Interpretability, Decision Trees, and Sequential Decision Making

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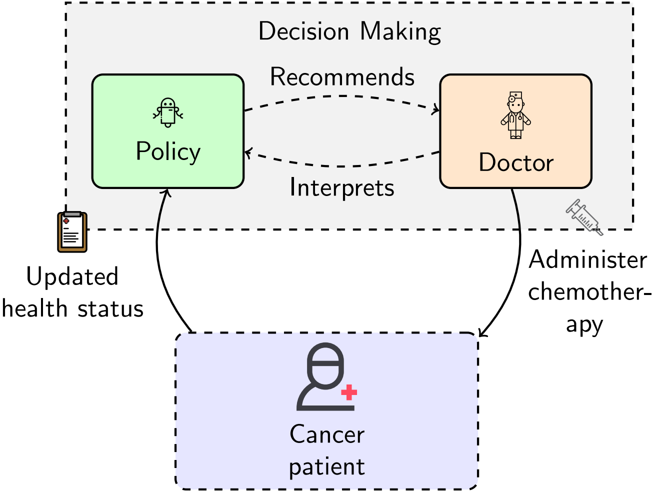
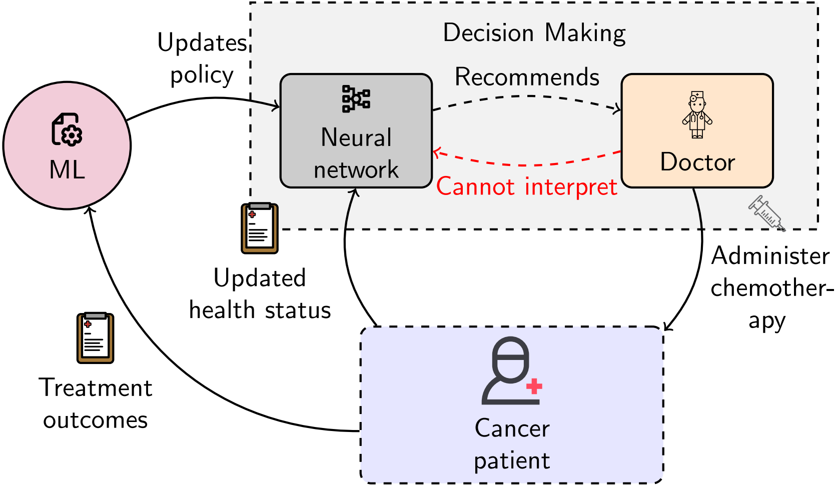
Sequential decision making (SDM)



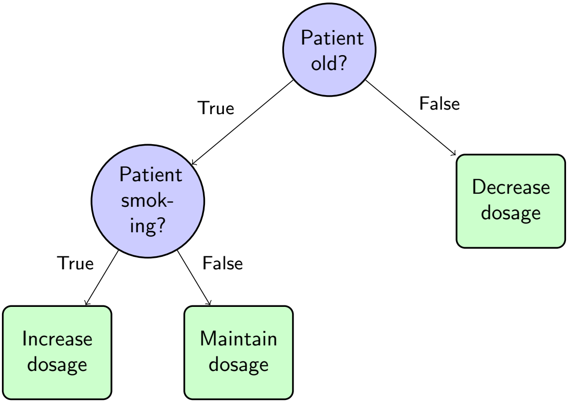
Sequential decision making in cancer treatment.

Machine learning (ML) of policies for SDM



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

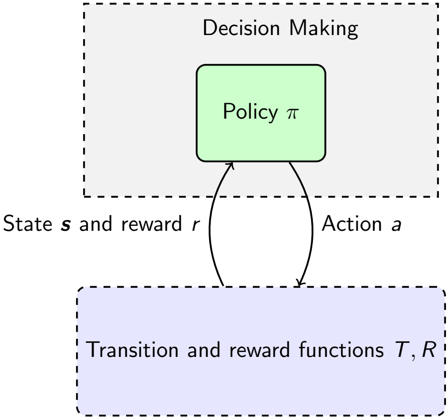
Decision trees



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

Successful algorithms for non-sequential learning: [Bre+84; BD17; Dem+22; VZ19; MMW22] . . . What about SDM?

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



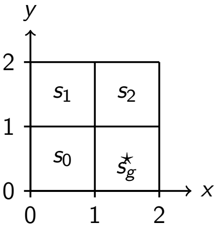
Markov decision processes [Put94].

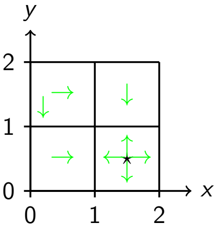
- RL [SB98] aims to find a policy, $\pi : S \to A$ that maximizes:

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

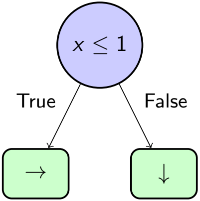
- Lots of succesful RL algorithms [SB98; Mni+15; Sch+17].
- No interpretability concerns.

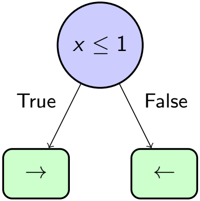
Grid world MDP





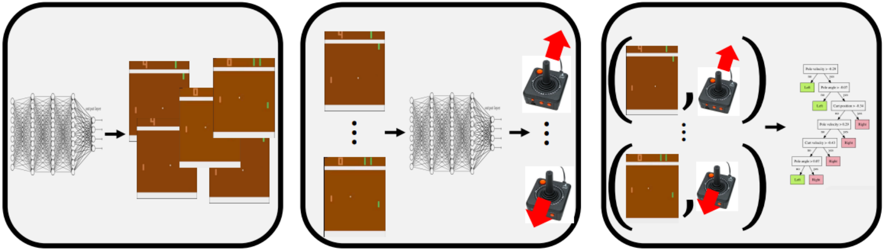
A grid world MDP and optimal actions.





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

Indirect approach: imitation learning



Step 1: Use NN to generate states

Step 2: Use NN to obtain actions

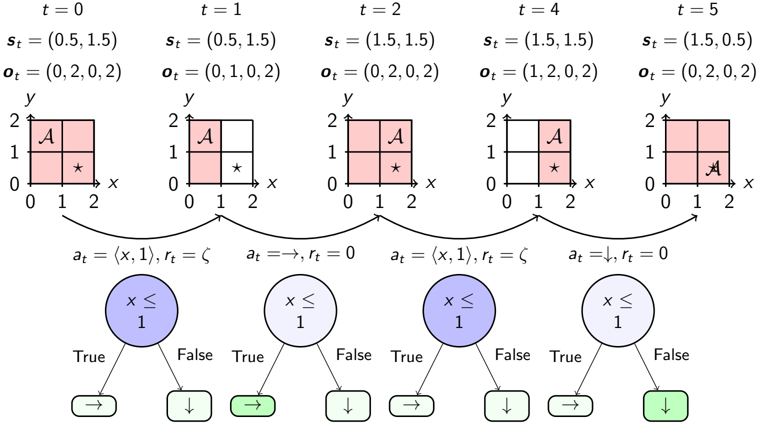
Step 3: Use supervised learning to train a decision tree

Imitation learning works well in practice to get interpretable policies [Mil+24; BPS18; RGB10] but no optimality guarantees.

Contributions

1. Why is learning optimal interpretable policies for sequential decision making difficult?
2. How to leverage sequential decision making to learn interpretable classifiers for supervised learning?
3. How to measure policy interpretability in sequential decision making?

Iterative bounding Markov decision processes (IBMDP)



Trajectory in an IBMDP of the grid world MDP [Top+21]. 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 **determinstic** 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 [Lit94]!

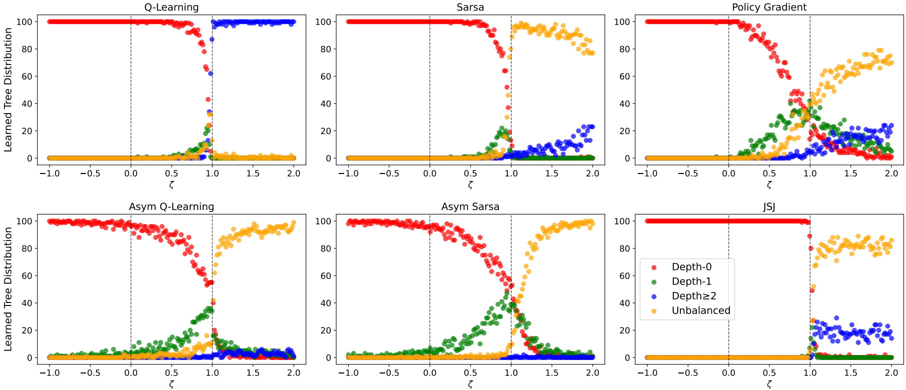
Re-formulation

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

$$\Leftrightarrow$$

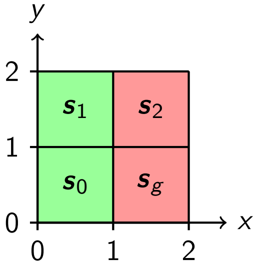
Q: How does RL perform for optimizing **deterministic** *and* **partially observable** *policies in IBMDPs?*

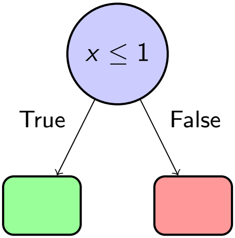
Result: RL cannot retrieve optimal depth-1 trees for the grid world MDP



Distributions of final tree policies learned with various (asymmetric) RL algorithms [SB98; SJJ94; LS98; BA22; BDA22] across 100 seeds. For each different performance-interpretability trade-off value ζ, each point represent the share of different trees.

Interesting sub-class of MDPs: classification MDPs

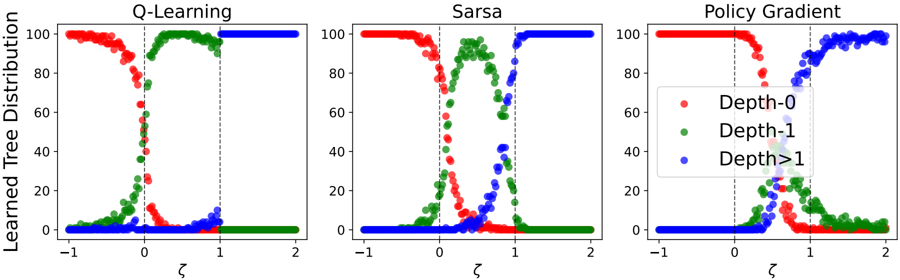




Classification MDP and the unique optimal depth-1 tree.

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

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



Distributions of final tree policies learned with various RL algorithms across 100 seeds. For each different performance-interpretability trade-off value ζ, each point represent the share of different trees.

Perspectives for direct RL of decision tree policies.

- Interpretability for SDM problems can be difficult because of **partial observability**.
- Should we focus on indirect approaches? Hybrid approaches [Wu+20]?
- Fixing the policy tree structure a priori (paramteric trees, [Mar+25])?
- Design algorithms that learn deterministic partially observable policies [LBE25; LEM25]?

RL works in classification MDPs

Q: Can we leverage SDM design new decision tree induction algorithms for the supervised learning setting? **A: Yes!**

Decision trees in supervised learning

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

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

- Trees **interpretable** and **competitive with neural nets** [GOV22].
- Greedy algorithms **sub-optimal accuracy**, but $\boldsymbol{O(2^D)}$ operations [Bre+84; Qui86; Qui93] .
- Optimal algorithms, **optimal accuracy**, but $\boldsymbol{O((2Np)^D)}$ operations (NP-hard) [BD17; Dem+22; LWD23; CRB24; HR76].
- In between optimal and greedy?

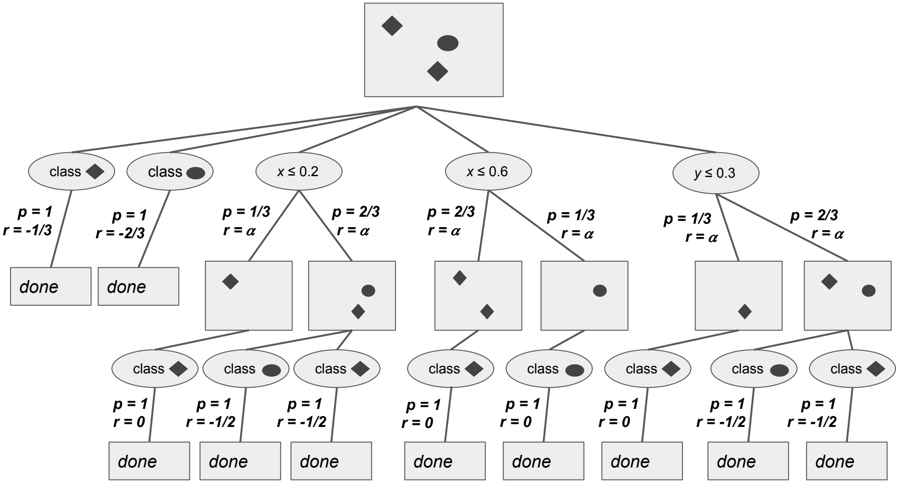
Decision tree induction as solving MDPs

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) $\mathcal{E}$, 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

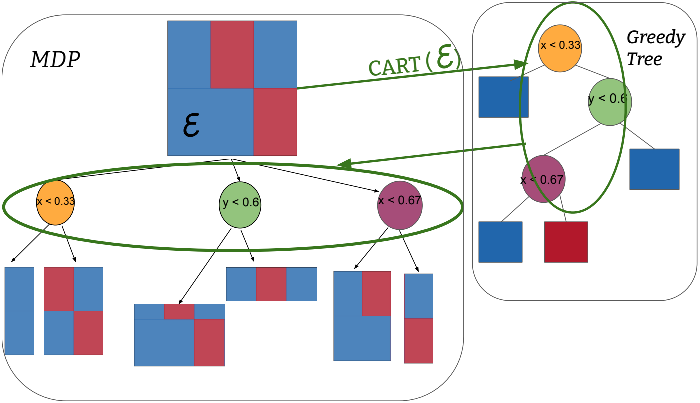


MDP formulation of a generic decision tree induction for a supervised learning task.

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 $\rightarrow$ **MDP state space size is $O(2^D)$**.
- Optimal algorithms consider all possible actions in each state $\rightarrow$ **MDP state space size is $O((2Np)^D)$**.
- Let's choose candidate actions adaptively $\rightarrow$ for each MDP state consider B actions: **state space size is $O((2B)^D)$**.

Dynamic Programming Decision Trees (DPDT)[1]



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

[1]Because states are entire datasets, we implement DPDT with a depth-first search to limit the space complexity.

Theoretical motivation

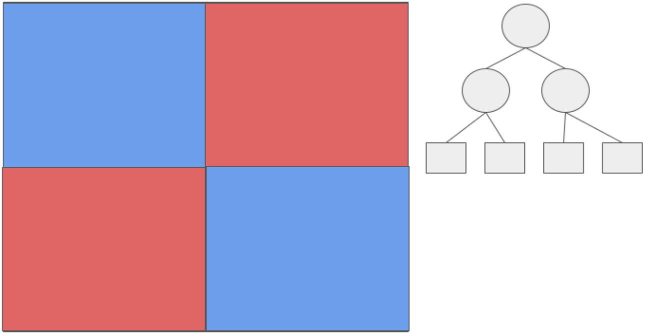
Theorem (DPDT trees are not worse than greedy trees)

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.

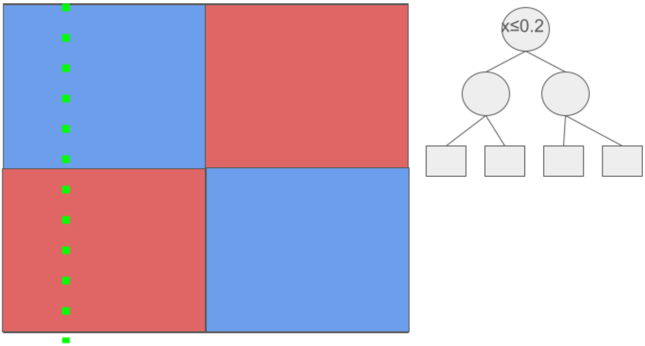
Theorem (DPDT trees can be strictly better than greedy trees)

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

DPDT trees can be strictly better than greedy trees



DPDT trees can be strictly better than greedy trees



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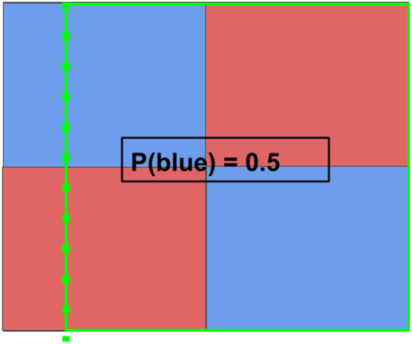

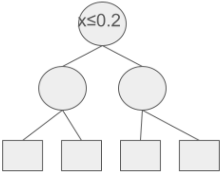

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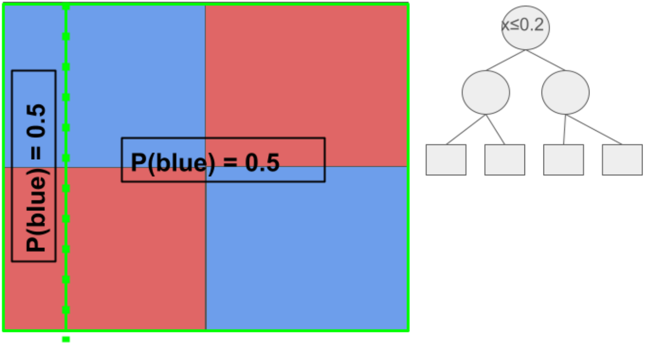

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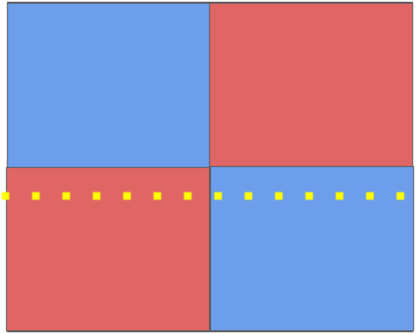

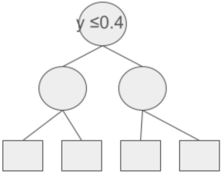

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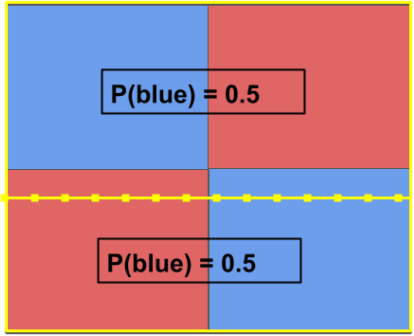

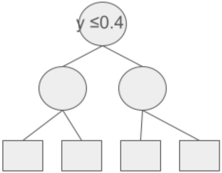

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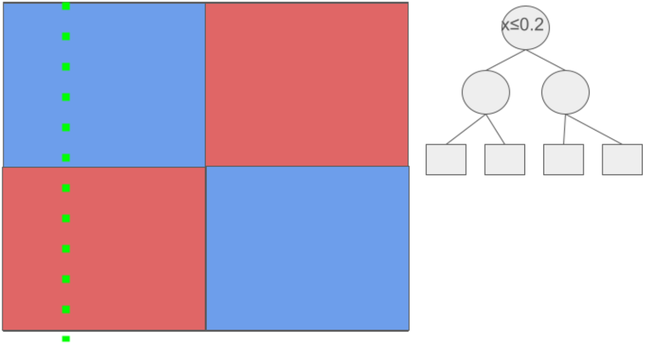

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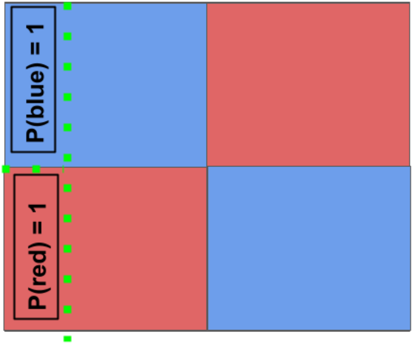

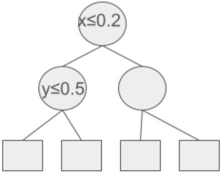

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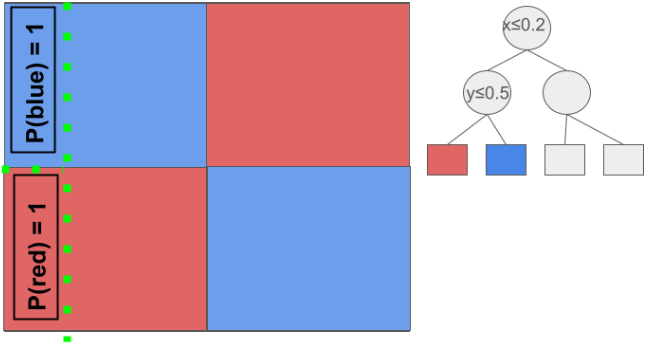

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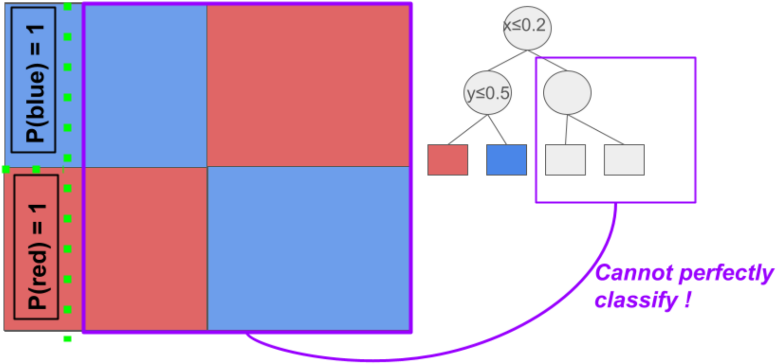
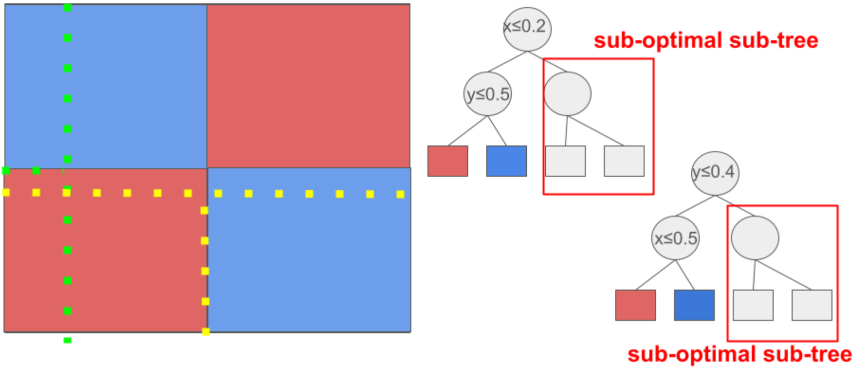


DPDT trees can be strictly better than greedy trees



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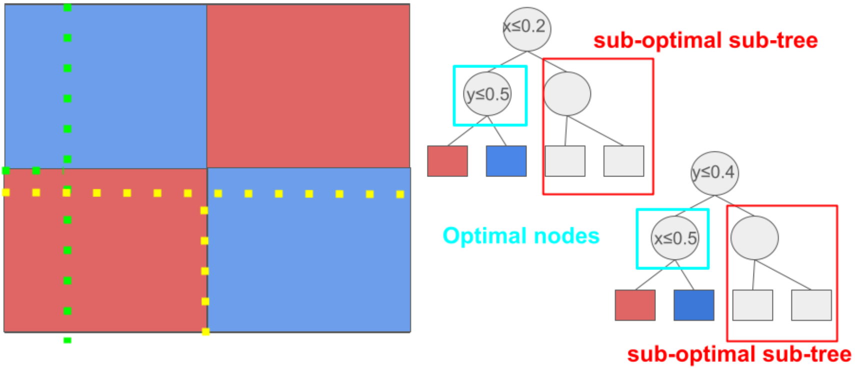

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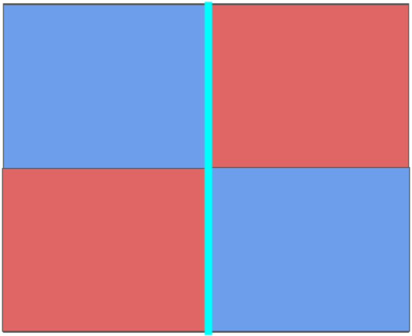
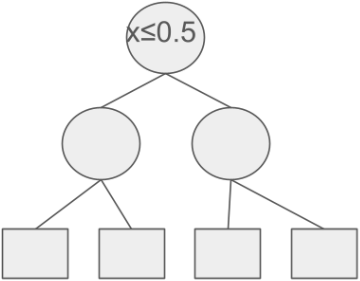
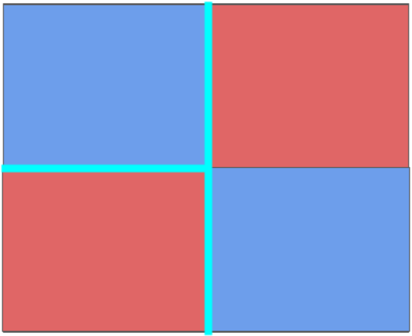
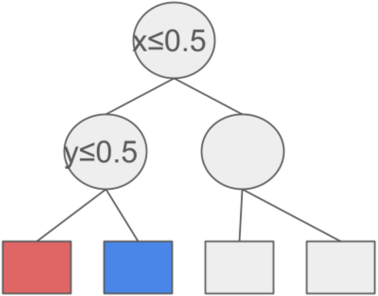


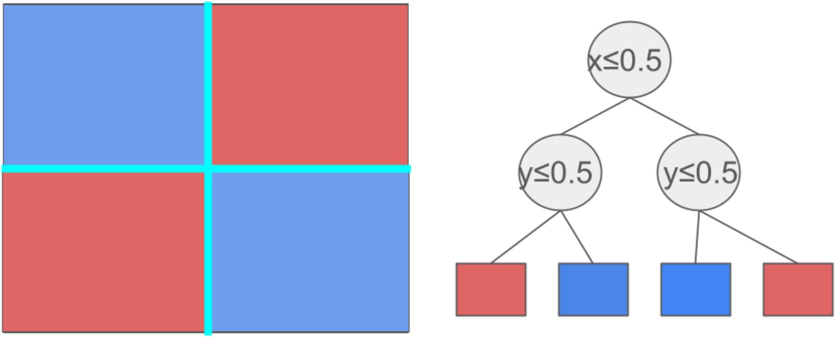


DPDT trees can be strictly better than greedy trees

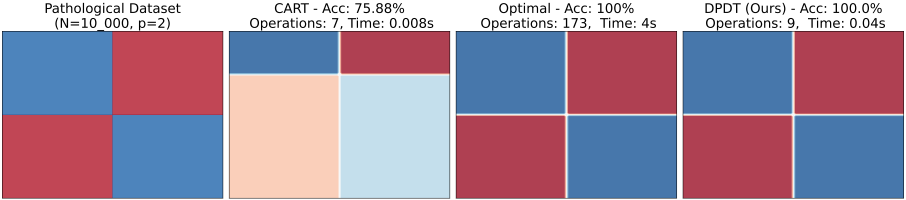




DPDT trees can be strictly better than greedy trees



Fast like greedy trees, accurate like optimal trees



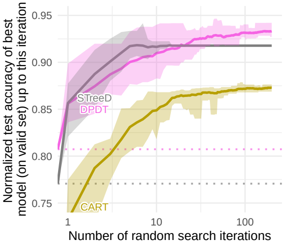
A checkers board data set highlights the limitations of existing works.

Comparing tree accuracy to complexity

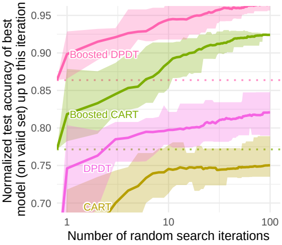
Train accuracy and operation count when learning depth-3 decision trees.

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

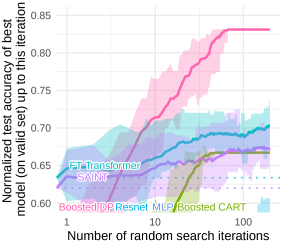
DPDT trees generalization



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



Boosted DPDT vs. Boosted CART



Boosted DPDT vs. other classifiers

Perspectives

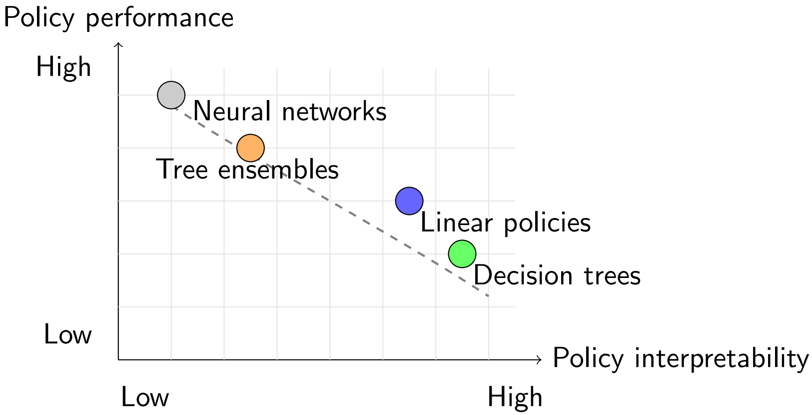
- New SOTA decision tree induction with dynamic programming in MDPs.
- What about using DPDT for indirect decision tree policy learning for SDM?
- What performances could we reach with an industry-grade implementation of XGboost+DPDT?

Let us take a step back

Q: Are decision trees really the most interpretable model?

A: It depends.

Policy interpretability



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

How to measure policy interpretability?

Challenges [Gla+24; Lip18; DK17]

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

The notion of *simulatability* [Lip18]

- 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 [Fre14; Lav99].
- Time to formally verify a policy decreases with interpretability [Bar+20].

A methodology to measure policy interpretability without humans

Simulatability [Lip18]

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 [Luo+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]
```

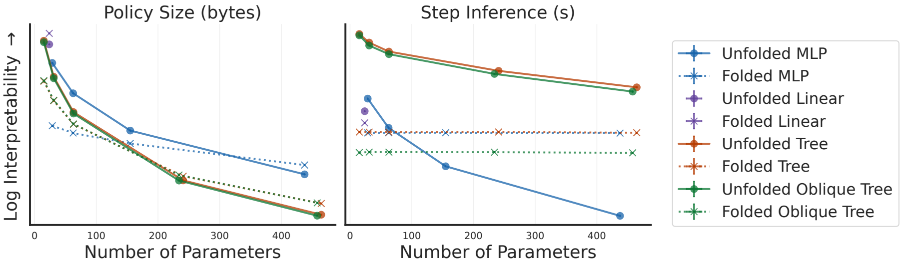
Empirical validation

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?

W

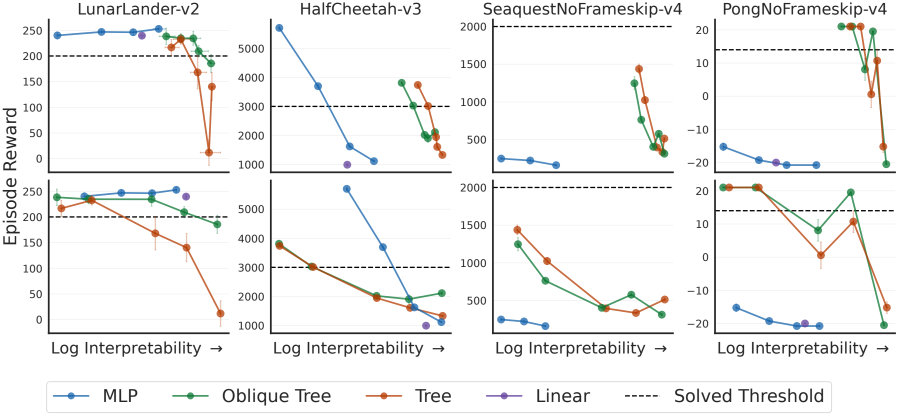
e imitate $\sim$ 40000 expert policies from `stable-baselines3` using various policy classes/nb parameters on various environments.

Result: unfolding policies is necessary to respect consensus



Aggregated policies interpretability on classic control environments

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.

Perspectives

- 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**.
  $\rightarrow$ Focus on indirect approaches and/or on POMDP research first.
- Fundamental challenges: **no definition**.
  $\rightarrow$ 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 [Nag+24].

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