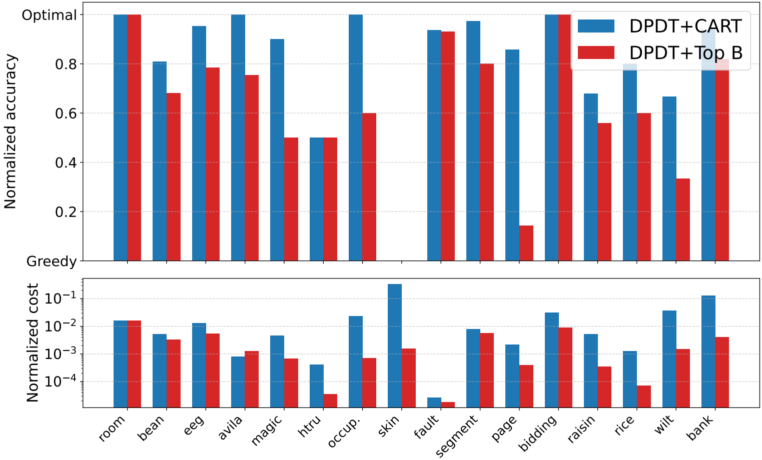

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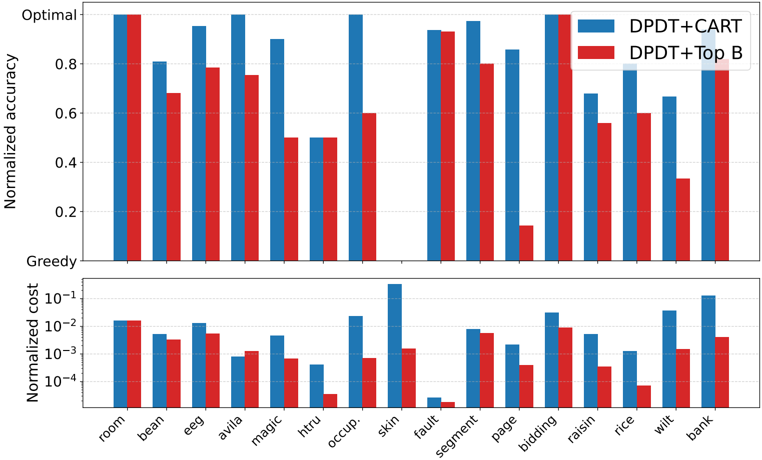

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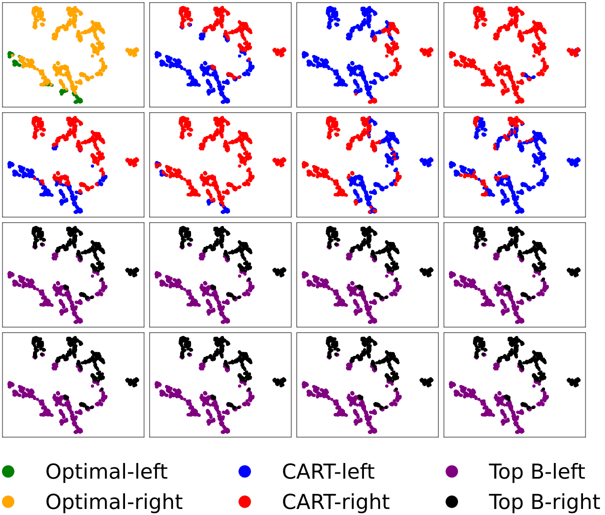
- DPDT trees can be strictly better than greedy trees.

CART generates more diverse splits than Top B for DPDT



T-SNE projection of candidate splits on the bank dataset.

Large scale evaluation of DPDT trees generalization

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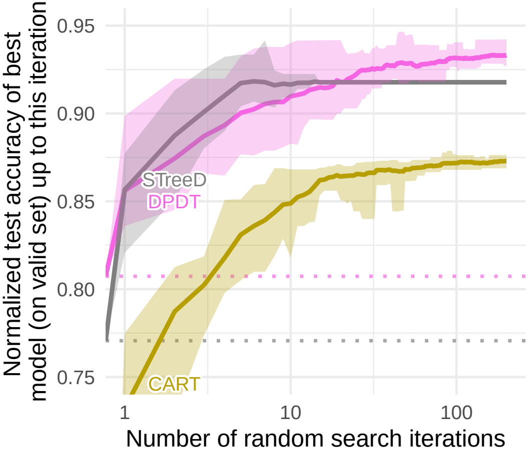

DPDT depth-5 trees vs. other detph-5 trees

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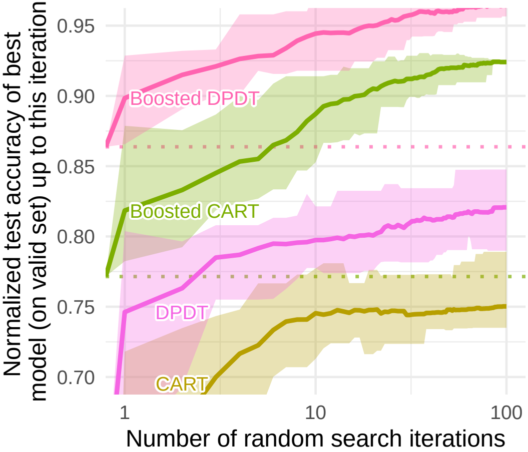

Boosted DPDT vs. Boosted CART

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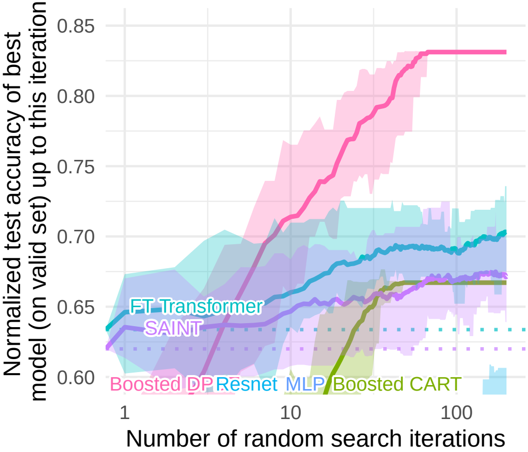

Boosted DPDT vs. other classifiers

Perspectives

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Let us take a step back

Q: Are decision trees really the most interpretable model?

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The notion of *simulatability* (Lipton 2018)

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The notion of *simulatability* (Lipton 2018)

- Interpretability ≃ **runtime in seconds?**
- Interpretability ≃ effort to read through the entire policy.

How to measure policy interpretability?

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How to compare policy of different classes?

- Different hardwares (CPUs vs GPUs).
- Different implementations (matrix operations vs fully sequentially) (Luo et al. 2024)

We propose policy unfolding

```
# Small ReLU MLP for Pendulum
def play(x):
    h_layer_0_0 = 1.68 * x[0] + -0.69 * x[1] + -0.74 * x[2] + -1.40
    h_layer_0_0 = max(0.0, h_layer_0_0)
    h_layer_0_1 = 0.20 * x[0] + 0.29 * x[1] + -0.021 * x[2] + 1.25
    h_layer_0_1 = max(0.0, h_layer_0_1)
    h_layer_0_2 = 0.33 * x[0] + -0.57 * x[1] + 0.47 * x[2] + 1.94
    h_layer_0_2 = max(0.0, h_layer_0_2)
    h_layer_0_3 = 1.39 * x[0] + 0.94 * x[1] + 0.50 * x[2] + -1.13
    h_layer_0_3 = max(0.0, h_layer_0_3)
    h_layer_1_0 = 1.16 * h_layer_0_0 + -1.59 * h_layer_0_1 + 0.95 * h_layer_0_2 +
      -1.22 * h_layer_0_3 + -0.54
    h_layer_1_0 = max(0.0, h_layer_1_0)
    h_layer_1_1 = -0.55 * h_layer_0_0 + 1.13 * h_layer_0_1 + -0.58 * h_layer_0_2
     + -0.72 * h_layer_0_3 + 1.56
    h_layer_1_1 = max(0.0, h_layer_1_1)
    h_layer_1_2 = 1.10 * h_layer_0_0 + -1.01 * h_layer_0_1 + 0.96 * h_layer_0_2 +
      -2.84 * h_layer_0_3 + -0.02
    h_layer_1_2 = max(0.0, h_layer_1_2)
    h_layer_1_3 = 0.27 * h_layer_0_0 + 0.44 * h_layer_0_1 + 0.39 * h_layer_0_2 +
     0.15 * h_layer_0_3 + -1.24
    h_layer_1_3 = max(0.0, h_layer_1_3)
    h_layer_2_0 = -2.80 * h_layer_1_0 + -0.60 * h_layer_1_1 + 3.07 * h_layer_1_2
     + -1.63 * h_layer_1_3 + -0.36
    y_0 = h_layer_2_0

    return [y_0]
```

Is time/size of unfolded policies a good proxy?

Setup

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

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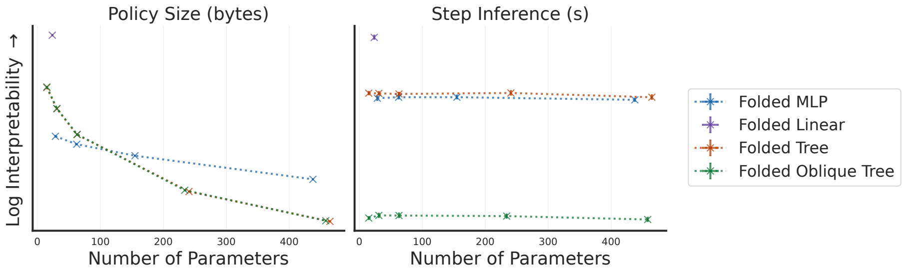

Aggregated policies interpretability on classic control environments

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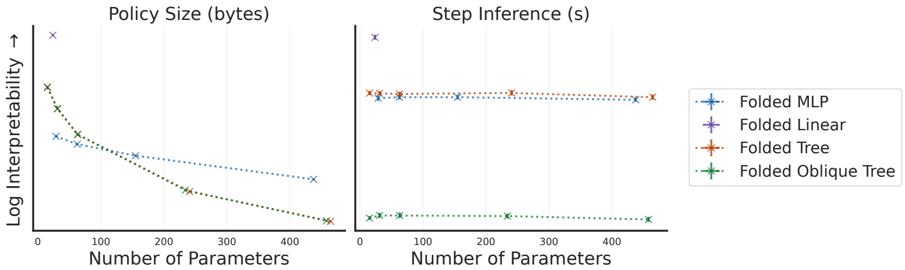

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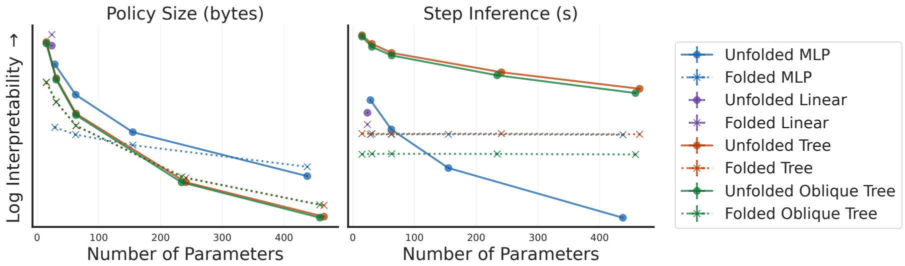

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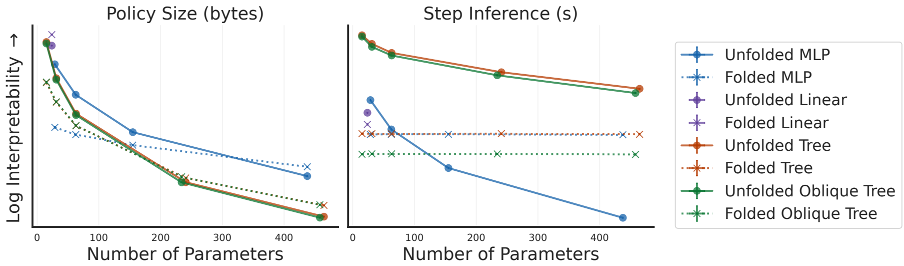

Aggregated policies interpretability on classic control environments

- ⚠Less parameters means more interpretability (Freitas 2014).
- Not always true that "trees are more interpretable than neural networks".

General perspectives

- **Technical challenges:** **learning interpretable policies for SDM involves partial observability.**
  → Focus on indirect approaches and/or on POMDP research first?
  → **Created opportunities for new decision tree algos for classif/regression (DPDT).**
- **Fundamental challenges:** **no concensus on interpretability definition**.
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Result: for similar problems, RL struggles more when there is partial observability

Success rates over thousands of RL runs with varying hyperparameters when learning different policies in the same IBMDP[2].

[2] We also observed similar results on classic controls and variants of the grid world MDP.

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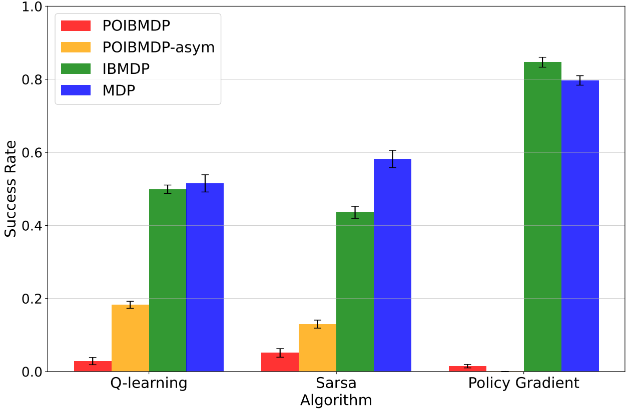

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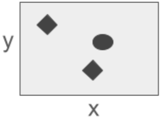
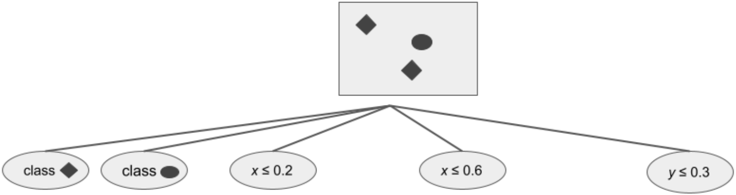
Decision tree induction as solving MDPs



Example of decision tree induction as an MDP.

Decision tree induction as solving MDPs



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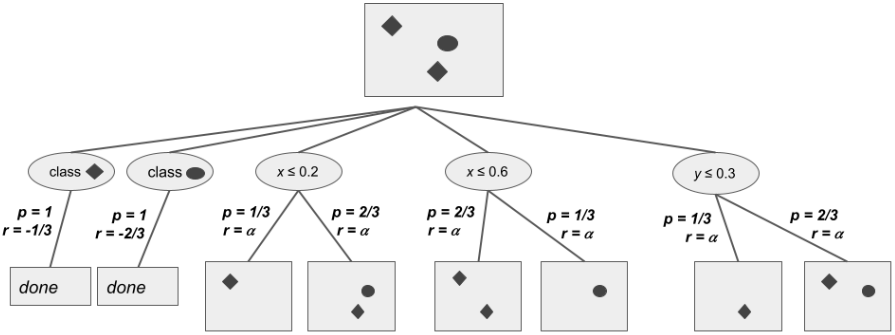

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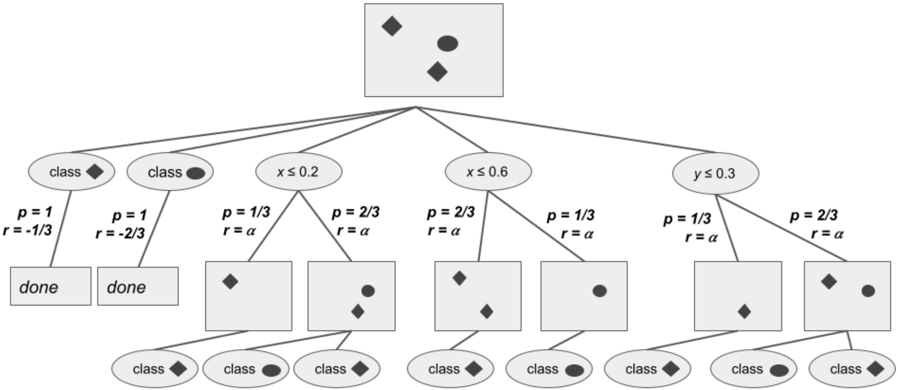

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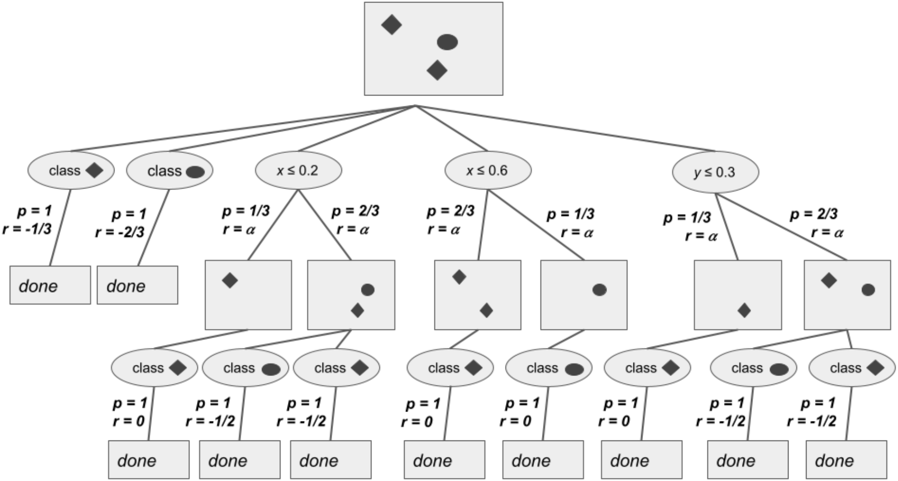
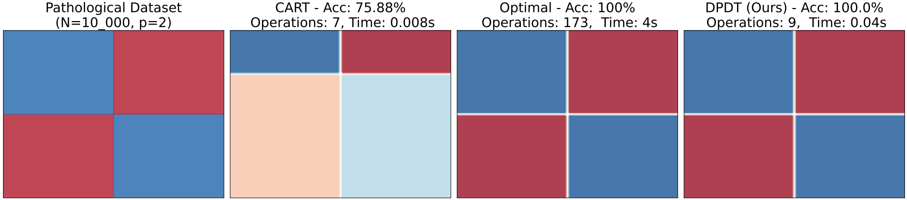


Example of decision tree induction as an MDP.

Fast like greedy trees, accurate like optimal trees



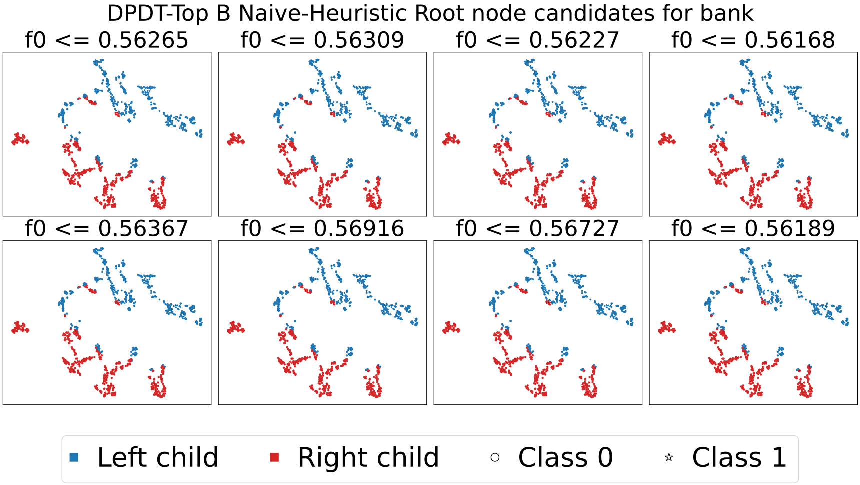
Comparison of greedy, optimal, and DPDT depth-2 trees on the checkersboard dataset.

Fast like greedy trees, accurate like optimal trees

Comparison of accuracies and operations for depth-3 trees.

	Accuracy						Operations					
Dataset	Opt	Greedy	DPDT				Opt	Greedy	DPDT			
			CART$^-$	CART$^+$	TopB$^-$	TopB$^+$			CART$^-$	CART$^+$	TopB$^-$	TopB$^+$
room	**0.992**	0.968	0.991	**0.992**	0.990	**0.992**	10^6	15	286	16100	111	16100
bean	**0.871**	0.777	0.812	0.853	0.804	0.841	$5 \cdot 10^6$	15	295	25900	112	16800
eeg	**0.708**	0.666	0.689	0.706	0.684	0.699	$2 \cdot 10^6$	13	289	26000	95	11000
avila	**0.585**	0.532	0.574	**0.585**	0.563	0.572	$3 \cdot 10^7$	9	268	24700	60	38900
magic	**0.831**	0.801	0.822	0.828	0.807	0.816	$6 \cdot 10^6$	15	298	28000	70	4190
htru	**0.981**	0.979	0.979	0.980	0.979	0.980	$6 \cdot 10^7$	15	295	25300	55	2180
occup.	**0.994**	0.989	0.991	**0.994**	0.990	0.992	$7 \cdot 10^5$	13	280	16300	33	510
skin	**0.969**	0.966	0.966	0.966	0.966	0.966	$7 \cdot 10^4$	15	301	23300	20	126
fault	**0.682**	0.553	0.672	0.674	0.672	0.673	$9 \cdot 10^8$	13	295	24200	111	16800
segment	**0.887**	0.574	0.812	0.879	0.786	0.825	$2 \cdot 10^6$	7	220	16300	68	11400
page	**0.971**	0.964	0.970	0.970	0.964	0.965	10^7	15	298	22400	701	4050
bidding	**0.993**	0.981	0.985	**0.993**	0.985	**0.993**	$3 \cdot 10^5$	13	256	9360	58	2700
raisin	**0.894**	0.869	0.879	0.886	0.875	0.883	$4 \cdot 10^6$	15	295	20900	48	1440
rice	**0.938**	0.933	0.934	0.937	0.933	0.936	$2 \cdot 10^7$	15	298	25500	49	1470
wilt	**0.996**	0.993	0.994	0.995	0.994	0.994	$3 \cdot 10^5$	13	274	11300	33	465
bank	**0.983**	0.933	0.971	0.980	0.951	0.974	$6 \cdot 10^4$	13	271	7990	26	256

CART generates more diverse splits than Top B



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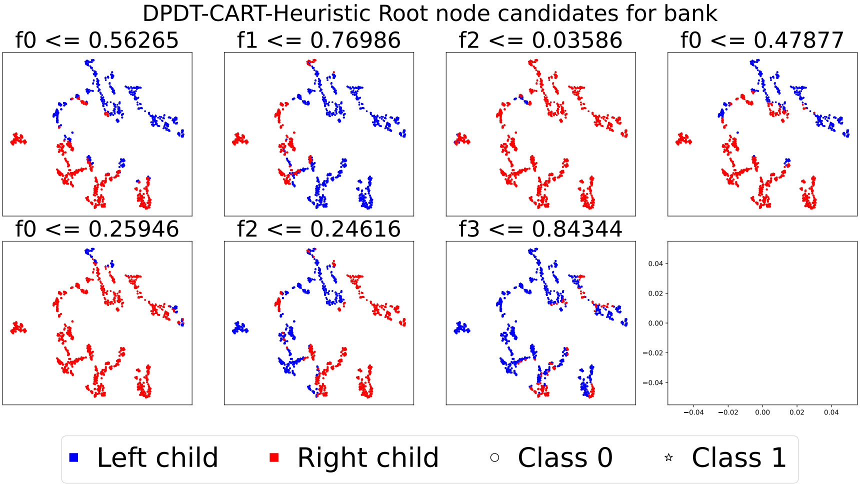

Why generating candidate splits with CART?

Theorem (DPDT trees are not worse than greedy trees)

The greedy tree is always a solution of the MDPs we solve. Because we solve the MDPs exactly with DP, if the greedy tree is the best solution, DPDT will find it.

Theorem (DPDT trees can be strictly better than greedy trees)

There exist a depth budget D and a dataset for which DPDT trees are strictly better than greedy trees.[a]

[a] cf. checkersboard dataset.

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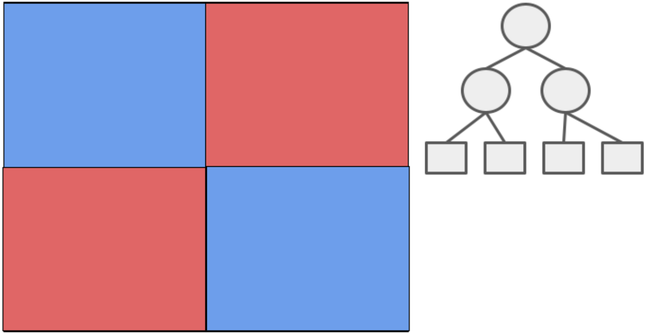

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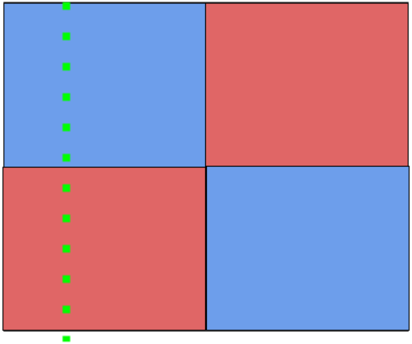

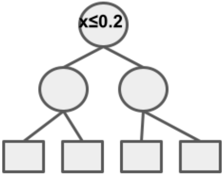

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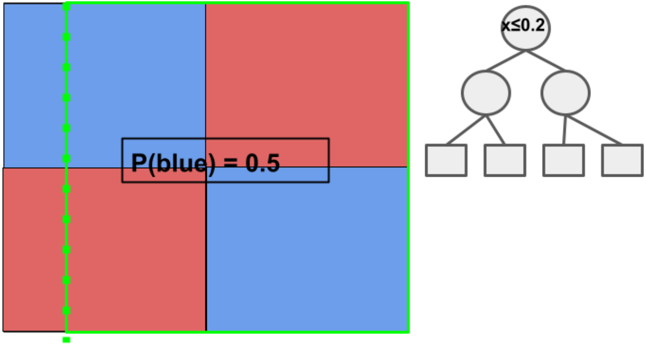
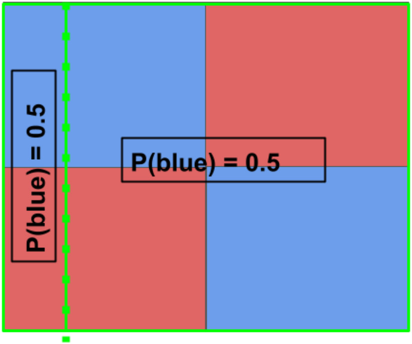
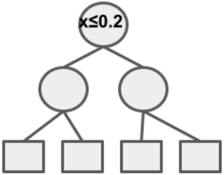
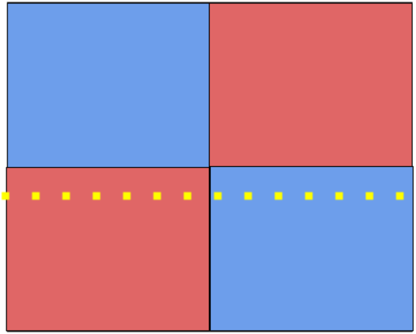


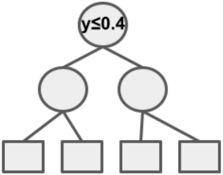
DPDT trees can be strictly better than greedy trees



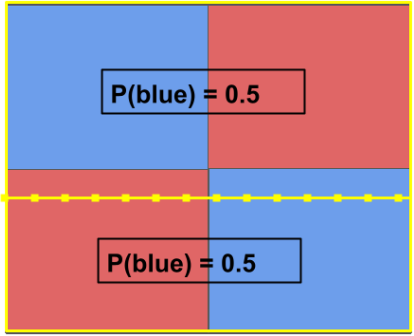


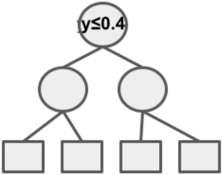
DPDT trees can be strictly better than greedy trees





DPDT trees can be strictly better than greedy trees





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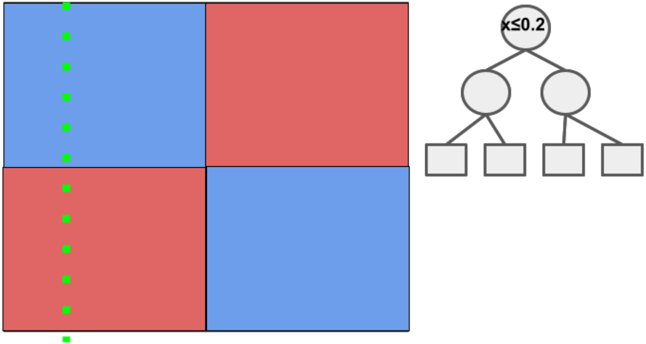

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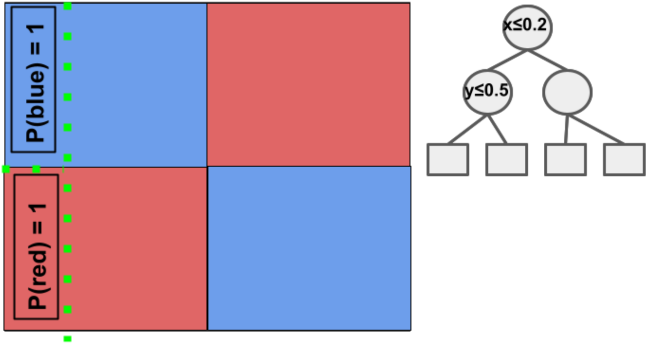

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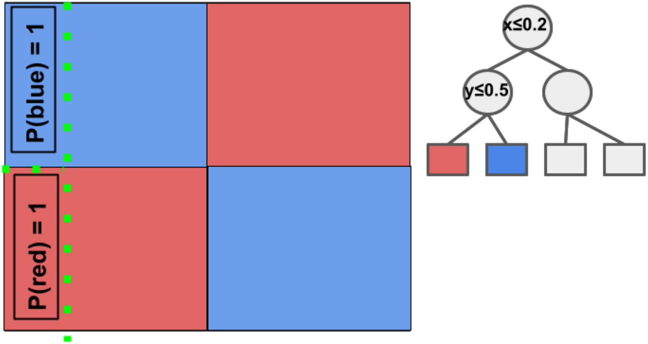
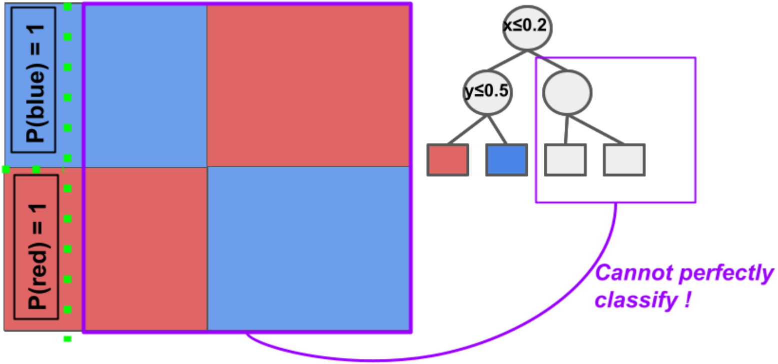


DPDT trees can be strictly better than greedy trees



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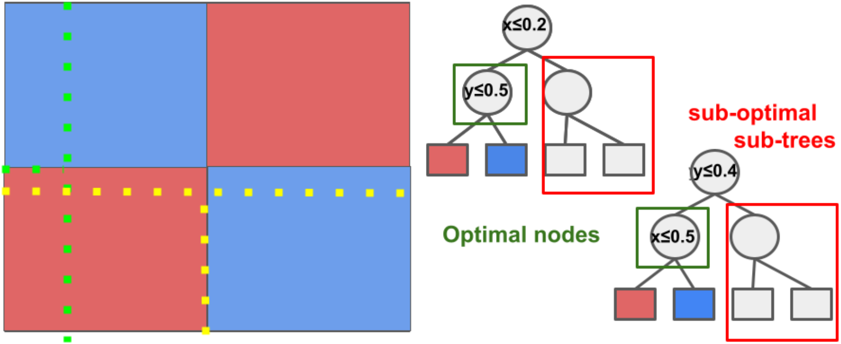
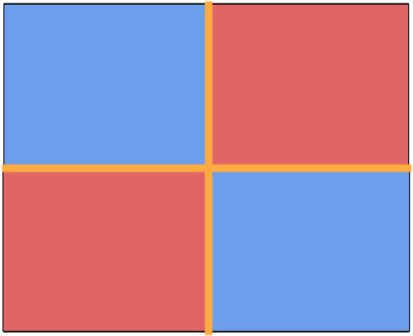
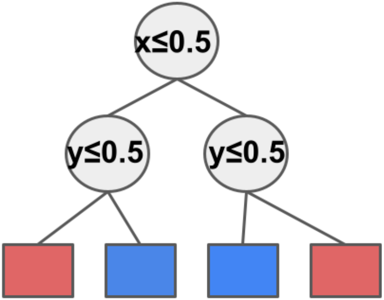
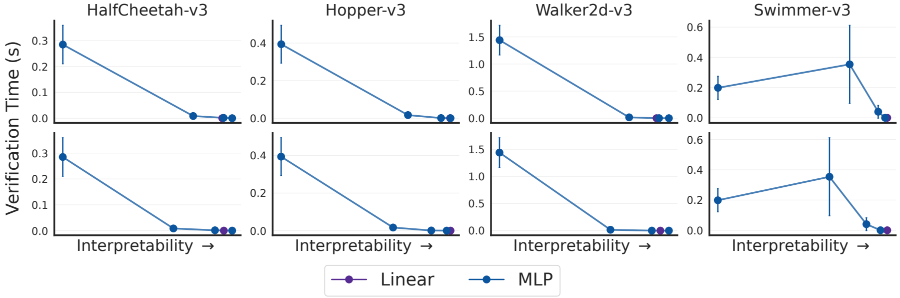


DPDT trees can be strictly better than greedy trees



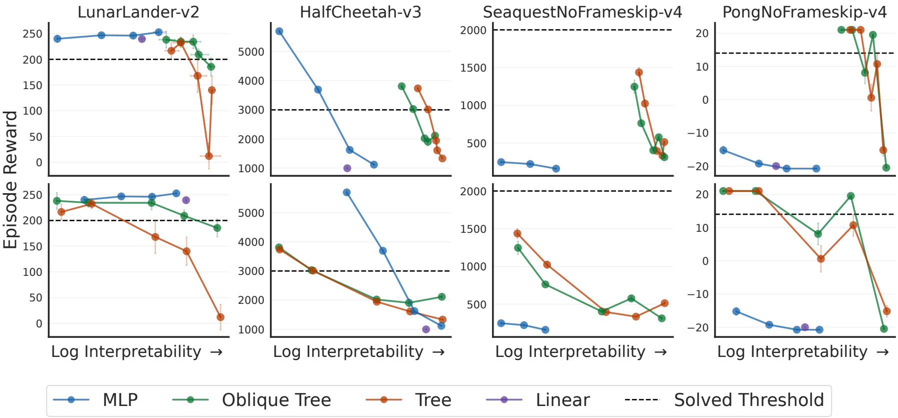


Result: verification time does scale with step inference time



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: there is no dominating policy class for all environments



Interpretability-Performance trade-offs. Top row, interpretability is measured with step inference times. Bottom row, the interpretability is measured with policy size.

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]
```