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Thèse présentée par **Hector Kohler**Soutenue le 1<sup>er</sup> **décembre 2025** 

En vue de l'obtention du grade de docteur de l'Université de Lille et de l'Inria

#### Discipline **Informatique** Spécialité **Informatique et Applications**

## Interpretabilité via l'Apprentissage Supervisé ou par Renforcement d'Arbres de Décisions

Thèse dirigée par Philippe Preux directeur

Riad Akrour co-directeur

#### Composition du jury

Rapporteurs René Descartes professeur à l'IHP

Denis Diderot directeur de recherche au CNRS

Examinateurs Victor Hugo professeur à l'ENS Lyon président du jury

Sophie Germain McF à l'Université de Paris 13 Joseph Fourier chargé de recherche à l'INRIA Paul Verlaine chargé de recherche hdr au CNRS

Invité George SAND

Directeurs de thèse Philippe Preux professeur à l'Université de Lille

Riad Akrour Inria

#### Colophon

Mémoire de thèse intitulé « Interpretabilité via l'Apprentissage Supervisé ou par Renforcement d'Arbres de Décisions », écrit par Hector Kohler, achevé le 25 juin 2025, composé au moyen du système de préparation de document LATEX et de la classe yathesis dédiée aux thèses préparées en France.





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Committee President

#### Université de Lille Inria

Doctoral School École Graduée MADIS-631
University Department Centre de Recherche en Informatique, Signal et Automatique de

Thesis defended by **Hector Kohler**Defended on **December 1, 2025** 

Lille

In order to become Doctor from Université de Lille and from Inria

Academic Field Computer Science
Speciality Computer Science and Applications

# Interpretability through Supervised or Reinforcement Learning of Decision Trees

Thesis supervised by Philippe Preux Supervisor

Riad Akrour Co-Supervisor

#### **Committee members**

Referees René Descartes Professor at IHP

Denis Diderot Senior Researcher at CNRS

Examiners Victor Hugo Professor at ENS Lyon

Sophie Germain Associate Professor at Université de

Paris 13

Joseph Fourier Junior Researcher at INRIA
Paul Verlaine HDR Junior Researcher at CNRS

Guest George SAND

Supervisors Philippe Preux Professor at Université de Lille

Riad Akrour Inria

Résumé vii

### Interpretabilité via l'Apprentissage Supervisé ou par Renforcement d'Arbres de Décisions

#### Résumé

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**Mots clés :** apprentissage par renforcement, arbres de décision, interprétabilité, méthodologie

viii Résumé

## Interpretability through Supervised or Reinforcement Learning of Decision Trees Abstract

In this Ph.D. thesis, we study algorithms to learn decision trees for classification and sequential decision making. Decision trees are interpretable because humans can read through the decision tree computations from the root to the leaves. This makes decision trees the go-to model when human verification is required like in medicine applications. However, decision trees are non-differentiable making them hard to optimize unlike neural networks that can be trained efficiently with gradient descent. Existing interpretable reinforcement learning approaches usually learn soft trees (non-interpretable as is) or are ad-hoc (train a neural network then fit a tree to it) potentially missing better solutions.

In the first part of this manuscript, we aim to directly learn decision trees for a Markov decision process with reinforcement learning. In practice we show that this amounts to solving a partially observable Markov decision process. Most existing RL algorithms are not suited for POMDPs. This parallel between decision tree learning with RL and POMDPs solving help us understand why in practice it is often easier to obtain a non-interpretable expert policy—a neural network—and then distillate it into a tree rather than learning the decision tree from scratch.

The second contribution from this work arose from the observation that looking for a deicison tree classifier (or regressor) can be seen as sequentially adding nodes to a tree to maximize the accuracy of predictions. We thus formulate decision tree induction as sloving a Markov decision problem and propose a new state-of-the-art algorithm that can be trained with supervised example data and generalizes well to unseen data.

Work from the previous parts rely on the hypothesis that decision trees are indeed an interpretable model that humans can use in sensitive applications. But is it really the case? In the last part of this thesis, we attempt to answer some more general questions about interpretability: can we measure interpretability without humans? And are decision trees really more interpretable than neural networks?

**Keywords:** reinforcement learning, deicision trees, interpretability, methodology

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### **Preliminary Concepts**

#### **Interpretable Sequential Decision Making**

#### What is Sequential Decision Making?

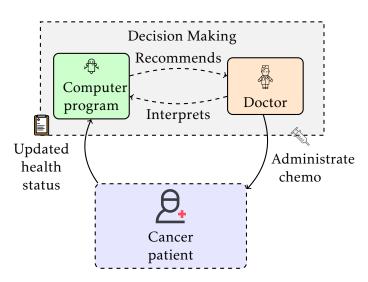


Figure 1 – Sequential decision making in cancer treatment. The AI system reacts to the patient's current state (tumor size, blood counts, etc.) and makes a recommendation to the doctor, who administers the chemotherapy to the patient. The patient's state is then updated, and this cycle repeats over time.

In this manuscript we study algorithms for sequential decision making. Humans engage in sequential decision making in all aspects of life. In medicine, doctors have to decide how much chemotherapy to administrate based on the patient's current health in order to cure [6]. In agriculture, agronomists have to decide when to fertilize next based on the current soil and weather conditions in

order to maximize plant growth [7]. In automotive, the auto-pilot system has to decide how to steer the wheel next based on lidar sensors in order to maintain a safe trajectory [11]. Those sequential decision making processes exhibits key similarities: an agent takes actions based on some current information to achieve some goal.

As computer scientists, we ought to design computer programs [9] that can help humans during those sequential decision making processes. For example, as depicted in Figure 1, a doctor could benefit from a program that would recommend the "best" treatment given the patient's state. Machine learning algorithms [22] output such helpful programs. For non-sequential decision making, when the doctor only takes one decision and does not need to react to the updated patient's health, e.g. making a diagnosis about cancer type, a program can be fitted to example data: given lots of patient records and the associated diagnoses, the program learns to make the same diagnosis a doctor would given the same patient record, this is *supervised* learning [12]. In the cancer treatment example, the doctor follows its patient through time and adapts its treatment to the changing health of the patient. In that case, machine learning, and in particular, reinforcement learning [19], can be used to teach the program how take decisions that lead to the patient recovery in the future based on how the patient's health changes from one chemo dose to another. Such machine learning algorithms train more and more performing program that make their way into our society to, e.g. identify digits on images [10], control tokamak fusion [4], or write the abstract of a scientific article [5].

However, the key problematic behind this manuscript is that those programs computations cannot be understood and verified by humans: the programs are black-box. Next, we describe the notion of interpretability that is key to ensure safe deployment of computer programs trained with machine learning in critical sectors like medicine.

#### What is Interpretability?

Originally, the etymology of "interpretability" is the Latin "interpretabilis" meaning "that can be understood and explained". According to the Oxford

English dictionary, the first recorded use of the english word "interpretability" dates back to 1854 when the british logician George Boole (Figure 2) described the addition of concepts:

I would remark in the first place that the generality of a method in Logic must very much depend upon the generality of its elementary processes and laws. We have, for instance, in the previous sections of this work investigated, among other things, the laws of that logical process of addition which is symbolized by the sign +. Now those laws have been determined from the study of instances, in all of which it has been a necessary condition, that the classes or things added together in thought should be mutually exclusive. The expression x + y seems indeed uninterpretable, unless it be assumed that the things represented by x and the things represented by y are entirely separate; that they embrace no individuals in common. And conditions analogous to this have been involved in those acts of conception from the study of which the laws of the other symbolical operations have been ascertained. The question then arises, whether it is necessary to restrict the application of these symbolical laws and processes by the same conditions of interpretability under which the knowledge of them was obtained. If such restriction is necessary, it is manifest that no such thing as a general method in Logic is possible. On the other hand, if such restriction is unnecessary, in what light are we to contemplate processes which appear to be uninterpretable in that sphere of thought which they are designed to aid? [2, p. 48]

What is remarkable is that the supposedly first recorded occurrence of "interpretability" was in the context of computer science. Boole asked: when can we meaningfully apply formal mathematical operations beyond the specific conditions under which we understand them? In Boole's era, the concern was whether logical operations like addition could be applied outside their original interpretable contexts—where symbols and their sum represent concepts that humans can understand, e.g. red + apples = red apples. Today, we face an analogous dilemma with machine learning algorithms: black-box programs like neural





Figure 2 – British logician and philosopher George Boole (1815-1864) next to its book *The Laws of Thoughts* (1854) that is the oldest known record of the word "interpretability".

netowrks [16], that learn complex unintelligible combinations of inputs (representations), are often deployed in contexts where computations should be understood by humans, e.g., in medicine [18].

In Figure 3a, we illustrate how existing machine learning algorithms *could* be used in principle to help with cancer treatment. In truth this should be prohibited without some kind of transparency in the program's recommendation: why did the program recommended such dosage? In Figure 3b, we illustrate how machine learning *should* be used in practice. We would ideally want doctors to have access to computer programs that can recommend "good" treatments and which recommendations are interpretable.

The key challenge of doing research in interpretability is the lack of formalism; there is no *formal* definition of what is an interpretable computer program. Hence, unlike for performance objectives which have well-defined optimization objective, e.g. maximizing accuracy (supervised learning) or maximizing rewards over time (reinforcement learning), it is not clear how to design machine learning algorithms to maximize interpretability of programs. Despite this lack of formalism the necessity of deploying interpretable models has sparked many works that we present next.



(a) Black-box approach using neural networks



(b) Interpretable approach using decision trees

FIGURE 3 – Comparison of sequential decision making approaches in cancer treatment. Top: A black-box neural network approach where the doctor cannot interpret the AI's recommendations. Bottom: An interpretable decision tree approach where the doctor can understand and verify the AI's recommendations. Both systems learn from treatment outcomes to improve their recommendations over time.

## What are existing approaches for learning interpretable programs?

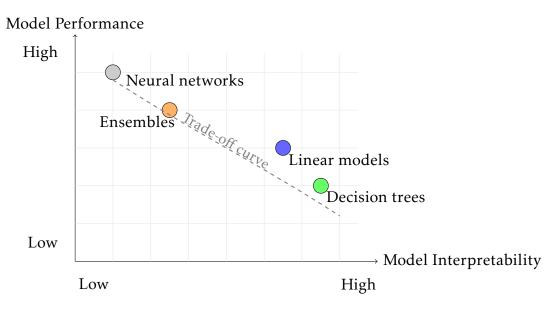


FIGURE 4 – The interpretability-performance trade-off in machine learning. Different program classes are positioned according to their typical interpretability and performance characteristics. The dashed line illustrates the general trade-off between these two properties.

Interpretable machine learning provides either local or global explanations [8]. Global methods output a program which all recommendations can be interpreted without additional computations, e.g. a decision tree [3]. On the other hand, local methods require additional computations but are agnostic to the program class: they can give an *approximate* interpretation of e.g. neural networks recommendations. In Figure 4 we present the popular trade-off between interpretability and performance of different program classes.

The most famous local explanation algorithm is LIME (Local Interpretable Model-agnostic Explanations) [15]. Given a program class, LIME works by perturbing the input and learning a simple interpretable model locally to explain that particular prediction. For each individual prediction, LIME provides explanations by identifying which features were most important for that specific decision. Hence, as stated above, LIME needs to learn a whole program per

recommendation that needs to be interpreted; this is a lot of computations.

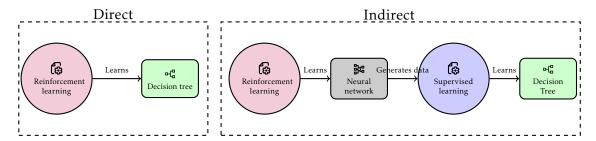


Figure 5 – Comparison of direct and indirect approaches for learning interpretable policies in sequential decision making

Global approaches are either direct or indirect [13]. Direct algorithms, such as decision tree induction [3], are algorithms that directly search a space of interpretable programs (see Figure 4). One of the key challenges that motivates this thesis is that decision tree induction is only defined for supervised learning but not for reinforcement learning. It means that to directly learn computer programs for interpretable sequential decision making, one has to design completely new algorithms. What most existing research have focused on so far, is to work around this confinement of decision tree induction to supervised learning and develop indirect methods. Indirect methods for interpretable sequential decision making-sometimes called post-hoc-start with the reinforcement learning of a non-interpretable computer program, e.g., deep reinforcement learning of a neural network, and then use supervised learning of an interpretable model with the objective to emulate the non-interpretable program. This approach is called behavior cloning or imitation learning [14, 17] and many, if not all, work on interpretable sequential decision making use this indirect approach[1, 23]. Figure 5 illustrates the key difference between these two approaches.

Researchers just recently started to study the advantage of direct over indirect learning of interpretable programs [20, 21]. In short, the motivation behind developing direct methods is to have the interpretable program optimized to solve your actual goal, e.g. patient treatment, while indirect methods learn an interpretable program that is optimized to match the behaviour of a non-interpretable model that was itself optimized to solve your goal. There is no guarantee that optimizing this indirect objective yields the "best" interpretability-performance

trade-offs. Hence, the ideal solution to interpretable sequential decision making would be to have global direct algorithms.

Next, we present the outline of this thesis.

#### **Outline of the Thesis**

In this thesis we take a stab at the difficult task of designing global direct algorithms for interpretable sequential decision making. In the first part of the manuscript we will present a mathematical formalism for the reinforcement learning of decision trees for sequential decision making. In particular we will show that indeed the direct approach can yield better trees than the indirect one. However the unfortunate key result from this opening part is that a good direct method cannot find decision trees for sequential decision making that are not very easy. Fortunately for us, in the second part of this manuscript, we show that some of these easy instances of interpretable sequential decision making tasks can be made *non*-sequential giving rise to a whole new decision tree induction algorithm for supervised learning. In particular, we thoroughly benchmark our new decision tree induction algorithm and claim the state-of-the-art for decision tree induction. Finally, after heavily studying decision trees and direct methods, we will leverage the diversity and simplicity of *indirect* methods to compare other model classes of programs and show that in some cases neural networks can be considered more interpretable than trees and there exist problems for which there is no need to trade-off performance for interpretability. We summarize the outline of the manuscript in Figure 6

#### **Technical Preliminaries**

#### What are decision trees?

As mentioned earlier, as opposed to neural networks, decision trees are supposedly very interpretable because they only apply boolean operations on the program input without relying on internal complex representations.

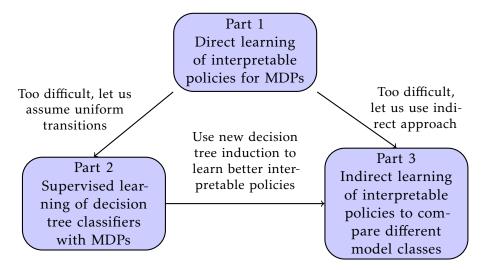


FIGURE 6 – Thesis structure showing the progression from direct reinforcement learning of decision tree policies (Chapter 1) to simplified approaches: supervised learning with uniform transitions (Chapter 2) and indirect learning methods (Chapter 3).

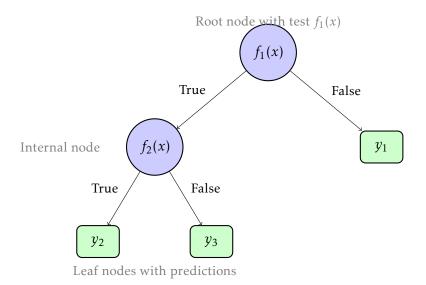


Figure 7 – A generic decision tree structure. Internal nodes contain test functions  $f_v(x): \mathcal{X} \to \{0,1\}$  that map input features to boolean values. Edges represent the outcomes of these tests (True/False), and leaf nodes contain predictions  $y_\ell \in \mathcal{Y}$ . For any input x, the tree defines a unique path from root to leaf.



Figure 8 – The american statistician Leo Breiman (1928-2005) author of *Classification and Regression Trees* (1984)

**Definition 1** (Decision tree). A decision tree is a rooted tree T = (V, E) where :

- Each internal node  $v \in V$  is associated with a test function  $f_v : \mathcal{X} \to \{0,1\}$  that maps input features  $x \in \mathcal{X}$  to a boolean.
- Each edge  $e \in E$  from an internal node corresponds to an outcome of the associated test function.
- Each leaf node  $\ell \in V$  is associated with a prediction  $y_{\ell} \in \mathcal{Y}$ , where  $\mathcal{Y}$  is the output space.
- For any input  $x \in \mathcal{X}$ , the tree defines a unique path from root to leaf, determining the prediction  $T(x) = y_{\ell}$  where  $\ell$  is the reached leaf.

#### How to learn decision trees?

The Classification and Regression Trees (CART) algorithm, developed by Leo Breiman and colleagues (Figure 8), is one of the most widely used methods for learning decision trees from supervised data. CART builds binary decision trees through a greedy, top-down approach that recursively partitions the feature space. At each internal node, the algorithm selects the feature and threshold that best splits the data according to a purity criterion such as the Gini impurity for classification or mean squared error for regression.

CART uses threshold-based test functions of the form  $f_v(x) = \mathbb{I}[x[feature] \le threshold]$  where  $\mathbb{I}[\cdot]$  is the indicator function, consistent with the general de-

cision tree definition above. The key idea is to find splits that maximize the homogeneity of the resulting subsets. For classification, this means finding test functions that separate different classes as cleanly as possible. The algorithm continues splitting until a stopping criterion is met, such as reaching a minimum number of samples per leaf or achieving sufficient purity. The complete CART procedure is detailed in Algorithm 1.

#### Markov decision processes/problems

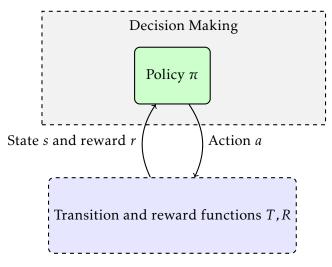


Figure 9 – Markov decision process

Markov decision processes (MDPs) were first introduced in the 1950s by Richard Bellman (cite). Informally, an MDP models how an agent acts over time to achieve its goal. At every timestep, the agent observes its current state, e.g. a patient weight and tumor size, and takes an action, e.g. injects a certain amount of chemotherapy. When doing a certain action in a certain state, the agent gets a reward that helps it evaluate the quality of its action with respect to its goal, e.g., the tumor size decrease when the agent has to cure cancer. Finally, the agent is provided with a new state, e.g. the updated patient state, and repeats this process over time. Following Martin L. Puterman's book on MDPs (cite), we formally define as follows.

**Definition 2** (Markov decision process). An MDP is a tuple  $\mathcal{M} = \langle S, A, R, T, T_0 \rangle$ 

#### Algorithme 1: CART Algorithm for Decision Tree Learning

```
Data : Training data (X, y) where X \in \mathbb{R}^{n \times d} and y \in \{1, 2, ..., K\}^n
Result : Decision tree T
Function BuildTree(X, y):
    if stopping criterion met then
        return leaf node with prediction MajorityClass(y)
    end
    (feature, threshold) \leftarrow BestSplit(X, y)
    if no valid split found then
     return leaf node with prediction MajorityClass(y)
    Split data : X_{left}, y_{left} = \{(x_i, y_i) : x_i[feature] \le threshold\}
                      X_{right}, y_{right} = \{(x_i, y_i) : x_i[feature] > threshold\}
    left\_child \leftarrow BuildTree(X_{left}, y_{left})
    right\_child \leftarrow BuildTree(X_{right}, y_{right})
    return internal node with test function
     f_v(x) = \mathbb{I}[x[feature] \le threshold] and children
     (left_child,right_child)
Function BestSplit(X, y):
    best\_gain \leftarrow 0
    best\_feature \leftarrow None
    best\_threshold \leftarrow None
    for each feature f \in \{1, 2, ..., d\} do
        for each unique value v in X[:, f] do
             y_{left} \leftarrow \{y_i : X[i, f] \le v\}
            y_{right} \leftarrow \{y_i : X[i, f] > v\}
             gain \leftarrow Gini(y) - \frac{|y_{left}|}{|y|}Gini(y_{left}) - \frac{|y_{right}|}{|y|}Gini(y_{right})
             if gain > best_gain then
                 best_gain ← gain
                 best_feature \leftarrow f
               best threshold \leftarrow v
             end
        end
    return (best_feature, best_threshold)
Function Gini(y):
    return 1 - \sum_{k=1}^{K} \left( \frac{|\{i: y_i = k\}|}{|y|} \right)^2 // Gini impurity
return BuildTree(X, y)
```

where:

- S is a finite set of states  $s \in \mathbb{R}^n$  representing all possible configurations of the environment.
- A is a finite set of actions  $a \in \mathbb{Z}^m$  available to the agent.
- $R: S \times A \to \mathbb{R}$  is the reward function that assigns a real-valued reward to each state-action pair.
- $T: S \times A \rightarrow \Delta(S)$  is the transition function that maps state-action pairs to probability distributions over next states, where  $\Delta(S)$  denotes the probability simplex over S.
- $T_0 \in \Delta(S)$  is the initial distribution over states.

Now we can also model the "goal" of the agent. Informally, the goal of an agent is to behave such that it gets as much reward as it can over time. For example, in the cancer treatment case, the best reward the agent can get is to completely get rid of the patient's tumor after some time. Furthermore, we want our agent to prefer behaviour that gets rid of the patient's tumor as fast as possible. We can formally model the agent's goal as an optimization problem as follows.

**Definition 3** (Markov decision problem). Given an MDP  $\mathcal{M} = \langle S, A, R, T, T_0 \rangle$ , the goal of an agent following policy  $\pi : S \to A$  is to maximize 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  $\gamma \in (0,1)$  is the discount factor that controls the trade-off between immediate and future rewards.

Hence, algorithms presented in this manuscript aim to find solutions to Markov decision problems, i.e. the optimal policy :  $\pi^* = \underset{\pi}{\operatorname{argmax}} J(\pi)$  For the rest of this text, we will use an abuse of notation and denote both a Markov decision process and the associated Markov decision problem by MDP.

#### **Exact solutions for Markov decision problems**

It is possible to compute the exact optimal policy  $\pi^*$  using dynamic programming (cite). Indeed, one can leverage the Markov property to find for all states the best action to take based on the reward of upcoming states.

**Definition 4** (Value of a state). The value of a state  $s \in S$  under policy  $\pi$  is the expected discounted sum of rewards starting from state s and following policy  $\pi$ :

$$V^{\pi}(s) = \mathbb{E}\left[\sum_{t=0}^{\infty} \gamma^{t} R(s_{t}, a_{t}) \mid s_{0} = s, a_{t} = \pi(s_{t}), s_{t+1} \sim T(s_{t}, a_{t})\right]$$

Applying the Markov property gives a recursive definition of the value of s under policy  $\pi$ :

$$V^{\pi}(s) = R(s, \pi(s)) + \gamma \sum_{s' \in S} T^{s'}(s, \pi(s)) V^{\pi}(s')$$

where  $T^{s'}(s, \pi(s))$  is the probability of transitioning to state s' when taking action  $\pi(s)$  in state s.

**Definition 5** (Optimal value of a state). The optimal value of a state  $s \in S$ ,  $V^*(s)$ , is the value of state s when following the optimal policy:  $V^{\pi^*}(s)$ .

$$V^{\star}(s) = V^{\pi^{\star}}(s) = \max_{\pi} [J(\pi)]$$

**Definition 6** (Optimal value of a state-action pair). The optimal value of a state-action pair  $(s, a) \in S \times A$ ,  $Q^*(s, a)$ , is the value of state s when taking action a and then following the optimal policy:  $V^{\pi^*}(s)$ .

$$Q^{\star}(s,a) = Q^{\pi^{\star}}(s) = R(s,a) + \gamma \sum_{s' \in S} V^{\star}(s')$$

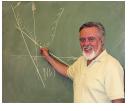
Hence, the algorithms we study in the thesis can also be seen as solving the problem :  $\pi^* = \underset{\pi}{\operatorname{argmax}} \mathbb{E}[V^{\pi}(s_0)|s_0 \sim T_0]$ . The well-known Value Iteration algorithm 2 solves this problem exactly (cite).

More realistically, neither the transition kernel *T* nor the reward function *R* of the MDP are known, e.g., the doctor can't **know** how the tumor and the patient

#### **Algorithme 2 :** Value Iteration

```
Data: MDP \mathcal{M} = \langle S, A, R, T, T_0 \rangle, convergence threshold \theta
Result : Optimal policy \pi^*
Initialize V(s) = 0 for all s \in S
repeat
     \Delta \leftarrow 0
     for each state s \in S do
          v \leftarrow V(s)
          V(s) \leftarrow \max_{a} \left[ R(s, a) + \gamma \sum_{s' \in S} T(s, a, s') V(s') \right] / / \text{ Bellman}
          optimality update
          \Delta \leftarrow \max(\Delta, |v - V(s)|)
     end
until \Delta < \theta;
for each state s \in S do
     \pi^*(s) \leftarrow \arg\max_a \left[ R(s, a) + \gamma \sum_{s' \in S} T(s, a, s') V(s') \right] / / \text{ Extract}
     optimal policy
end
```

health will change after a dose of chemotherapy, it can only **observe** the change. This distinction between the information available to the agent is paralleled with the distinction between dynamic programming and reinforcement learning (RL) that we describe next.







(b) M.L. Puterman



(c) A. Barto



(d) R. Sutton

FIGURE 10 – The godfathers of sequential decision making. Andrew Barto and Richard Sutton are the ACM Turing Prize 2024 laureate and share an advisor advisee relationship.

#### Reinforcement learning of approximate solutions to MDPs

Reinforcement learning algorithms popularized by Richard Sutton (Figure 10) (cite) don't **compute** an optimal policy but rather **learn** an approximate one based on sequences of observations  $(s_t, a_t, r_t, s_{t+1})_t$ . RL algorithms usually fall into two categories: value-based (cite) and policy gradient (cite). The first group of RL algorithms computes an approximation of  $V^*$  using temporal difference learning, while the second class leverages the policy gradient theorem to approximate  $\pi^*$ . Examples of these approaches are shown in Algorithms 3 and 4.

```
Algorithme 3: Value-based RL (Q-Learning)

Data: MDP \mathcal{M} = \langle S, A, R, T, T_0 \rangle, learning rate \alpha, exploration rate \epsilon

Result: Policy \pi

Initialize Q(s,a) = 0 for all s \in S, a \in A

for each episode do

Initialize state s_0 \sim T_0

for each step t do

Choose action a_t using \epsilon-greedy: a_t = \arg\max_a Q(s_t, a) with prob.

1 - \epsilon

Take action a_t, observe r_t = R(s_t, a_t) and s_{t+1} \sim T(s_t, a_t)

Q(s_t, a_t) \leftarrow Q(s_t, a_t) + \alpha[r_t + \gamma \max_{a'} Q(s_{t+1}, a') - Q(s_t, a_t)]

s_t \leftarrow s_{t+1}

end

end

end

\pi(s) = \arg\max_a Q(s, a) // Extract greedy policy
```

Both classes of algorithms are known to converge to the optimal value or policy under some conditions (cite) and have known great successes in real-world applications (cite). The books from Puterman, Bertsekas, Sutton and Barto, offer a great overview of MDPs and algorithm to solve them. There are many other ways to learn policies such as simple random search (cite) or model-based reinforcement learning. However, not many algorithms consider the learning of policies that can be easily understood by humans which we discuss next and that is the core of this manuscript.

#### **Algorithme 4 :** Policy Gradient RL (REINFORCE)

```
Data: MDP \mathcal{M} = \langle S, A, R, T, T_0 \rangle, learning rate \alpha, policy parameters \theta

Result: Policy \pi_{\theta}

Initialize policy parameters \theta

for each episode do

Generate trajectory \tau = (s_0, a_0, r_0, s_1, a_1, r_1, ...) following \pi_{\theta}

for each timestep t in trajectory do

G_t \leftarrow \sum_{k=t}^T \gamma^{k-t} r_k // Compute return

G_t \leftarrow G_t \nabla_{\theta} \log \pi_{\theta}(a_t|s_t) // Compute General end

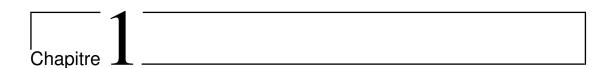
end
```

## Première partie

A difficult problem : Learning Decision Trees for MDP

I have not failed. I've just found 10.000 ways that won't work.

Thomas A. Edison



## A failing direct interpretable reinforcement learning algorithm

#### 1.1 Iterative Bounding Markov Decision Processes

We start by considering a very basic Markov decision process (def) for which we would like decision tree (def) policies.

In 2021, Topin et. al. introduced Iterative Bounding Markov decision process (IBMPD) (cite). It is, to the best of our knowledge, the only work in which decision tree policies are *grown* using the RL object (def). We insist here on *growing* to refer to trees whose nodes and leaves structure is not knows *a priori* as opposed to parametric trees—trees which structure is fixed— and can be optimized with the policy gradient theorem (cite). In supervised learning a similar distinction exists too (cite).

The policy gradient theorem or random search can also be used in to learn linear policies (cite) that should be more interpretable than deep neural netwok. In this seminal work Topin et. al., formulate learning a decision tree policy for an MDP as solving an augmented MDP where some actions are adding decision nodes to a tree structure or taking base actions. (figure) More interestingly, IBMDP can generalize to any sort of tree-like policies where nodes need only to be binary functions of features.

#### 1.2 Litterature and results on POMDPs

CITE ALL NAMES OF THIS PARTICULAR POMDP (c.f. Olivier Buffet) Without mentionning explicitely Topin et.al. propose to learning in IBMDPs by solving a Partially Observable MDP (cite). POMDPs are notorously more difficult to solve than MDPs (cite). In particular, not all policies for  $\mathcal{M}_IB$  are decision tree policies for  $\mathcal{M}$ . Only policies from partial observation to actions are trees. Hence learning a decision tree policy for an MDP can be done by learning a deterministic and reactive policy for a POMDP. In general, this problem cannot be solved exactly with dynamic programming because of intrinsic POMDP limitations described in the work of Michael Littman (cite).

We will show that three of those limitations arise in direct interpretable RL:

- 1. The optimal policy in a POMDP can be stochastic
- 2. The optimal policy in a POMDP does not necessarily maximizes all state values simultaneously
- 3. Q-Learning like algorithms do not necessirily converge to the optimal Q-values.

In addition to those limitaions that are inherited from POMDPs, IBMDPs bring their own intrinsic challenges:

- 1. The action space might need to be state dependent
- 2. It is hard to align RL agents for IBMDPs

#### 1.3 IBMDP and Didactic example

Given an MDP  $\mathcal{M} = \langle S, A, R, T, T_0 \rangle$ , an Iterative Bounding Markov decision process is defined as follows.

**Definition 7.** Given an MDP  $\mathcal{M} = \langle S, A, R, T, T_0 \rangle$ , an Iterative Bounding Markov decision process  $\mathcal{M}_{IB}$  is a tuble  $\langle S, O, A, A_{IG}, R, \zeta, T, T_0, P \rangle$ . The IBMDP is an augmented version of an MDP. The states in an IBMPD are concatenations of  $s \in S \subset [L_1, U_1] \times \cdots \times [L_n, U_n] \subsetneq \mathbb{R}^n$  and bounding values  $o = (L_0) \in O$ 

#### 1.3.1 An MDP for which we want a decision tree policy

(figure) Do figure of POMDP graphical models with grid world. We consider a  $2\times2$  grid world Markov Decision Process (MDP) defined as follows :

- **States**: Four cells labeled  $S_0$ ,  $S_1$ ,  $S_2$ , and G (goal state) arranged in a 2×2 grid.
- **Actions**: At each state, the agent can move right  $(\rightarrow)$  or down  $(\downarrow)$  up  $(\uparrow)$  or left  $(\leftarrow)$ .
- **Transitions**: Movements are deterministic, following the direction of the chosen action. Actions that would lead outside the grid leave the agent in the same state.
- **Rewards**: All transitions yield a reward of 0, except for any action taken from the goal state *G*, which yields a reward of 1.
- **Objective**: Maximize the expected discounted cumulative reward.

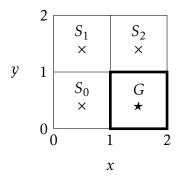


Figure 1.1 – The 2×2 grid world environment with states  $S_0$ ,  $S_1$ ,  $S_2$ , and goal state G.

In the next chapter we show the limitation of both direct and indirect approaches for this problem.



## An attempt at Reinforcement Learning of Policies

#### 2.1 Grid World tabular solutions

In this section, for the sake of example, we assume that a dictionary with 4 key-value pais is less interpretable than a depth-1 decision tree. In Figure 2.1, we illustrate *a*–there are others–tabular optimal policy for the grid world MDP described in the previous section, i.e. that maximizes the objective (cite). In any starting state, the agent will move towards the abosrbing state with positive reward.

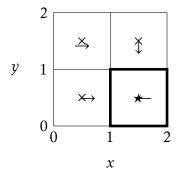


FIGURE 2.1 – An optimal tabular policy for the grid world.

For this grid world, there exist optimal decision tree policies. In particular

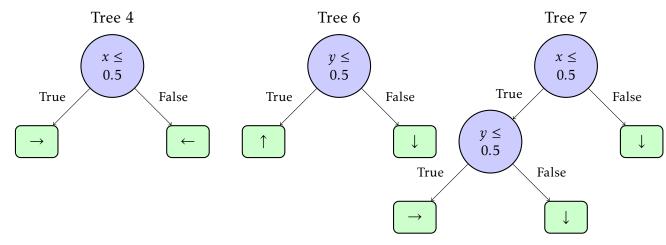


FIGURE 2.2 – Some optimal decision tree policies.

Tree 4 and 6 are have very good interpretability-performance trade-offs (smallest tree that can get the maximum MDP reward). In the rest of this section we shall attempt to *learn* those trees from data.

#### 2.2 Method

Let us compute the objective value (cite) for the trees presented above. We will identify the range of  $\zeta$  values—the interpretability penalty—for which the depth-1 tree is optimal. Let us compute the objective values of the most rewarded tree for each tree structure.

**Depth-0 decision tree :** has only one leaf node that takes a single base action indefinitely. For this type of tree the best reward achievable is to take actions that maximize the probability of reaching the objective  $\rightarrow$  or  $\downarrow$ . In that case the objective value of such tree is : In the goal state G = (1,0), the value of the

2.2. Method 27

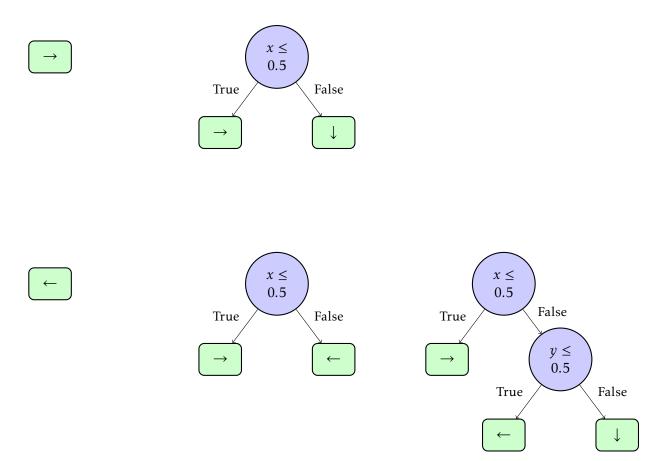


FIGURE 2.3 – Examples of decision trees for different policies in the grid world. Each tree represents a different policy, from simple single-action policies to more complex conditional policies.

depth-0 tree  $T_0$  is:

$$V_G^{T_0} = 1 + \gamma + \gamma^2 + \dots$$
$$= \sum_{t=0}^{\infty} \gamma^t$$
$$= \frac{1}{1 - \gamma}$$

In the state (0,0) when the policy repeats going right respectively in the state (0,1) when the policy repeats going down, the value is :

$$V_{S_0}^{T_0} = 0 + \gamma V_g^{T_0}$$
$$= \gamma V_G^{T_0}$$

In the other states the policy never gets positive rewards;  $V_{S_1}^{T_0} = V_{S_2}^{T_0} = 0$ . Hence:

$$J(\mathcal{T}_0) = \frac{1}{4} V_G^{\mathcal{T}_0} + \frac{1}{4} V_{S_0}^{\mathcal{T}_0} + \frac{1}{4} V_{S_1}^{\mathcal{T}_0} + \frac{1}{4} V_{S_2}^{\mathcal{T}_0}$$

$$= \frac{1}{4} V_G^{\mathcal{T}_0} + \frac{1}{4} \gamma V_G^{\mathcal{T}_0} + 0 + 0$$

$$= \frac{1}{4} \frac{1}{1 - \gamma} + \frac{1}{4} \gamma \frac{1}{1 - \gamma}$$

$$= \frac{1 + \gamma}{4(1 - \gamma)}$$

**Depth-1 decision tree :** has one root node that tests  $x \le 0.5$  (respectively  $y \le 0.5$ ) and two leaf nodes  $\to$  and  $\downarrow$ . In the goal state G = (1,0), the depth-1 decision tree policy cycles between taking an information gathering action  $x \le 0.5$  and moving down to get a positive reward for which it gets the returns :

$$V_G^{\mathcal{T}_1} = \zeta + \gamma + \gamma^2 \zeta + \gamma^3 \dots$$

$$= \sum_{t=0}^{\infty} \gamma^{2t} \zeta + \sum_{t=0}^{\infty} \gamma^{2t+1}$$

$$= \frac{\zeta + \gamma}{1 - \gamma^2}$$

2.2. Method 29

In states  $S_0 = (0,0)$  and  $S_2 = (1,1)$ , the value of the depth-1 decision tree policy is the return when taking one information gathering action  $x \le 0.5$ , then moving right or down, then following the policy from the goal state G:

$$\begin{aligned} V_{S_0}^{T_1} &= \zeta + \gamma 0 + \gamma^2 V_G^{T_1} \\ &= \zeta + \gamma^2 V_G^{T_1} \\ &= V_{S_2}^{T_1} \end{aligned}$$

Similarly the value of the depth-1 decision tree policy in state  $S_1 = (0,1)$  is the value of taking one information gathering action then moving right to  $S_2$  then following the policy in  $S_2$ :

$$\begin{split} V_{S_1}^{T_1} &= \zeta + \gamma 0 + \gamma^2 V_{S_2}^{T_1} \\ &= \zeta + \gamma^2 V_{S_2}^{T_1} \\ &= \zeta + \gamma^2 (\zeta + \gamma^2 V_G^{T_1}) \\ &= \zeta + \gamma^2 \zeta + \gamma^4 V_G^{T_1} \end{split}$$

The objective value of the depth-1 decision tree policy is:

$$\begin{split} J(\mathcal{T}_1) &= \frac{1}{4} V_G^{\mathcal{T}_1} + \frac{2}{4} V_{S_2}^{\mathcal{T}_1} + \frac{1}{4} V_{S_1}^{\mathcal{T}_1} \\ &= \frac{1}{4} \frac{\zeta + \gamma}{1 - \gamma^2} + \frac{2}{4} (\zeta + \gamma^2 \frac{\zeta + \gamma}{1 - \gamma^2}) + \frac{1}{4} (\zeta + \gamma^2 \zeta + \gamma^4 \frac{\zeta + \gamma}{1 - \gamma^2}) \\ &= \frac{1}{4} \frac{\zeta + \gamma}{1 - \gamma^2} + \frac{2}{4} (\frac{\zeta + \gamma^3}{1 - \gamma^2}) + \frac{1}{4} (\frac{\zeta + \gamma^5}{1 - \gamma^2}) \\ &= \frac{4\zeta + \gamma + 2\gamma^3 + \gamma^5}{4(1 - \gamma^2)} \end{split}$$

**Unbalanced depth-2 decision tree :** the unbalanced depth-2 decision tree takes an information gathering action  $x \le 0.5$  then either takes the  $\downarrow$  action or takes a second information  $y \le 0.5$  followed by  $\rightarrow$  or  $\downarrow$ . In states G and  $S_2$ , the value of the unbalanced tree is the same as for the depth-1 tree. In states  $S_0$  and  $S_1$ , the policy takes two information gathering actions before taking a base

action and so on:

$$V_{S_0}^{T_u} = \zeta + \gamma \zeta + \gamma^2 0 + \gamma^3 V_G^{T_1}$$

$$V_{S_1}^{T_u} = \zeta + \gamma \zeta + \gamma^2 0 + \gamma^3 V_{S_0}^{T_u}$$

$$= \zeta + \gamma \zeta + \gamma^2 0 + \gamma^3 (\zeta + \gamma \zeta + \gamma^2 0 + \gamma^3 V_G^{T_1})$$

$$= \zeta + \gamma \zeta + \gamma^3 \zeta + \gamma^4 \zeta + \gamma^6 V_G^{T_1}$$

We get:

$$\begin{split} J(\mathcal{T}_{u}) &= \frac{1}{4}V_{G}^{\mathcal{T}_{u}} + \frac{1}{4}V_{S_{0}}^{\mathcal{T}_{u}} + \frac{1}{4}V_{S_{1}}^{\mathcal{T}_{u}} + \frac{1}{4}V_{S_{2}}^{\mathcal{T}_{u}} \\ &= \frac{1}{4}V_{G}^{\mathcal{T}_{1}} + \frac{1}{4}(\zeta + \gamma\zeta + \gamma^{3}V_{G}^{\mathcal{T}_{1}}) + \frac{1}{4}(\zeta + \gamma\zeta + \gamma^{3}\zeta + \gamma^{4}\zeta + \gamma^{6}V_{G}^{\mathcal{T}_{1}}) + \frac{1}{4}V_{S_{2}}^{\mathcal{T}_{1}} \\ &= \frac{1}{4}(\frac{\zeta + \gamma}{1 - \gamma^{2}}) + \frac{1}{4}(\frac{\gamma\zeta + \gamma^{4} + \zeta - \gamma^{2}\zeta}{1 - \gamma^{2}}) + \frac{1}{4}(\zeta + \gamma\zeta + \gamma^{3}\zeta + \gamma^{4}\zeta + \gamma^{6}V_{G}^{\mathcal{T}_{1}}) + \frac{1}{4}V_{S_{2}}^{\mathcal{T}_{1}} \\ &= \frac{1}{4}(\frac{\zeta + \gamma}{1 - \gamma^{2}}) + \frac{1}{4}(\frac{\gamma\zeta + \gamma^{4} + \zeta - \gamma^{2}\zeta}{1 - \gamma^{2}}) + \frac{1}{4}(\frac{\zeta + \gamma\zeta - \gamma^{2}\zeta - \gamma^{5}\zeta + \gamma^{6}\zeta + \gamma^{7}}{1 - \gamma^{2}}) + \frac{1}{4}V_{S_{2}}^{\mathcal{T}_{1}} \\ &= \frac{1}{4}(\frac{\zeta + \gamma}{1 - \gamma^{2}}) + \frac{1}{4}(\frac{\gamma\zeta + \gamma^{4} + \zeta - \gamma^{2}\zeta}{1 - \gamma^{2}}) + \frac{1}{4}(\frac{\zeta + \gamma\zeta - \gamma^{2}\zeta - \gamma^{5}\zeta + \gamma^{6}\zeta + \gamma^{7}}{1 - \gamma^{2}}) + \frac{1}{4}(\frac{\zeta + \gamma^{3}}{1 - \gamma^{2}}) \\ &= \frac{\zeta(4 + 2\gamma - 2\gamma^{2} - \gamma^{5} + \gamma^{6}) + \gamma + \gamma^{3} + \gamma^{4} + \gamma^{7}}{4(1 - \gamma^{2})} \end{split}$$

**The balanced depth-2 decision tree:** alternates in every state between taking the two available information gathering actions and then a base action. The value of the policy in the goal state is:

$$\begin{split} V_G^{\mathcal{T}_2} &= \zeta + \gamma \zeta + \gamma^2 + \gamma^3 \zeta + \gamma^4 \zeta + \dots \\ &= \sum_{t=0}^{\infty} \gamma^{3t} \zeta + \sum_{t=0}^{\infty} \gamma^{3t+1} \zeta + \sum_{t=0}^{\infty} \gamma^{3t+2} \\ &= \frac{\zeta}{1 - \gamma^3} + \frac{\gamma \zeta}{1 - \gamma^3} + \frac{\gamma^2}{1 - \gamma^3} \end{split}$$

2.3. Results

Following the same reasoning for other states we find the objective value for the depth-2 decision tree policy to be :

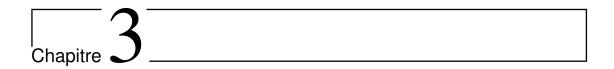
$$\begin{split} J(\mathcal{T}_2) &= \frac{1}{4} V_G^{\mathcal{T}_2} + \frac{2}{4} V_{S_2}^{\mathcal{T}_2} + \frac{1}{4} V_{S_1}^{\mathcal{T}_2} \\ &= \frac{1}{4} V_G^{\mathcal{T}_2} + \frac{2}{4} (\zeta + \gamma \zeta + \gamma^2 0 + \gamma^3 V_G^{\mathcal{T}_2}) + \frac{1}{4} (\zeta + \gamma \zeta + \gamma^2 0 + \gamma^3 \zeta + \gamma^4 \zeta + \gamma^5 0 + \gamma^6 V_G^{\mathcal{T}_2}) \\ &= \frac{\zeta (3 + 3\gamma) + \gamma^2 + \gamma^5 + \gamma^8}{4(1 - \gamma^3)} \end{split}$$

#### 2.3 Results

#### 2.3.1 Reinforcement Learning

stochastic policies

#### 2.3.2 Asymmetric RL



## Conclusion

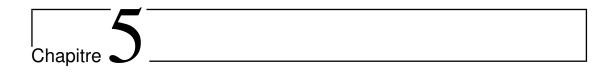
3.1 What happens when the MDP's transitions are independent of the current state?

# Deuxième partie

# An easier problem : Learning Decision Trees for MDPs that are Classification tasks

Chapitre 4

## DPDT-intro



# DPDT-paper

Chapitre 6

# Conclusion

# Troisième partie

Beyond Decision Trees: what can be done with other Interpretable Policies?

# Conclusion générale

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## Programmes informatiques

Les listings suivants sont au cœur de notre travail.

Listing A.1 – Il est l'heure

```
#include <stdio.h>
 int heures, minutes, secondes;
2
3
4
 5
6
          print_heure
                                 * /
7
 / *
                                 * /
8
    But:
 /*
9
      Imprime 1'heure
10
           _____*
11
  /*___Interface:_____*/
12
  /*___Utilise_les_variables_globales_____*/
13
  /*____heures,_minutes,_secondes_____*/
14
  /*_____*/
15
16
17
  void_print_heure(void)
18
  19
  20
21
 __printf("_%d_minute", minutes);
 """ if " (minutes" > "1) "printf("s");
22
23
 24 \__if_(secondes_>_1)_printf("s");
```

```
25 | Listing A.2 - Factorielle

1 | int factorielle(int n)
2 | {
3 | if (n > 2) return n * factorielle(n - 1);
4 | return n;
5 | }
```

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