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Fluents valuation in Deep Reinforcement Learning agents for non-Markovian goals

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Nomenclature

AFW	Alternating Automaton on finite Words, page 14
DFA	Deterministic Finite-state Automaton, page 15
DGM	Directed Graphical Model, page 18
DQN	Deep Q-Network algorithm, page 24
FOL	First-Order Logic, page 8
LDL_f	Linear Dynamic Logic of finite traces, page 11
LTL	Linear Temporal Logic, page 7
LTL_f	Linear Temporal Logic of finite traces, page 8
MDP	Markov Decision Process, page 17
MSO	Monadic Second-Order Logic, page 8
NFA	Nondeterministic Finite-state Automaton, page 14
NMRDP	Non-Markovian Reward Decision Process, page 30
NN	Neural Network, page 23
NNF	Negation Normal Form, page 15
PDL	Propositional Dynamic Logic, page 8
POMDP	Partially Observable Markov Decision Process, page 27
RL	Reinforcement Learning, page 17
SGD	Stochastic Gradient Descent algorithm, page 24

Chapter 1

Introduction

A classic and important branch of Artificial Intelligence (AI) aims at developing agents that select their actions through a form of logic reasoning, such as planning. One of the main advantages of these approaches is that reasoning proceeds by manipulating *abstractions*. In fact, in logic, we can define symbols that represent any meaningful event or condition that should be considered. For example, some propositional symbols might represent conditions such as “the door is closed” or “I am holding an object”, etc. We’ll also call these propositional symbols with the term “*fluents*” (a name that suggests how their truth can change over time).

These reasoning methods based on logics are powerful but they imply one fundamental ability: at each instant, the agent must be able to decide whether those propositions are true. This means that all symbols that represent conditions which happen to be true in the environment, must be true for the agent. This “grounding” process can be really hard in complex environments, because the agent’s sensors may return a noisy and multidimensional output, that is difficult to interpret.

Reinforcement Learning (RL) is a successful field of AI, in which the agent’s goal is to learn a policy that maximizes the rewards received. We could argue that RL does not require the valuations just mentioned. Still, rewards and punishments must be somehow supplied in response to desirable and undesirable events. We could consider of providing these feedbacks with programmed ad-hoc conditions, but this can be easily done just for the simulations we create. Furthermore, as we will see, complex and non-Markovian tasks can only be solved through a combination of both RL and logic-based methods; thus, introducing all the needs of the latter.

With this thesis, we defined and implemented an agent based on temporal logics and Deep Reinforcement Learning. This required to investigate new ways to solve the fluents valuation problem that has been just described, for a specific class of environments and fluents. In Section 1.2, the goal and the achievements of this work will be described more precisely.

1.1 Related works

Reinforcement Learning (RL) is an area of Machine Learning in which the agent is trained by sending rewards and punishments in response to its actions. This technique can be also used in unknown environments, where a model of the dynamics is not available, because the agent learns by trying all actions and by remembering those that lead to the highest rewards. As we will see in Chapter 3, most RL algorithms assume that the environment can be modelled with a Markov Decision Process (MDP). Many learning algorithms exist in this setting [22].

Neural Networks (NN) have brought new possibilities for RL: in Deep Reinforcement Learning (Deep RL), the agent employs a neural network as a very expressive function approximator for the quantities it is trying to learn [9]. For example, the optimal q-value is an important quantity in RL, that the agents are usually designed to learn from the observations received. The Deep Q-Network (DQN) algorithm [17] is one of the first to successfully employ neural networks in RL. They have shown that a Deep RL agent can be trained directly from complex observations such as the frames of a video game. Without any modification, the same agent has been able to learn and reach human-level performances in many of these games.

Games have always been a classic benchmark for AI algorithms, because they provide various levels of complexity, they have few and strict rules, and they are easy to implement and simulate. Regarding Deep RL, many authors have tested their algorithms on the collection of video games “Atari 2600” [2]. In this thesis, we’ll use and experiment with the same environments.

The reinforcement learning algorithm we’ve adopted is called Double DQN [25]. The motivation of this choice is that this is a relatively simple algorithm, based on DQN, which has also proven to be successful for the specific environments that we’ll use in our experiments [16]. In fact, among Q-Network algorithms, the only ones that were able to clearly achieve superior performances in most of these games combined many of the others DQN variants [12].

If we look at the results in [16], DQN agents are able to learn excellent policies for many games. However, for many other environments of the same collection, the agents struggle to learn and, in some cases, it doesn’t learn anything at all. The worst performances have been measured for the *Montezuma’s Revenge* environment. Even in the works that followed, the only methods that were able to achieve good policies in this game adopted some form of expert imitation and manual restarts [15]. In Section 3.3, we’ll investigate the main cause of these difficulties.

As we will see throughout this thesis, a promising solution for these environments is the construction provided in [3] and [5]. The former work [3] has shown that a Non-Markovian Reward Decision Process (NMRDP) can be easily declared with

linear-time temporal logics, and it has provided a translation from this NMRDP to a classic MDP. The logics they used are LTL_f and LDL_f . This idea was initially introduced in [1] for a linear temporal logic of the past. The latter work [5], instead, has shown that through a similar construction, it's possible to influence the agent's optimal behaviour by declaring additional non-Markovian rewards that are learnt in conjunction with the original rewards. This paper named this additional module with "Restraining Bolt". Thorough this thesis, it may be practical to use this name to refer to this logic construction.

1.2 Objective and results

This work started with the following goal: defining and implementing a Deep RL agent that, through the Restraining Bolt, is able to achieve non-Markovian tasks. This first objective has been accomplished, but the Restrained Bolt is a method based on logic, and, as we’ve already anticipated in this introduction, it requires to correctly value the fluents we define. Since the environments adopted in Deep RL have much more complex observation spaces, it has been necessary to investigate new ways to solve the problem of the fluents valuation, at least for a specific class of fluents and observations.

Thus, it is possible to isolate two groups of contributions of this thesis: those concerning the definition of a Deep RL agent for non-Markovian goals, and those related to methods for learning the fluents’ valuation function. Regarding the former, in this thesis:

- We provide a flexible implementation of the Restraining Bolt method, described in [5] and [3].
- We proposed a neural network architecture for a Deep RL agent that allowed to successfully employ the Restraining Bolt also in Deep Reinforcement Learning.
- Tests have been conducted in a video game called *Montezuma’s Revenge*, the hardest game (for a RL agent) in the Atari 2600 collection [16]. We’ve shown that the agent can be successfully guided through the initial room of the game, with low manual intervention.

The latter topic, instead, received much attention in this thesis: how is it possible to learn a function that, given an observation of the environment, predicts whether the fluents we have defined are true? As we may recognise, this problem is really general, and we must restrict to a specific class of fluents and observations. Observations will be frames of the Atari games, and fluents will be propositions decidable from a single frame. Every choice or assumption that further restricts the applicability of the proposed method will be pointed out along the text. Still, there are some interesting achievements of this work that are to be highlighted:

- We don’t manually assign a meaning to some Boolean features. Instead, this is an initial investigation about how to proceed in the opposite direction: we first define a set of symbols, then we learn their valuation function.
- We adopt the temporal logic LDL_f as a formalism to define some temporal constraints that our fluents are always expected to satisfy. Candidate valuation functions will be checked against these constraints.

- The training algorithm won't require any manual annotation, nor labelled datasets at all.
- We propose an architecture, based on Deep Belief Networks, that by reducing the input space dimensionality, binds the valuations to some visual features that are recognizable in the image.

All these ideas have been implemented in a Python software and tested on games of the Atari collection.

Finally, we also strongly contributed to the development of the `f1loat` package [6], a Python software for the conversion of LTL_f and LDL_f formulae to the associated automaton (NFA or DFA).

1.3 Structure of the thesis

The rest of this thesis is structured as follows:

2 – Temporal logics and Linear Dynamic Logic

Temporal logics are an important formalism for this work and will be used throughout the text. This chapter introduces the reader to concepts such as: fluents, traces and linear-time temporal logics. Then, we will define the Linear Dynamic Logic (LDL_f), that is the specific temporal logic used in this text.

3 – Deep Reinforcement Learning for non-Markovian goals

In this chapter, we will see how to design Deep RL agents able to achieve non-Markovian goals. In Sections 3.1 and 3.2 we thoroughly explain the basic concepts behind RL and Deep RL. Then, in Section 3.3, we will analyze what happens when the most common assumptions of RL (and of Deep RL) are falsified. A solution for these complex RL problems will be presented in Section 3.4, where we illustrate the Restraining Bolt method. This chapter ends with Section 3.5, where we propose an original model that allows to apply the previous solution also in the context of Deep RL.

4 – Learning to value fluents in games

In this important chapter we propose a model for the valuation function of the fluents. We'll also propose a training algorithm for this model that doesn't require labelled datasets at all.

5 – AtariEyes package

This chapter presents the software that implements all the concepts presented in the previous chapters. We will first review its features and its functionality from a user perspective, then the most interesting implementation details will follow.

6 – Experiments

This chapter contains experiments and training outcomes in two Atari games. The experiments will be finalized to test: the effectiveness of the proposed method for learning the valuation functions; the capabilities of the “restrained” Deep RL agents.

7 – Conclusions and future work

In this final chapter, we draw the main conclusions that can be derived from this work, the strength of this approach and its weakness, and all the possibilities for improvement.

Chapter 2

Temporal logics and Linear Dynamic Logic

2.1 Temporal logics on finite traces

Temporal logics are a class of formal languages, more precisely modal logics, that allow to talk about properties and events over time [10]. Among all formalisms, we care about logics that assume a linear time, as opposed to branching, and a discrete sequence of instants, instead of continuous time. In computer science, the most famous logic in this group is the Pnueli's Linear Temporal Logic (LTL) [19].

The assumptions about the nature of time directly reflect to the type of structures these logics are interpreted on: their models are tuples $\mathcal{M} = \langle T, \prec, V \rangle$, where T is a discrete set of time instants, such as \mathbb{N} , \prec is a complete ordering relation on T , like $<$, and V is a valuation function $V : T \times \mathcal{F} \rightarrow \{true, false\}$. For a logic that defines a set \mathcal{F} of proposition symbols, the function V assigns a truth value to each of them, in every instant of time. The symbols in \mathcal{F} represent atomic propositions which may or may not hold in different time instants. They are also called “fluents” (or simply propositional symbols, in this thesis). An equivalent and compact way of defining such structures is with *traces*. A trace π is a sequence $\pi_0\pi_1 \dots \pi_n$, where each element is a propositional interpretation of the fluents \mathcal{F} . Each symbol π_i in the sequence is the set of true symbols at time i : $\pi_i \in 2^{\mathcal{F}}$. The i -th element is also denoted with $\pi(i)$. $\pi(i, j)$ represents the trace between instants i and j : $\pi_i, \pi_{i+1}, \dots, \pi_{j-1}$.

LTL is a logic that only allows to talk about the future. The semantics of its temporal operators, neXt \circ , Until \mathcal{U} , and of those derived, eventually \Diamond , always \Box , can only access future instants on the sequence. Interpretations for this logic are infinite traces with a first instant, which are equivalent to valuations on the temporal frame $\langle \mathbb{N}, < \rangle$.

As it has been pointed out in [4], most practical uses of LTL interpret the formulae on *finite* traces, not infinite. The pure existence of a last instant of time has strong consequences on the meaning of all formulae, because operators semantics need to handle such instant differently. For example, the “always” operator \Box translates to “until the last instant”, quite naturally. However, the formula $\Box\Diamond\varphi$ no longer requires that φ becomes true an infinite number of times (in LTL, this formula represents the “response” property); instead, it is satisfied exactly by those traces in which φ is true at the last instant. So, it assumes a completely different meaning. Furthermore, both $\Box\Diamond\varphi$ and $\Diamond\Box\varphi$ become equivalent to $\Diamond(\text{Last} \wedge \varphi)$: something that doesn’t happen in standard LTL¹. From this example, it should be clear that the expressive power of the language has changed, and LTL interpreted over finite traces should be regarded as a different logic, that we will denote with LTL_f . More precisely, over infinite linearly-ordered interpretations, LTL has the same expressive power of Monadic Second Order Logic (MSO), while LTL_f is equivalent to First-Order Logic (FOL) and star-free regular expressions, which are strictly less expressive than MSO.

In the next section, we will define a temporal logic, called LDL_f , that was purposefully devised to be interpreted over finite traces. This is the formalism that we will use, in Section 3.4, to declare plans and desired behaviours. However, many useful temporal properties can be also expressed with LTL_f . So, one may also use as alternative formalisms LTL_f or any temporal logic over finite traces that can be translated to equivalent finite-state automata; even temporal logics of the past [1].

In Section 2.3, we will define the Linear Dynamic Logic of finite traces (LDL_f) [4]. Its syntax combines regular expressions and propositional logic, just like Propositional Dynamic Logic (PDL) does [8][24]. So, we will review regular expressions first.

¹*Last* is an abbreviation for $\neg\bigcirc\text{true}$ and it evaluates to true at last instant only. So, $\Diamond(\text{Last} \wedge \varphi)$ means: eventually, at the last instant, φ is true.

2.2 Regular Temporal Specifications

Regular languages are the class of languages exactly recognized by finite state automata and regular expressions [13]. So, we will use regular expressions as a compact formalism to specify them. Regular expressions are usually said to accept strings. Traces are in fact strings, whose symbols $s \in 2^{\mathcal{F}}$ are propositional interpretations of the fluents \mathcal{F} . Such regular expressions would be:

$$\rho ::= \emptyset \mid s \mid \rho_1 + \rho_2 \mid \rho_1; \rho_2 \mid \rho^* \quad (2.1)$$

where \emptyset denotes the empty language, $s \in 2^{\mathcal{F}}$ is a symbol, $+$ is the disjunction of two constraints, $;$ concatenates two expressions, and ρ^* requires an arbitrary repetition on ρ . Parentheses can be used to group expressions with any precedence. Regular expressions are a basic formalism in computer science and they won't be covered here. The notable difference, though, is that the symbols found in the trace, hence of the regular expression, are propositional interpretations (i.e. sets of true fluents).

Example 1. Briefly, the regular expression $\rho := (\{A\}^* + \{B\}^*); \{\}$ accepts the following traces:

$$\begin{aligned} \pi_a &:= \langle \{A\}, \{A\}, \{A\}, \{\} \rangle \\ \pi_b &:= \langle \{B\}, \{\} \rangle \\ \pi_c &:= \langle \{\} \rangle \end{aligned}$$

but not $\pi_d := \langle \{A, B\} \rangle$.

We call the regular expressions of equation (2.1) Regular Temporal Specifications RE_f , because they are interpreted on finite linear temporal structures. Unfortunately, writing specifications in terms of single interpretations can be very cumbersome, as we lack a construct for negation and all sets need to match exactly. Instead, we can substitute the symbols $s \in 2^{\mathcal{F}}$ with formulae of Propositional Logic. In fact, a propositional formula ϕ concisely represents all interpretations that satisfy it: $\text{Sat}(\phi) := \{s \in 2^{\mathcal{F}} \mid s \models \phi\}$.

The new definition for the syntax of Regular Temporal Specifications RE_f is:

$$\rho ::= \phi \mid \rho_1 + \rho_2 \mid \rho_1; \rho_2 \mid \rho^* \quad (2.2)$$

where ϕ is a propositional formula on the set of atomic symbols \mathcal{F} . The language generated by a RE_f ρ , denoted $\mathcal{L}(\rho)$, is the set of traces that match the temporal specification. The only difference with regular expressions standard semantics is

that a symbol $s \in 2^{\mathcal{F}}$ matches a propositional formula ϕ if and only if $s \in \text{Sat}(\phi)$. A trace that match the regular expression $\pi \in \mathcal{L}(\rho)$ is said to be generated or accepted by the specification ρ .

Example 2. As an example, let's define a RE_f expression $\rho := \text{true}; (\neg B)^*; (A \wedge B)$ and the following traces:

$$\pi_a := \langle \{\}, \{A\}, \{A\}, \{A, B\} \rangle$$

$$\pi_b := \langle \{B\}, \{A, B\} \rangle$$

$$\pi_c := \langle \{A, B\}, \{B\}, \{B\} \rangle$$

The first two traces are accepted by the expression, $\pi_a, \pi_b \in \mathcal{L}(\rho)$, but the third is not, $\pi_c \notin \mathcal{L}(\rho)$. Of course, the symbols A and B may represent any meaningful property of the environment that we may want to ensure at some time instants.

2.3 Linear Dynamic Logic

2.3.1 Definition

We can now move on to the *Linear Dynamic Logic of finite traces* (LDL_f). This logic was first defined in [4]. The definition we see here, also adopted in this thesis, is a small variant that can also be interpreted over the empty trace, $\pi_\epsilon = \langle \rangle$, unlike most logics, which assume a non-empty temporal domain T . This definition appears in [3].

Definition 1. A LDL_f formula φ is built as follows:

$$\begin{aligned}\varphi &::= tt \mid \neg\varphi \mid \varphi_1 \wedge \varphi_2 \mid \langle \rho \rangle \varphi \\ \rho &::= \phi \mid \varphi? \mid \rho_1 + \rho_2 \mid \rho_1; \rho_2 \mid \rho^*\end{aligned}\tag{2.3}$$

where tt is a constant that stands for logical true and ϕ is a propositional formula over a set of symbols \mathcal{F} . We also define the following abbreviations:

$$\begin{aligned}ff &:= \neg tt & [\rho]\varphi &:= \neg \langle \rho \rangle \neg \varphi & \phi &:= \langle \phi \rangle tt \\ End &:= [true]ff & Last &:= \langle true \rangle End\end{aligned}$$

together with all those of propositional logic, which are all to be considered part of the language.

The syntax just defined is really similar to PDL [8], a well known and successful formalism in Computer Science for describing states and events of programs. However, LDL_f formulae are interpreted over finite traces instead of Labelled Transition Systems.

Example 3. All the following formulae are all well-formed:

$$\begin{aligned}A \vee \neg B \\ \langle A; B^* \rangle (A \wedge B) \\ [true^*] \neg C \\ [A^*] \langle \neg B \rangle tt \wedge [true^*; C]ff \\ [A?; B]B\end{aligned}$$

Instead, these are not:

$$\langle tt \rangle A \quad \langle A \rangle \quad [A]B [A]B \quad B?$$

Before moving to the semantics, we can intuitively understand the meaning of these constructs. A LDL_f formula φ is a combination of temporal expressions,

$\langle \rho \rangle, [\rho]$, and propositional formulae. The former are modal expressions that allow to make statements that refer to future instants. $\langle \rho \rangle \varphi$ states that, from the current step i , there exists a future instant j , such that the path $\pi(i, j)$ is accepted by the $\text{RE}_f \rho$, and φ is satisfied at step j . Essentially, as in PDL, regular expressions are used to select some future states in which the formulae that follow should hold. Similarly, $[\rho] \varphi$ states that, from the current step, all executions satisfying ρ are such that their last instant satisfy φ . There is a clear similarity between $\langle \rangle, []$ operators and \exists, \forall from first-order logic, because we defined them to obey a similar relation to the De Morgan rule. In fact, if we consider the set S_ρ of future instants that are selected by a regular expression ρ , $\langle \rho \rangle$ can be read as “*there exists* one instant in S_ρ such that ...”, and $[\rho]$ is read as “*for all* instants in S_ρ ...”.

The LDL_f semantics is defined in terms of finite traces. We denote with $|\pi|$ the length of the trace π , i.e. the total number of time instants. Also, for non-empty traces, *last* refers to the index of the last instant in the sequence: $\text{last} := |\pi| - 1$.

Definition 2. Given a finite trace π , we inductively define when a LDL_f formula φ is true in π at time i , in symbols $\pi, i \models \varphi$, as follows:

$$\begin{aligned}
& \pi, i \models tt \\
& \pi, i \models \neg \varphi \quad \text{iff} \quad \pi, i \not\models \varphi \\
& \pi, i \models \varphi_1 \wedge \varphi_2 \quad \text{iff} \quad \pi, i \models \varphi_1 \quad \text{and} \quad \pi, i \models \varphi_2 \\
& \pi, i \models \langle \phi \rangle \varphi \quad \text{iff} \quad i < |\pi| \quad \text{and} \quad \pi(i) \models \phi \quad \text{and} \quad \pi, i+1 \models \varphi \\
& \quad \text{(for a propositional formula } \phi) \\
& \pi, i \models \langle \rho_1 + \rho_2 \rangle \varphi \quad \text{iff} \quad \pi, i \models \langle \rho_1 \rangle \varphi \vee \langle \rho_2 \rangle \varphi \\
& \pi, i \models \langle \rho_1; \rho_2 \rangle \varphi \quad \text{iff} \quad \pi, i \models \langle \rho_1 \rangle \langle \rho_2 \rangle \varphi \\
& \pi, i \models \langle \psi? \rangle \varphi \quad \text{iff} \quad \pi, i \models \psi \quad \text{and} \quad \pi, i \models \varphi \\
& \pi, i \models \langle \rho^* \rangle \varphi \quad \text{iff} \quad \pi, i \models \varphi \quad \text{or} \\
& \quad i < |\pi| \quad \text{and} \quad \pi, i \models \langle \rho \rangle \langle \rho^* \rangle \varphi \quad \text{and} \quad \rho \text{ is not test-only}
\end{aligned}$$

We say that ρ is test-only if it is a RE_f whose atoms are only tests $\psi?$.

Definition 3. A LDL_f formula φ is *true* in (or, is satisfied by) a trace π , written $\pi \models \varphi$, if $\pi, 0 \models \varphi$.

Definition 4. A LDL_f formula φ is *satisfiable* if there exists a trace that satisfy it; it is *valid* if it is true in every trace. A formula φ logically implies a formula φ' , in notation $\varphi \models \varphi'$, if for every trace π , we have that $\pi \models \varphi$ implies $\pi \models \varphi'$.

Example 4. We'll now list few examples that may help to better understand the

semantics just defined. Given the following trace,

$$\pi_a := \langle \{A\}, \{A\}, \{A, B\} \rangle$$

we have²:

$$\begin{array}{ll} \pi_a, 2 \models A \wedge B & \pi_a, 1 \not\models B \\ \pi_a \models \langle A^* \rangle (A \wedge B) & \pi_a \not\models [A^*]B \\ \pi_a \models [(\neg B)^*]A & \pi_a \not\models \langle A; B \rangle tt \end{array}$$

Now that the fundamental mechanics are clear, we can highlight some peculiarities of the language:

- The test operator “?” is typical of PDL. In the middle of a RE_f computation, I can check whether a condition is verified before moving on. As we can see from Definition 1, the condition is a full LDL_f formula; so it acts as a powerful look-ahead operation.
- The two expressions *true* and *tt* may mistakenly look equivalent at first sight. Instead, *tt* is an atomic formula that is *always* satisfied (it evaluates to logical true); while *true* is a propositional formula and, as such, it is an abbreviation for $\langle \text{true} \rangle tt$. The latter is satisfied if and only if there exists at least one next instant in the trace.
- According to the semantics of $\langle \phi \rangle \varphi$, if we evaluate this formula on the last instant of a trace, φ needs to be verified at step *last* + 1. This is fine, indeed. As the truth of $\pi, i \models \varphi$, with $i \geq |\pi|$, is perfectly defined in LDL_f (and it’s equivalent to $\langle \rangle \models \varphi$).

The last observation has some profound consequences that we should consider when writing the formulae. Let’s suppose we want to encode that *A* must always hold, just like the LTL_f sentence “always *A*”, $\Box A$. The LDL_f formula $[true^*]A$ doesn’t represent this concept; instead, it is unsatisfiable. What we’re actually saying is that at each point of the trace, even at the end, *A* must follow; which is impossible. What we meant is $[true^*](A \vee \text{End})$, or $[true^*; (\neg \text{End})?]A$.

In [4] (De Giacomo and Vardi) some important theorems have been established for LDL_f ³:

²We shouldn’t get confused about the different uses of the angle brackets: in $\langle \{A\}, \{A, B\} \rangle$, they delimit a sequence of sets (that is a trace); in the formula $\langle A^*; true \rangle B$, instead, they represent the temporal operator containing a regular temporal specification.

³The following theorems have been proved in [4] for the original definition of LDL_f , which is slightly different. The same results are valid for the empty trace variant presented here.

Theorem 1. *LTL_f and RE_f formulae can be translated to LDL_f in linear time.*

Theorem 2. *LDL_f has the same expressive power of MSO (Monadic Second-Order logic) over finite traces.*

Theorem 3. *Satisfiability, validity and logical implication for LDL_f formulae are PSPACE-complete.*

2.3.2 Automaton translation

Automata are a well-established common formalism for talking about languages. The set of traces that satisfy a formula form a language, in fact. What we're looking for is an equivalent automaton \mathcal{A}_φ that accepts exactly the same traces that satisfy a given LDL_f formula φ . As we will see, this translation is indeed possible, because to every LDL_f formula, it can be associated an equivalent alternating automaton on finite words. We assume the reader is acquainted with basic automata theory, such as DFAs, NFAs [13].

Alternating automaton

Definition 5. An *Alternating Automaton on finite Words* (AFW) is a tuple $\mathcal{A} := \langle \Sigma, Q, q_0, \delta, F \rangle$, where Σ is a finite nonempty alphabet, Q is a finite nonempty set of states, $q_0 \in Q$ is the initial state, $F \subseteq Q$ is a set of final states, and $\delta : Q \times \Sigma \rightarrow \mathcal{B}^+(Q)$ is the transition function. $\mathcal{B}^+(Q)$ denotes the set of all positive boolean functions composed from the set of atoms Q , together with *true* and *false*.

Let's define a word $w := \sigma w'$, with $\sigma \in \Sigma$ and $w' \in \Sigma^*$. In a *Nondeterministic Finite-state Automaton* (NFA), a transition $\delta(q_0, \sigma) = \{q_1, q_2, q_3\}$ means that input word, w , is accepted iff w' is accepted by *any* of the runs continuing from q_1 , q_2 , or q_3 (a run accepts if it ends up in a final state). We could also write this transition as $\delta(q_0, \sigma) = (q_1 \vee q_2 \vee q_3)$, because the agent can “choose” among these states. The dual operation is to require that *all* the following runs needs to be accepting: $\delta(q_0, \sigma) = (q_1 \wedge q_2 \wedge q_3)$. The transition function of an AFW adopts boolean functions without negations to allow both conjunctions and disjunctions. For example, we may write $\delta(q_0, \sigma) = q_1 \wedge (q_2 \vee q_3)$. Due to conjunctions, the AFW is usually thought to be in multiple states at the same time. An AFW, \mathcal{A} , accepts a word w iff there exists a run of \mathcal{A} on w such that all the current states at the end of the computation are either final or are labelled with *true*⁴. For a more precise description of runs and acceptance condition of AFWs, see [26].

⁴ $\delta(q, \sigma) = \text{true}$ can be considered as an empty conjunction of states: this branch of the computation accepts without the need of further tests.

Surprisingly, alternating automata have the same expressive power as NFA, but they are exponentially more succinct. So, it is possible to transform any AFW to an equivalent NFA that has an exponentially bigger state space. Therefore, we can also build an equivalent *Deterministic Finite-state Automaton* (DFA) through a double exponential transformation. The AFW-to-NFA transformation is provided in [26].

Delta function

In this section, given a LDL_f formula φ , we define its associated AFW, $\mathcal{A}_\varphi := \langle \Sigma, Q, q_0, \delta, F \rangle$. The alphabet, $\Sigma := 2^{\mathcal{F}}$, is the set of all propositional interpretations for the fluents \mathcal{F} (we will indicate them with $\Pi \in \Sigma$). It will be handy to use LDL_f formulae to refer to the states $q \in Q$: each formula will be an (implicitly quoted) identifier for a state. Formally, the set Q is the Fisher-Ladner closure of φ extended with two special constructs, but we don't need to define it explicitly. The initial state is $q_0 := \varphi$. The set of final states is empty, $F := \{\}$, so acceptance can only be ensured by reaching *true*. We now assume that the formula φ has been already transformed in Negation Normal Form (NNF), through a function $\text{nnf}(\cdot)$. A formula is in NNF if negations only appear in front of atomic propositions. We can finally define the transition function, also called the *delta function*, as:

$$\begin{aligned}
\delta(tt, \Pi) &= \text{true} \\
\delta(ff, \Pi) &= \text{false} \\
\delta(\phi, \Pi) &= \delta(\langle \phi \rangle tt, \Pi) \quad (\phi \text{ propositional}) \\
\delta(\varphi_1 \wedge \varphi_2, \Pi) &= \delta(\varphi_1, \Pi) \wedge \delta(\varphi_2, \Pi) \\
\delta(\varphi_1 \vee \varphi_2, \Pi) &= \delta(\varphi_1, \Pi) \vee \delta(\varphi_2, \Pi) \\
\delta(\langle \phi \rangle \varphi, \Pi) &= \begin{cases} \mathbf{E}(\varphi) & \text{if } \Pi \models \phi \\ \text{false} & \text{if } \Pi \not\models \phi \end{cases} \quad (\phi \text{ propositional}) \\
\delta(\langle \psi? \rangle \varphi, \Pi) &= \delta(\psi, \Pi) \wedge \delta(\varphi, \Pi) \\
\delta(\langle \rho_1 + \rho_2 \rangle \varphi, \Pi) &= \delta(\langle \rho_1 \rangle \varphi, \Pi) \vee \delta(\langle \rho_2 \rangle \varphi, \Pi) \\
\delta(\langle \rho_1; \rho_2 \rangle \varphi, \Pi) &= \delta(\langle \rho_1 \rangle \langle \rho_2 \rangle \varphi, \Pi) \\
\delta(\langle \rho^* \rangle \varphi, \Pi) &= \delta(\varphi, \Pi) \vee \delta(\langle \rho \rangle \mathbf{F}_{\langle \rho^* \rangle} \varphi, \Pi) \\
\delta([\phi] \varphi, \Pi) &= \begin{cases} \mathbf{E}(\varphi) & \text{if } \Pi \models \phi \\ \text{true} & \text{if } \Pi \not\models \phi \end{cases} \quad (\phi \text{ propositional}) \\
\delta([\psi?] \varphi, \Pi) &= \delta(\text{nnf}(\neg \psi), \Pi) \vee \delta(\varphi, \Pi) \\
\delta([\rho_1 + \rho_2] \varphi, \Pi) &= \delta([\rho_1] \varphi, \Pi) \wedge \delta([\rho_2] \varphi, \Pi) \\
\delta([\rho_1; \rho_2] \varphi, \Pi) &= \delta([\rho_1][\rho_2] \varphi, \Pi)
\end{aligned} \tag{2.4}$$

$$\begin{aligned}
\delta([\rho^*]\varphi, \Pi) &= \delta(\varphi, \Pi) \wedge \delta([\rho]\mathbf{T}_{[\rho^*]\varphi}, \Pi) \\
\delta(\mathbf{F}_\varphi, \Pi) &= \text{false} \\
\delta(\mathbf{T}_\varphi, \Pi) &= \text{true}
\end{aligned}$$

where $\mathbf{E}(\varphi)$ recursively replaces in φ all occurrences of atoms of the form \mathbf{T}_ψ and \mathbf{F}_ψ by $\mathbf{E}(\psi)$; and $\delta(\varphi, \epsilon)$ is defined inductively as above, except for the following base cases:

$$\delta(\langle \phi \rangle \varphi, \epsilon) = \text{false} \quad \delta([\phi]\varphi, \epsilon) = \text{true} \quad (\phi \text{ propositional})$$

The role of \mathbf{T}_φ and \mathbf{F}_φ is to evaluate as *true/false* or as φ depending on the context. This allows to respect the “test-only” requirement in Definition 2 for the star operator.

Let φ be an LDL_f formula and \mathcal{A}_φ the corresponding AFW of equation 2.4. Then, for every trace π , we have that $\pi \models \varphi$ if and only if \mathcal{A}_φ accepts π . Also, the space-size of \mathcal{A}_φ is linear in the size of φ . Since the emptiness problem for AFWs is PSPACE-complete, we get a proof for Theorem 3 on page 14.

DFA are the easiest automata to visualize and simulate. A LDL_f formula can be translated to an equivalent DFA through the following transformations: $\text{LDL}_f \rightarrow \text{AFW} \rightarrow \text{NFA} \rightarrow \text{DFA}$. Although the asymptotic worst-case cost of this algorithm is already the best known (which doubly-exponential on the size of the formula), it is possible to combine some or all of these steps in a single algorithm, that may allow some optimizations. A LDL_f -to-NFA algorithm is presented in [3]; while a LDL_f -to-DFA is described in [7].

Chapter 3

Deep Reinforcement Learning for non-Markovian goals

3.1 Reinforcement Learning

In this section, we will briefly review the most important aspects of classic *Reinforcement Learning* (RL). These concepts are relevant because they are also found in Deep Reinforcement Learning (Deep RL), which is a central component of the agent we will design. Excellent references for these topics are [22], [21], and [18] for graphical models.

In AI, we commonly isolate two entities, the agent and the environment, which continuously interact. At each instant, the agent receives observations from the environment and it executes actions in response. In RL specifically, the agent observes the current state of the environment and a numerical reward. The environment produces high rewards in response to desirable events. The agent's goal is to maximize the rewards received. The basic setup is illustrated in Figure 3.1.

3.1.1 Markov Decision Processes

Most RL algorithms assume that the environment dynamics can be modelled with a *Markov Decision Process* (MDP). They do so, because under the independence

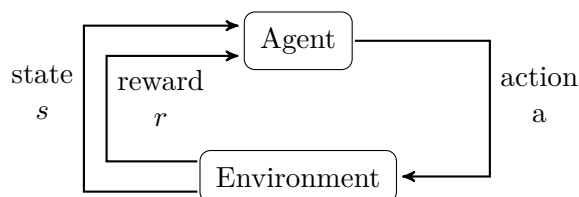


Figure 3.1. How agent and environment interact in RL.

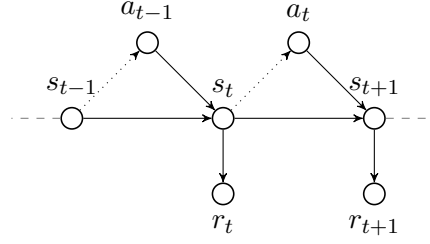


Figure 3.2. The directed graphical model of an MDP.

assumptions taken by MDP, it's possible to efficiently find the optimal agent's policy.

Definition 6. A Markov Decision Process is a tuple $\langle S, A, T, R, \gamma \rangle$, where: S is the set of states of the environment; A is the action space; $T : S \times A \times S \rightarrow \mathbb{R}$ is the transition function, which, for $T(s_t, a_t, s_{t+1})$, returns the probability $p(s_{t+1} \mid s_t, a_t)$ of the transition $s_t \xrightarrow{a_t} s_{t+1}$; $R : S \times A \times S \rightarrow \mathbb{R}$ is the reward function; and $\gamma \in [0, 1]$ is called “discount factor”¹.

In a RL problem, the functions T and R are unknown. The agent can only learn them by taking each action and observing the outcomes. Even if they are unknown, by assuming that they can be modelled with functions $S \times A \times S \rightarrow \mathbb{R}$, we introduce some Markov assumptions. In particular, we assume that the next state of the environment is conditionally independent on the whole history, given the previous state and action: $s_{t+1} \perp s_0, \dots, s_{t-1} \mid s_t, a_t$. Similarly, the reward only depends on the last transition of the environment. Although it's not required by the model, it is common that rewards are computed just from desirable configurations of the environment s_t , not from specific transitions (s_{t-1}, a_{t-1}, s_t) . All these assumptions are summarized in the Directed Graphical Model (DGM) of Figure 3.2. In a DGM, edges indicate direct conditional probabilities, while missing arcs indicate conditionally independent variables. In Figure 3.2, the lack of any arrow between s_{t-1} and s_{t+1} means that future states, hence the rewards, do not depend on the past history, given the current state s_t . This is the essence of a Markov assumption.

Example 5. Tic-Tac-Toe, Chess and many other board games can be modelled with an MDP. Even games with dice, such as Backgammon. To do so, we define as state space S the set of configurations of the board, and a reward function $R(s)$ that returns 1, if the configuration s is a win, -1 for a loss, and 0 otherwise. Even though most games are deterministic, the presence of an opponent makes the transition function T of the MDP nondeterministic. What these games have in common, is that the player gets to see the complete state of the game, which is the current

¹In this chapter, variables with an integer subscript or index refer to the value at the discrete time indicated.

configuration of the board. Future states of the game and rewards only depend on the current situation, not on the whole play. In Chess, for example, we can determine whether a configuration is a win or loss just by looking for a checkmate; there is no need to ask the players how the game has been carried out.

Proving that Markovian T and R exist is easy for board games, because the rules of the game define them. As we will see in Section 3.3, when T is unknown, as always happens in the real-world, it's much more difficult to prove that we're in fact facing an MDP.

3.1.2 Optimal policies

The *policy* is the criterion the agent uses to select the actions to perform. If the environment dynamics can be modelled with an MDP, the optimal action at time t only depends on s_t . So, there must exist an optimal policy as $\rho_* : S \rightarrow A$. However, due to common estimation errors, it is always better to prefer nondeterministic policies, which return a probability distribution over the actions. The action at time t will be sampled according to $a_t \sim \rho(s_t)$. This dependency is represented by the dotted arrows of Figure 3.2. A policy that is a function only of the state is called “stationary”.

We will now introduce few basic quantities of RL that serve to define what it means for an action or a policy to be optimal. The *discounted return* G is the combination of all rewards collected:

$$G := r_0 + \gamma r_1 + \gamma^2 r_2 + \cdots = \sum_{t=0}^T \gamma^t r_t \quad (3.1)$$

The discount factor, $0 \leq \gamma \leq 1$, decides the relative importance of immediate and future rewards. Usually, this factor is strictly less than 1 because this stimulates the agent to achieve rewards as soon as possible. It also produces a finite discounted reward, even for an infinite run, where $T \rightarrow \infty$. Since the environments we will experiment with are video games, each play is an episode and the total number of steps in each episode is finite.

It is now clear, that the optimal policy should always maximize the expected discounted return. The *value function* of a policy ρ computes this quantity from each state s :

$$v_\rho(s) := \mathbb{E}_\rho[G \mid s_0 = s] \quad (3.2)$$

which is the expected value of G , when the agent starts from state s and it follows the policy ρ . The notation \mathbb{E}_ρ indicates that the estimation assumes that the actions are sampled according to ρ . Finally, we can define the *optimal policy* ρ_* as the one

maximizing the value function at all states:

$$\rho_* : \quad v_{\rho_*}(s) \geq v_{\rho}(s) \quad \forall s \in S, \quad \text{for all } \rho \quad (3.3)$$

The typical Reinforcement Learning problem is to find the optimal policy for an MDP with unknown T and R .

The *action-value function* of a policy ρ is a similar measure to the value function:

$$q_{\rho}(s, a) := \mathbb{E}_{\rho}[G \mid s_0 = s, a_0 = a] \quad (3.4)$$

which also forces the first action to be a . Since the agent can only observe outcomes of single actions, this is usually a much more convenient form for updating the estimate of the expected discounted return. Most important, the optimal policy can be simply expressed as:

$$\rho_*(s) = \arg \max_{a \in A} q_{\rho_*}(s, a) \quad (3.5)$$

So, instead of learning the optimal policy directly, we can learn the optimal state-value function, q_{ρ_*} (also denoted with q_*). Fortunately, we don't need ρ_* to value q_* because, assuming optimality, we know it satisfies the Bellman optimality equation:

$$q_*(s, a) = \mathbb{E} [r_{t+1} + \gamma \max_{a'} q_*(s_{t+1}, a') \mid s_t = s, a_t = a] \quad (3.6)$$

$$= \sum_{s', r'} p(s', r' \mid s, a) (r' + \gamma \max_{a'} q_*(s', a')) \quad (3.7)$$

for any t .

Many learning algorithms exist for estimating q_* . Briefly, on-policy algorithms, estimate q_{ρ} of the policy ρ that is being used and improved, $\rho \rightarrow \rho_*$; off-policy algorithms, instead, act according to any exploration policy ρ_e and directly estimate q_* . Two famous algorithms in these classes are SARSA and Q-learning, respectively. The one used in this thesis is derived from the latter.

3.1.3 Exploration policies

If q_* were known, equation (3.5) would be enough to always select the optimal action. Generalizing for any q , we call that the *greedy policy*, because it always selects the best action according to q :

$$\rho_q(s) := \arg \max_{a \in A} q(s, a) \quad (3.8)$$

Unfortunately, while learning, we only have a rough estimate of the optimal function, $\hat{q} \approx q_*$. Being greedy with respect to sub-optimal values is dangerous, because the agent may deterministically select actions that repeatedly lead to dead-ends. To

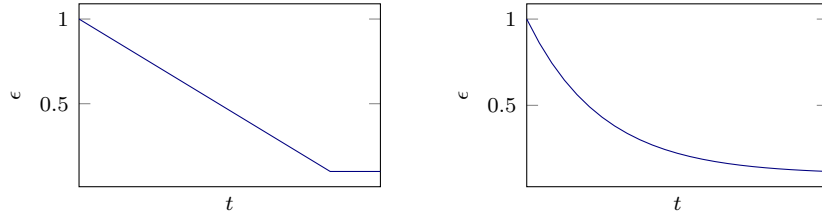


Figure 3.3. Probability of a random action over time: ϵ with linear decay (left), ϵ with exponential decay (right).

mitigate this issue, we can choose some actions at random. The ϵ -greedy policy is defined as:

$$\rho_{q,\epsilon}(s) := \begin{cases} \text{random action } a \in A & \text{with probability } \epsilon \\ \arg \max_{a \in A} q(s, a) & \text{otherwise} \end{cases} \quad (3.9)$$

More precisely, random actions are sampled from a uniform distribution over the set of actions A . By making random moves, the agent might escape from suboptimal environment configurations. If $\epsilon = 1$, definition (3.9) reduces to the random policy:

$$\rho_r(s) := \text{random action } a \in A \quad (3.10)$$

When training begins, the agent has no clue about the optimal q -function. It can just try out all actions by executing the random policy. In this phase, the agent receives low rewards but observes a lot of different outcomes for its actions. This is the purpose of exploration. After a while, the agent can begin to trust in its predictions. So, it may gradually choose the most promising actions in order to achieve higher rewards. This is the exploitation phase. The exploitation–exploration trade-off is a fundamental problem in AI. Unfortunately, there’s no general solution in RL, because the agent has no way to tell when the policy is “good enough”. Usually, we need to try some compromises between the two.

To address this issue, during training, the agent can act according to a policy that is initially stochastic but gradually approaches the greedy policy, over time. There are many ways to do this. One of the most simple options is to select the ϵ -greedy policy of equation (3.9) with ϵ that varies over time according to some schedule. Figure 3.3 shows two common possibilities. On the left-hand figure, the probability of a random action is linearly decreased over time, while on the right, it follows an exponential decay. In both cases ϵ never becomes zero, because that would effectively terminate the learning process. The rate of this decrease is a hyperparameter that can be tuned.

The most important policies are those just described. They can be directly used in a RL algorithm or combined to create more complex policies. The variants

designed in this thesis will be presented in the next chapters. With “exploration policy” we refer to any policy that has a strong component of nondeterminism and it’s suitable to drive the agent’s behaviour during training.

3.2 Deep Reinforcement Learning

Classic RL algorithms, such as SARSA and Q-learning, are tabular methods. In fact, they store and update the estimate for each pair (s, a) independently. Unfortunately, this requires discrete and small states and actions spaces. To overcome this very limiting assumption, we need parametrized value functions and policies. *Deep Reinforcement Learning* (Deep RL) is a recent field of RL in which Neural Networks (NN) are used as powerful function approximators for policies or value functions.

The main advantage of NNs, and parametric models in general, is that they can be trained in high-dimensional and continuous input spaces. In fact, a good fit does not require a complete exploration of the input space, which may be unfeasible or impossible. Instead, they are trained with some form of Stochastic Gradient Descent on the set of parameters from input-output samples. Then, the model can be able to generalize to inputs that have been never observed, in a meaningful way.

Unfortunately, due to approximation and parametrization, Deep RL algorithms allow very little guarantees about convergence and optimality. Even if the input space would be explored completely, updates for recent samples would also affect the regions previously visited. In fact, any effective Deep RL algorithm introduces some techniques in order to generate a stable training.

3.2.1 Environment: Atari 2600 games

The Atari 2600 is a video game platform that was developed in 1977. There are hundreds of classic games available to play: Space Invaders, Ms. Pacman, Breakout and many others. The screen is 160 pixels wide and 210 pixels high, with RGB colors of 8-bits depth. The joystick has 9 positions (3 for each axis) and one button, for a total of 18 possible actions. For this reason, we'll only focus on RL methods for discrete action spaces.

The Arcade Learning Environment [2] is a simple interface to the Atari 2600 emulator. It allows agents to play and be trained on these games. At each step, the agent chooses one of the 18 actions available and receives in return a frame of the game and a reward. The reward is the increment in the player's score for the original game. This is really the same interface that a human player would use. Figure 3.4 shows the frames from few games in this collection.

Although these games come from an early stage of video games development, they represent the appropriate challenge for current (Deep) Reinforcement Learning agents. In fact, many papers tested their RL algorithms on these games [17][16][25][12]. In this thesis, we also tested with some of these environments. We will also show how improve on the hardest game in this collection for a RL agent: Montezuma's

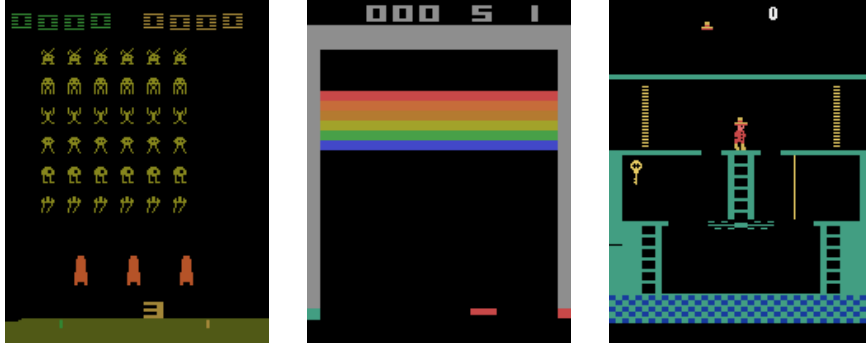


Figure 3.4. Initial frames of some Atari 2600 games (left to right): Space Invaders, Breakout, Montezuma's Revenge.

Revenge.

3.2.2 Deep Q-Network

The *Deep Q-Network* (DQN) [17] was the first algorithm to successfully combine deep learning models and Reinforcement Learning. Although many basic ideas presented here have been already introduced by the Neural Fitted Q iteration algorithm [20], DQN addressed some causes of training instability. They also demonstrated that exactly the same agent can be trained in many Atari games and achieve human-level performances in many of those [16]. These promising results sparked a lively interest in Deep RL, recently.

In DQN, the state-action value is approximated by a deep neural network $Q(s, a; \theta)$, on the parameters θ , that we call Q-Network. The purpose of learning, is to train this network to approximate the optimal q-function: $\hat{\theta} : Q(s, a; \hat{\theta}) \approx q_*(s, a)$. Then, the estimated optimal policy will be:

$$\hat{\rho}(s) = \arg \max_{a \in A} Q(s, a; \hat{\theta}) \quad (3.11)$$

A trained network, for each input (s, a) , should return the expected value of some target $y_{s,a}$. To do so, we select the parameters that minimize the squared difference between the estimates and the targets:

$$\text{loss}(\theta) := (Q(s, a; \theta) - y_{s,a})^2 \quad (3.12)$$

Since this is a Q-Network, the targets are the optimal state-action values $q_*(s, a)$ that the net should estimate. The loss (3.12) contains some random variables. So, we minimize it through any stochastic optimization algorithm. In Stochastic Gradient Descent (SGD), at each step t , we observe an input (s_t, a_t) and the associated target

y_t . Then, we take a small step toward the negative gradient of the loss:

$$\theta_{t+1} = \theta_t - \alpha \nabla_{\theta} \left((Q(s_t, a_t; \theta) - y_t)^2 \right) \Big|_{\theta=\theta_t} \quad (3.13)$$

in which $0 < \alpha < 1$ is a small learning rate. This equation is not the only update rule possible. There are more advanced optimization algorithms, such as: Momentum, RMSprop and Adam. In this thesis, we’ve mostly experimented with Adam.

What has just been described is the usual way of fitting a neural network to a dataset of samples. In RL, however, the targets $q_*(s_t, a_t)$ are unknown, because they depend recursively from the same optimal q-function that we’re trying to learn (see equation (3.7)). In classic RL, this is not a problem: the 1-step approximation of the q-values (derived from equation (3.7)),

$$y_t := r_{t+1} + \gamma \max_{a \in A} \hat{q}(s_{t+1}, a) \quad (3.14)$$

or the n-step approximation, are a valid targets for the function \hat{q} . By updating toward these values on the whole input space, convergence is guaranteed. In other words, targets can be estimates themselves.

With neural networks, instead, any update to the parameters also affects the target, because the weights have a global influence on the function. It’s not possible apply a correction for just one tiny region of the input space (nor it’s desirable, after all). It has been shown [20], that due to this effect, propagating errors slow down convergence or even render the training unstable. To address this issue one must ensure that the targets do not move much.

The DQN [17] algorithm addresses this issue in two ways. First, the targets in equation (3.14) are not generated by the network that is being trained, $Q(s, a; \theta)$, but they are computed from a second net, $Q(s, a; \theta')$. Every C iterations, the target net is updated to match the trained net, with the assignment: $\theta' \leftarrow \theta$. This keeps the targets constant for C steps and helps to stabilize the training.

Second, the network is not trained from the last sample, but from transitions of the recent experience. At each step, the agent acts according to some exploration policy, $a_t \sim \rho_e$. Each transition, of the form $\langle s_t, a_t, r_{t+1}, s_{t+1} \rangle$, is recorded in a buffer of size n_r , called “experience replay”. Then, at each training step, we sample a number of n_b transitions, thus creating a batch, and we perform an update $\theta_{i+1} = \theta_i - \alpha g_i$ on the cumulative gradient g_i of the whole batch.

DQN also includes a number of heuristics that greatly help the training but are specific to the Atari 2600 environments:

- Rewards can be really high, so they are limited in the range $[-1, +1]$; this is called *reward clipping*. It helps to keep the same learning rate for diverse games.

- The agent has a single life available. When a life is lost, the episode ends. This prevents the agent to rely on restarts.
- The frames are slightly down-scaled to further reduce the resolution, they are transformed to gray-scale and mapped to the range $[-1, +1]$. These are common preprocessing steps for NNs.
- Every observation is composed by the last 4 frames stacked together. This allows the agent to observe how the objects in the scene move. See Section 3.3 and Example 7 on page 30.

The algorithm used in this thesis is called *Double DQN* [25]. It is a slight variant of DQN, so all details mentioned so far also apply. The motivation of this algorithm is a known issue of Q-learning: it is likely to make overoptimistic value estimates. To show this, let's rewrite the targets of (3.14) as:

$$y_t := r_{t+1} + \gamma Q(s_{t+1}, \arg \max_{a \in A} Q(s_{t+1}, a; \theta_t); \theta_t) \quad (3.15)$$

where the estimates \hat{q} are computed with the Q-Network. This form makes more evident that the same model is used both to select the next greedy action and to estimate the q-value of state s_t . As result, any action with an overestimated q-value will be selected and its value propagated. To remove this bias, Double DQN decouple the two operations by using different sets of parameters, $\theta^{(1)}$ and $\theta^{(2)}$. The targets y_t are computed as:

$$y_t := r_{t+1} + \gamma Q(s_{t+1}, \arg \max_{a \in A} Q(s_{t+1}, a; \theta_t^{(1)}); \theta_t^{(2)}) \quad (3.16)$$

Then, just the parameters $\theta^{(1)}$ are updated toward this targets; this is called the online network. With random chance, the roles of the two parameters are continuously swapped at each step.

To compute the target, we need to compute the q-values for all actions in state s_{t+1} . To speed up this computation, the network is defined as a function that takes in input a state and computes a vector of state-action values, one for each action. So, just one forward pass is required to select the next action. Common Q-Networks for images are composed of a number of convolutional layers and some fully-connected layers. The specific structure may change, and the network used will be defined in the implementation section.

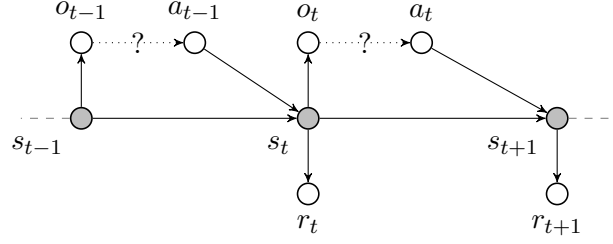


Figure 3.5. The Directed Graphical Model of a POMDP. Gray nodes are unobservable. For simplicity, the rewards in this graph depend just on the current state s_t , not on transitions (s_t, a_t, s_{t+1}) .

3.3 Non-Markovian goals

The goal of a RL agent is to maximize the rewards received. A goal, or a task, is said *non-Markovian* if the rewards do not satisfy the Markov assumption on rewards, i.e:

$$r_{t+1} \not\perp s_i, a_i, r_i \mid s_t, a_t \quad \text{for some } t, i, \text{ with } 0 \leq i < t \quad (3.17)$$

Of course, this can happen only if the environment cannot be modelled with an MDP. Excellent algorithms exist for MDPs; instead, non-Markovian goals are much more difficult to learn. There are two main causes for non-Markovian rewards: partial observations and temporally-extended tasks. We'll thoroughly analyze both scenarios.

3.3.1 Partial observations

Up to this point, we didn't need to distinguish between observations and states. In fact, we assumed that the agent can directly observe the environment states and act accordingly (we defined the policy as a function of the state). Unfortunately, this is often not the case: we only get to see something that depends on the current state, but it's not. These systems can be modelled with a *Partially Observable Markov Decision Process* (POMDP). POMDPs are a generalization of MDPs for partial observations. From now on, we will denote with S the environment state space and with Ω the observation space. Formally, a discrete-time POMDP is a 7-tuple $\langle S, A, T, R, \Omega, O, \gamma \rangle$, where S, A, T, R are defined as in MDPs, Ω is the observation space, and O is the observation function $O : S \rightarrow \Omega$.

The graphical model of a POMDP is shown in Figure 3.5. The sequence of states $\langle s_0, s_1, \dots \rangle$, which is the environment dynamics, still satisfies the Markov assumption (it forms a Markov chain). In a POMDP, this dynamics exists but is unobservable. What we can see, instead, is a sequence of observations $\langle o_0, o_1, \dots \rangle$. Each of them is generated from the corresponding state, through the (possibly nondeterministic)

observation function. Actions and policies can only act in response to observations, not states.

The dotted arrows in Figure 3.5 have a question mark on them, because that dependency is our choice. As designers, we're free to select the informations that the agent should take into account when selecting an action. Is the last observation enough to decide? Or, more precisely, among all possible policies, do non-Markovian goals always admit an optimal policy of the form $\rho_* : \Omega \rightarrow A$? Unfortunately, the answer is no. As we will see, other informations are needed.

If the transition and observation functions are known, a common solution is to estimate the states and decide the action from this belief. With deterministic functions, the agent can iteratively restrict the set of possible states by eliminating those inconsistent with the observations received. More commonly, these functions are nondeterministic. In this case, probabilistic methods can be effective estimation algorithms. The iterative probabilistic filter applied to the sequence of observations would produce the belief distribution of the current state. We can represent the general procedure, at any instant t , with the following computation:

$$\begin{array}{ccc} \langle o_0, o_1, \dots, o_t \rangle & \searrow & \\ & b(s_t) & \longrightarrow a_t \\ \langle a_0, a_1, \dots, a_{t-1} \rangle & \nearrow & \end{array}$$

where $b(s)$ denotes the belief of s , being either a set of states or a probability distribution. Since these beliefs depend on the whole sequence of observations, also the next action is implicitly based on the whole history.

Standard RL algorithms cannot be applied to POMDPs, because the state space is not observable. Also, since we commonly assume the transition and observation functions to be unknown, no estimation could be carried out anyway. There is a clear difference between MDPs and POMDPs. Still, RL algorithms are frequently applied to POMDPs. Not surprisingly, they perform very poorly on these environments. See, for example, the games with worst performances in [16]. This is a subtle mistake, because determining whether we're observing the state space is the same as answering the following question: does the observation space capture the whole dynamics of the system? Or, more precisely, does an equivalent MDP $\langle \Omega, A, T_\Omega, R_\Omega, \gamma' \rangle$, that produces the same rewards, exist? If both $T_\Omega : \Omega \times A \times \Omega \rightarrow \mathbb{R}$ and $R_\Omega : \Omega \times A \times \Omega \rightarrow \mathbb{R}$ exist and produce the same rewards, the environment can be successfully modelled and solved with an MDP. Figure 3.6 represents this situation.

Example 6. As we've seen from Example 5 on page 18, the game of Chess can be modelled with an MDP if we consider as states the vectors of positions of all pieces

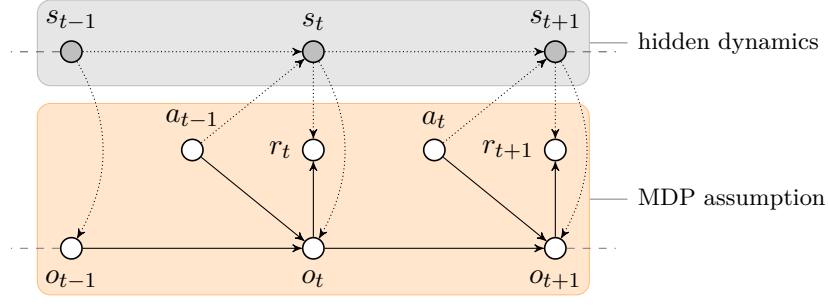


Figure 3.6. The dotted arrows $\cdots \rightarrow$ represent the dependencies in a POMDP model. Solid arrows \rightarrow show the MDP model over the same quantities.

on the board. Let's suppose, instead, the observations available are images of the board after each move (if the pieces can be distinguished, these could even come from a real play). Each image completely captures the state of the game because, for each move of the agent and the opponent, we're able to accurately predict the image that will follow. This is a transition T_Ω over images. Similarly, a reward function R_Ω can simply return $+1$ or -1 for images with checkmates and 0 otherwise. These functions can be unknown and don't need to be defined.

Suppose, instead, that the agent can only observe the left-hand side of the board (columns a-d, for example). In this case, each image provides an incomplete view over the state of the game. In fact, in order to determine the best action we must consider whether there are some attacking pieces on the hidden region. In this case, classic RL algorithms would perform poorly, because without any memory about the position of the hidden pieces, it's not possible to predict the next image and reward from the current observation.

Example 7. Let's consider a classic control problem: the swing-up of an inverted pendulum. A pendulum can freely rotate by 360° around a hinge. The agent, at each discrete time step, can apply torques to this active joint. The goal is to stabilize the pendulum in the upward position, which is the configuration of unstable equilibrium. In order to solve this problem with Reinforcement Learning, we need to define the spaces S and A of the MDP. In this domain, actions are continuous torques, which may be represented in a normalized range: $A := [-1, +1] \subseteq \mathbb{R}$. The angle of the pendulum θ with respect to some fixed reference completely determines the position of the masses. Is the reward Markovian with respect to $S := \{\theta \in [-\pi, +\pi]\}$? No, because the agent is rewarded when the pendulum *stops* in the upward position. So, the appropriate state space consists of both θ and $\dot{\theta}$ (or, rather its discrete-time approximation).

Including the momentum in the state space is very common for mechanical systems. However, this can be also necessary for games. In fact, just looking at a

single frame, the agent has no clue about how all the elements in the picture are moving. For example, in a video game where the agent has to hit a moving ball, the optimal policy certainly needs to observe also its direction.

3.3.2 Temporally-extended goals

The previous section has shown how partial observations may falsify the Markov assumption on rewards. A second possibility is to have a complete observation of the state ($\Omega = S$) but a task that is intrinsically non-Markovian. In this case, each reward is computed from the whole history of events

$$r_t = R(\langle s_0, s_1, \dots, s_t \rangle) \quad \forall t \in \mathbb{Z} \quad (3.18)$$

with $R : S^* \rightarrow \mathbb{R}$. The sequence of states $\pi := \langle s_0, s_1, \dots, s_t \rangle$ will be also called execution *trace*. In general, with the term “trace” we indicate any sequence that is produced during a run. We adopt a similar notation to those we’ve seen for interpretations of temporal logics.

Goals defined by rewards of equation (3.18) are said “temporally-extended” because they take into account multiple timesteps. Why should we define a reward function that is explicitly non-Markovian? One possibility is that we might want our agent to drive the environment through a *sequence* of states, instead of just reaching a single configuration. However, as we will see, we don’t need to restrict to sequences, because we may define very complex reward functions.

Example 8. Let’s suppose the agent can control a light bulb through a switch, and we want the light to be set on, then off again. The agent will be rewarded if, at the end of the episode, the light has been set on only once. The environment is extremely simple: its state may be completely described by a Boolean variable, “lightOn”, which reflects the status of the light. Still, in order to valuate whether the task has been accomplished, it’s not sufficient to check whether the light is off at the end of the episode; we also need to ensure that, *during the whole episode*, it has been switched on only once.

We now define a model that, by generalizing MDPs, can describe this large class of problems.

Definition 7. A *Non-Markovian Reward Decision Process* (NMRDP) [1] is a tuple $\langle S, A, T, R, \gamma \rangle$, where S, A, T, γ are defined as for MDPs, and $R : S^* \rightarrow \mathbb{R}$ is a non-Markovian reward function, which computes the reward at time t as $r_t = R(\langle s_0, s_1, \dots, s_t \rangle)$.

Every NMRDP admits an optimal policy as $\rho_* : S^* \rightarrow A$, which computes actions from the history of states. So, we’ll only consider policies with this form. In order to

define optimality, we would need to proceed as for MDPs, by defining value functions. However, this is slightly more complex, since as a consequence of non-Markovian rewards, value functions can only predict the future expected discounted return, if the past history is given. They effectively compare policies on traces, rather than single states. The simplest case is the valuation of any initial state, whose value function is [1]:

$$v_\rho(\langle s_0 \rangle) := \mathbb{E}_\rho \left[\sum_{t=0}^T \gamma^t R(\langle s_0, s_1, \dots, s_t \rangle) \right] \quad (3.19)$$

Informally, an NMRDP policy ρ_* is optimal if it maximizes the value function of future states. However, we won't further delve into the definition of optimality and value functions, because common solution methods (that we'll see in Section 3.4.1) transform NMRDPs into standard MDPs, that we already know how to solve.

NMRDP with LDL_f rewards

Non-Markovian reward functions have huge domains. Defining them by listing all the traces that should be (positively or negatively) rewarded is unfeasible, even for the simplest cases. Fortunately, as we already know from Chapter 2, temporal logics are powerful formalisms that allow to concisely define groups of traces. So, a very effective way to declare non-Markovian rewards is through a set of pairs $\{(\varphi_i, r_i)_{i=1}^m\}$, where each φ_i is a LDL_f formula and r_i is its associated reward [3]. The reward r_i will be produced whenever a trace satisfies φ_i . So, the reward function is defined as:

$$R(\pi) := \sum_{i: \pi \models \varphi_i} r_i \quad (3.20)$$

It follows that an equivalent way to define NMRDPs is: $\langle S, A, T, \{(\varphi_i, r_i)_{i=1}^m\}, \gamma \rangle$.

In this thesis, rewards will be always declared with LDL_f formulae. However, the same discussion also applies to LTL_f . Also, we may have noticed that the adoption of temporal logics requires a state space that is composed of propositional interpretations. This will be addressed in Section 3.4.2.

3.4 Reinforcement Learning with LDL_f specifications

This section illustrates how to learn optimal policies for a large class of problems among those introduced in Section 3.3. The main idea behind the techniques presented here is to formulate an appropriate NMRDPs with LDL_f rewards, and to solve it through an equivalent Markov Decision Process. Since many learning algorithms exist for MDPs, this translation can be considered as a solution for the original problem.

3.4.1 RL for NMRDPs with LDL_f rewards

RL for NMRDPs

Before looking at the construction, we need to define what is an *equivalent* MDP and what are its properties.

Definition 8. [1] An NMRDP $\mathcal{N} := \langle S, A, T, R, \gamma \rangle$ is *equivalent* to an extended MDP $\mathcal{M} := \langle S', A, T', R', \gamma \rangle$ if there exist two functions $\tau : S' \rightarrow S$ and $\sigma : S \rightarrow S'$ such that:

1. $\forall s \in S : \tau(\sigma(s)) = s$;
2. $\forall s_1, s_2 \in S$ and $s'_1 \in S'$: if $T(s_1, a, s_2) > 0$ and $\tau(s'_1) = s_1$, there exists a unique $s'_2 \in S'$ such that $\tau(s'_2) = s_2$ and $T'(s'_1, a, s'_2) = T(s_1, a, s_2)$.
3. For any feasible trajectory $\langle s_0, a_1, \dots, s_{n-1}, a_n \rangle$ of \mathcal{N} and $\langle s'_0, a_1, \dots, s'_{n-1}, a_n \rangle$ of \mathcal{M} , such that $\tau(s'_i) = s_i$ and $\sigma(s_0) = s'_0$, we have $R(\langle s_0, a_1, \dots, s_{n-1}, a_n \rangle) = R'(\langle s'_0, a_1, \dots, s'_{n-1}, a_n \rangle)$.

Conditions 1 and 2 require that every feasible trajectory of the NMRDP can be simulated with a trajectory of the MDP. Condition 3 forces corresponding trajectories to produce the same rewards. So, the equivalent MDP completely captures the dynamics of the NMRDP. As we will see, in order to do this, the new state space S' needs to include the old states S and some history-related informations. Since S' is always larger than S , the equivalent MDP is also called “extended”.

Definition 9. [1] Let $\rho' : S' \rightarrow A$ be a policy for the MDP \mathcal{M} . The corresponding policy $\rho : S^* \rightarrow A$ of the NMRDP \mathcal{N} is defined as $\rho(\langle s_0, \dots, s_n \rangle) := \rho'(s'_n)$ where $\langle s'_0, \dots, s'_n \rangle$ is the corresponding trajectory for $\langle s_0, \dots, s_n \rangle$.

As we can see ρ' , is a stationary policy. A very important result that allows to correlate the solutions between the two classes of problems is the following:

Theorem 4. [1] For any policy ρ' for the MDP \mathcal{M} , its corresponding policy ρ for the NMRDP \mathcal{N} , and $s \in S$, we have $v_\rho(s) = v_{\rho'}(\sigma(s))$.²

As a corollary of the previous theorem, any optimal policy of the MDP has a corresponding policy that is optimal for the NMRDP. This is the result we were looking for: by applying classic RL algorithms, we can learn optimal policies of MDPs that apply to their equivalent NMRDP. In practice, we don't need to translate the policy ρ' to the non-stationary equivalent ρ . It is possible to apply the trained RL agent directly to the NMRDP, by continuously transforming each observation s through the translation function $\sigma : S \rightarrow S'$.

LDL_f rewards

We will now define a specific MDP expansion for NMRDPs with LDL_f rewards. In fact, if the rewards are specified through LDL_f or LTL_f, it is possible to create extended MDPs that are very compact. We recall that a NMRDP with LDL_f rewards is a tuple $\mathcal{N} := \langle S, A, T, \{(\varphi_i, r_i)_{i=1}^m\}, \gamma \rangle$, where $S := 2^{\mathcal{F}}$ is a set of propositional interpretations and φ_i are LDL_f formulae on the set of fluents \mathcal{F} .

First, using the methods presented in Section 2.3.2, we transform each reward formula φ_i to its associated minimal DFA, $\mathcal{A}_i := \langle 2^{\mathcal{F}}, Q_i, q_{i0}, \delta_i, F_i \rangle$. Then, we state the following:

Definition 10. [3] Given an NMRDP with LDL_f rewards $\mathcal{N} = \langle S, A, T, \{(\varphi_i, r_i)_{i=1}^m\}, \gamma \rangle$, we define the equivalent extended MDP $\mathcal{M} := \langle S', A', T', R', \gamma \rangle$, where:

- $S' := Q_1 \times \dots \times Q_m \times S$ is the set of states
- $A' := A$
- $T' : S' \times A' \times S' \rightarrow [0, 1]$ is defined as:

$$T'((q_1, \dots, q_m, s), a, (q'_1, \dots, q'_m, s')) := \begin{cases} T(s, a, s') & \text{if } \forall i : \delta_i(q_i, s') = q'_i \\ 0 & \text{otherwise} \end{cases}$$

- $R' : S' \rightarrow \mathbb{R}$ is defined as³:

$$R((q_1, \dots, q_m, s)) := \sum_{i : q_i \in F_i} r_i$$

²In this equation, v refers to the value function for NMRDPs and MDPs respectively.

³There is a slight difference with the original definition in [3], which accounts for a small notation difference in some previous definitions: $R(s_t)$ is assumed to produce r_t , not r_{t+1} .

As we can see from this definition, the extended MDP augments the original model with all the automata \mathcal{A}_i corresponding to the m temporal goals. After each observation, both the original system and every component \mathcal{A}_i are advanced accordingly, in parallel. The reward function, which is now Markovian, can produce the same rewards as in the original formulation (see equation (3.20)) because all the necessary information has been included in the state space.

Theorem 5. [3] *The NMRDP with LDL_f rewards $\mathcal{N} = \langle S, A, T, \{(\varphi_i, r_i)_{i=1}^m\}, \gamma \rangle$ is equivalent to the MDP \mathcal{M} of Definition 10.*

The last theorem states that our construction creates an equivalent MDP, according to the Definition 8. Any NMRDP can be formulated as an MDP, if enough history is included in the state space. So, what is really interesting about this translation is that the expanded MDP has a minimal state space. This is possible because the current state of the automaton \mathcal{A}_i is a sufficient information that retains just enough history to render the rewards r_i Markovian. We have:

Theorem 6. [3] *If every automaton \mathcal{A}_i ($1 \leq i \leq m$) is minimal, then the extended MDP of Definition 10 is minimal.*

To recap, in this section, we’ve shown how to train an agent on a Non-Markovian Reward Decision Process, by applying classic RL algorithms on the equivalent MDP. Once the relevant fluents have been selected, we need to express our goal as LDL_f conditions that are associated to a positive reward (or, maybe, conditions for negative rewards). We will see some practical examples in the following section, where we study how to deal with multiple representations of the same configuration of the environment.

3.4.2 RL with LDL_f restraining specifications

Multiple representations

The solution for NMRDPs that we’ve seen in the previous section is elegant and effective. However, at first sight, it may only seem applicable in very simple state spaces, that are composed of Boolean valuations for sets of fluents (for example, at some time t , we might have a state s_t in which: $\{\text{HaveKey} = \text{True}, \text{DoorClosed} = \text{False}\}$). This is not true, because we must remember that the NMRDP is just a model that we’ve defined. We’re free to adopt a new formalism, where the sequence of observations produced by the environment is decoupled from the trace where our formulae are interpreted on. The ideas presented here have been developed in [5].

Let’s denote with W the set of world states. This is an abstract representation of the environment configuration that is inaccessible to the agent. Instead, it receives

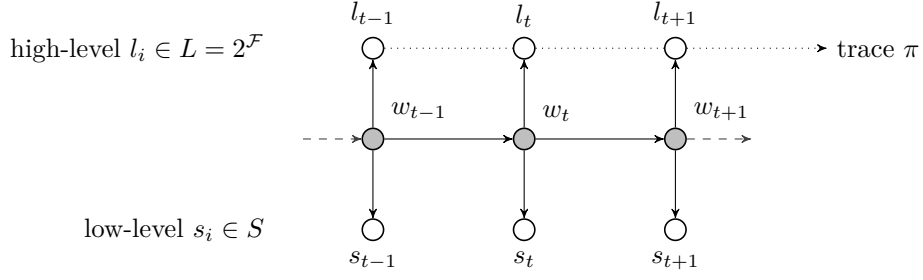


Figure 3.7. Every world state generates both high-level and low-level configurations.

observations that directly depend on these states. We can represent this sensory input with a function $f_S : W \rightarrow S$. Frequently, S is a multidimensional space, so the observations $s \in S$ are also called *features vectors*, or simply *features*. Assuming that these features are the state space of a Markov Decision Process, we can apply RL on S .

We now assume that there is a second function $f_L : W \rightarrow L$, with $L := 2^{\mathcal{F}}$, that given a world state, assigns a truth value to all fluents in \mathcal{F} . This creates two representations with different roles: S is a *low-level* features space that can be complex, noisy and difficult to interpret directly; L is a *high-level* logic representation of the same world states. To any configuration $w \in W$ corresponds a pair of the representations $s \in S$ and $l \in L$. See Figure 3.7.

This distinction is powerful: it allows us to declare temporally-extended goals with LDL_f on the set of fluents \mathcal{F} , while the agent receives and works with a different set of features. We now formally define a specific problem that is possible thanks to this distinction.

Restraining Specifications

Consider a Reinforcement Learning agent on the MDP $\mathcal{M} := \langle S, A, T, R \rangle^4$. This already defines the environment dynamics and the agent's optimal policy. We now want to modify the agent's behaviour by declaring an additional temporally-extended goal on some fluents \mathcal{F} . The purpose is to train an agent that pursues the original rewards, while complying with the additional specification we provided. As we know from Section 3.3.2, the LDL_f goals are just a clever way of declaring a non-Markovian reward function. These will be summed with the original rewards, so that the agent will try to pursue both⁵. We call this additional module, which

⁴The discount factor has been omitted in this section, because it doesn't apply to the problems we study here. So, it may be simply regarded as tunable parameter.

⁵The agent can behave optimally with respect to this combination, but this doesn't necessarily mean that this is the policy we were looking for. Finding the appropriate combination of rewards is a general issue in RL.

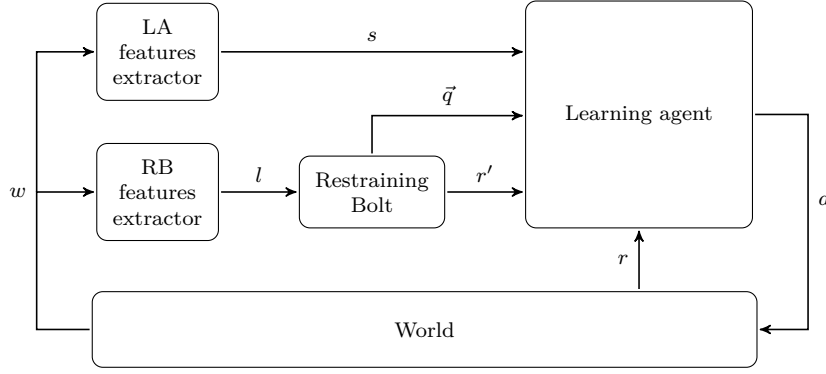


Figure 3.8. Learning agent with Restraining Bolt applied. r is the classic MDP reward; r' is the additional non-Markovian reward generated.

reads the current fluents' configuration and sends the non-Markovian reward back, as the “Restraining Bolt” [5]. This term, borrowed from Science Fiction, suggests that with this additional construction, we're able to modify the “natural” agent's behaviour. In this context, the LDL_f goals $\{(\varphi_i, r'_i)_{i=1}^m\}$ are referred to as “restraining specifications”. The general setup is presented in Figure 3.8. Notice, in particular, that the learning agent has access to the original observations s and rewards r , and the additional non-Markovian rewards r' . The quantity \vec{q} will be discussed shortly. Let's now formalize this problem.

Definition 11. [5] A *RL problem with LDL_f restraining specifications* is a pair $\langle \mathcal{M}, RB \rangle$, where: $\mathcal{M} := \langle S, A, T, R \rangle$ represents a learning agent, and $RB := \langle L, \{(\varphi_i, r'_i)_{i=1}^m\} \rangle$ is a Restraining Bolt formed by a set of LDL_f formulae φ_i over \mathcal{F} with associated rewards r'_i .

We can't simply apply a RL algorithm on the rewards r_i, r'_i over the state space S , because r'_i are non-Markovian in S . What we can do, instead, is to formulate a NMRDP with LDL_f rewards, that we already know how to solve. The complete proof is shown in [5] and [7]. What we see here is a shorter explanation that just highlights the main concepts.

We first observe that, in Definition 11, the MDP and the Restraining Bolt are completely distinct; their only interaction is in the sum of the rewards they produce (let's denote with $\bar{r}_i := r_i + r'_i$ the combined reward). So, to simplify the computation, we may keep these two problems separate, transform the restraining specifications to their equivalent MDP and combine them later. This is possible because, given two MDPs, $\mathcal{M}_a = \langle S_a, A, T_a, R_a \rangle$ and $\mathcal{M}_b = \langle S_b, A, T_b, R_b \rangle$, the following $\mathcal{M}_{ab} := \langle S_{ab}, A, T_{ab}, R_{ab} \rangle$, with states $S_{ab} := S_a \times S_b$, transition function $T_{ab} : S_{ab} \times A \times S_{ab} \rightarrow \mathbb{R}$ and rewards

$$R_{ab}((s_a, s_b), a, (s'_a, s'_b)) := R_a(s_a, a, s'_a) + R_b(s_b, a, s'_b)$$

is still an MDP. Note that we didn't define T_{ab} . This is not required, as in RL, it is sufficient that this unknown function exists; and by the laws of probability, this is certainly the case, because the existence of T_a and T_b is a stronger requirement.

Every Restraining Bolt $RB = \langle L, \{(\varphi_i, r'_i)_{i=1}^m\} \rangle$ defines a NMRDP with LDLf rewards $\mathcal{N}_{RB} := \langle L, A, T_L, \{(\varphi_i, r'_i)_{i=1}^m\} \rangle$, with states $L = 2^{\mathcal{F}}$ and T_L as the unknown transition function over fluents configurations. This is a problem that we already know how to solve. By directly applying Definition 10, we can write the extended MDP $\mathcal{M}_{RB} := \langle S_{rb}, A, T_{rb}, R_{rb} \rangle$ that is equivalent to the NMRDP \mathcal{N}_{RB} . Notice in particular, that the state space becomes: $S_{rb} := Q_1 \times \dots \times Q_m \times L$, where each Q_i is the set of states of the i -th automaton. For brevity, we will denote elements of $Q_1 \times \dots \times Q_m$ with \vec{q} , because they are vectors of automaton states.

We can now combine the original MDP \mathcal{M} with the one generated from the Restraining Bolt \mathcal{M}_{RB} , just like we've done for \mathcal{M}_{ab} , to obtain a new unified MDP that is defined as $\mathcal{M}' := \langle S', A, T', R' \rangle$, where:

- $S' := Q_1 \times \dots \times Q_m \times L \times S$
- $T' : S' \times A \times S' \rightarrow \mathbb{R}$ with:

$$T'((q_1, \dots, q_m, l, s), a, (q'_1, \dots, q'_m, l', s')) := \begin{cases} T_{l,s}((l, s), a, (l', s')) & \text{if } \forall i : \delta_i(q_i, l') = q'_i \\ 0 & \text{otherwise} \end{cases}$$

- $R' : S' \times A \times S' \rightarrow \mathbb{R}$ with:

$$R'((q_1, \dots, q_m, l, s), a, (q'_1, \dots, q'_m, l', s')) := \sum_{i: q'_i \in F_i} r'_i + R(s, a, s')$$

Both $T_{l,s}$, that is the joint transition function of the symbols s and l , and the original reward function, R , are unknown: we only observe the samples produced while the agent plays. Instead, we have to move all automata and return the associated rewards, because this is a dynamics we've defined.

To this point, we've reduced the original problem of Definition 11 to standard RL on the MDP \mathcal{M}' . However, we can move one step further. In fact, the combined rewards \bar{r}_i do not depend on the fluents configurations $l_i \in L$, if both s_i and \vec{q}_i are given, that is:

$$\bar{r}_t \perp l_0, \dots, l_t \mid \vec{q}_t, s_t \quad \text{for any } t$$

This means that an optimal policy exists for \mathcal{M}' with the form: $\rho_* : Q_1 \times \dots \times Q_m \times S \rightarrow A$. To prove it formally, we would need to show that the value of any

state (\vec{q}, l, s) , defined in equation (3.2), does not depend on l . We finally get to the following result:

Theorem 7. [5] *RL with LDL_f restraining specifications $\langle \mathcal{M}, RB \rangle$, with $\mathcal{M} = \langle S, A, T, R \rangle$ and $RB = \langle L, \{(\varphi_i, r'_i)_{i=1}^m\} \rangle$, can be reduced to RL over the MDP $\mathcal{M}'' := \langle Q_1 \times \dots \times Q_m \times S, A, T'', R'' \rangle$, and optimal policies for $\langle \mathcal{M}, RB \rangle$ can be learnt by learning corresponding optimal policies for \mathcal{M}'' .*

If we denote with S'' the state space $Q_1 \times \dots \times Q_m \times S$, the functions T'' and R'' are partially unknown functions $S'' \times A \times S'' \rightarrow R$, that are defined respectively as T' and R' , marginalized with respect to L . With the MDP \mathcal{M}'' , we assumed that at each instant t , we observe the current state (\vec{q}_t, s_t) . This is true for s_t , but not for \vec{q}_t . What we can do instead, is receiving an observation of the symbols l_t , moving all the automata accordingly, and collecting the resulting states \vec{q}_t . So, the new state (\vec{q}_t, s_t) is composed of the computed vector of automata states, and the observed symbols s_t . The symbols L don't need to be passed to the learning agent. Refer to Figure 3.8, once again.

3.4.3 Restraining Bolt for partial observations

We've thoroughly analyzed solutions for the non-Markovian goals of Section 3.3.2: namely, temporally-extended goals. We've solve them both in isolation, and as additional restraining specifications in preexisting MDPs. We now want to ask: is it possible to address partial observations, which is the second source of non-Markovian goals, in a similar way? In many cases, the answer is yes. Although, as we will see in a moment, this may not be possible or practical for every problem.

Partially observable environments would be properly modelled with POMDPs $\langle W, A, T, R, \Omega, O \rangle$, because they define an observation function $O : W \rightarrow \Omega$ that maps world states to observations. However, in RL, this function is unknown and the states W are inaccessible for the agent. So, the simplest approach is to learn a policy directly from the observation space, $\rho : \Omega \rightarrow A$, as if the system were an MDP with states Ω (see Figure 3.6 on page 29). As we've noted, this can lead to very poor performances, because rewards can be non-Markovian with respect to the observations.

Now, let's define a set of fluents \mathcal{F} that represent Boolean conditions whose truth can be valuated from the observations Ω . Similarly to the previous section, to each hidden environment state corresponds a low-level feature $o \in \Omega$ and a high-level symbol $l \in 2^{\mathcal{F}}$. In Figure 3.9, the environment is assumed to generate the observation o , on which we have no control. Instead, the feature extractor indicates that we're free to choose and generate our high-level alphabet.

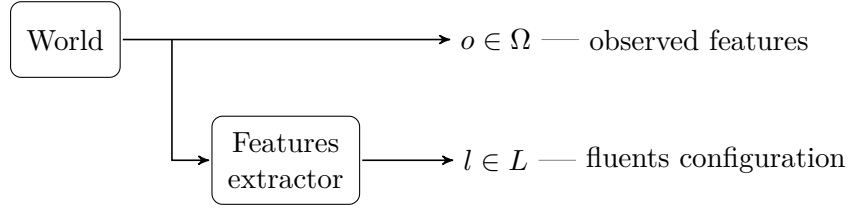


Figure 3.9. Fluents configurations are computed from observations of the environment.

Suppose our goal is to define a function that generates the same rewards as the environment. Since the rewards are non-Markovian with respect to the observations, they will certainly be non-Markovian with respect to the fluents configurations which are computed from them. So, what we can do is to define a NMRDP with LDL_f rewards from the fluents \mathcal{F} , that produces the same rewards r as the environment. In order to do this, we will certainly select as fluents all the conditions which are relevant for deciding whether the reward should be supplied.

Example 9. Let's extend Example 8. An agent can control a light bulb through a switch, but now it can capture images of the room. Suppose the environment rewards the agent with the same condition of the previous example: the light must have been switched on, then off, only once during the episode. Our goal is to emulate this reward with a NMRDP with LDL_f rewards. First, we define a fluent *LightOn*, representing the status of the light. The features extractor, from images of the room in which the light is on, would produce *LightOn* = *true* (or $l = \{\text{LightOn}\}$), and false otherwise. Now we state the following LDL_f goal:

$$\varphi_1 := \langle (\neg \text{LightOn})^*; \text{LightOn}^+; (\neg \text{LightOn})^+ \rangle \text{End}$$

where ρ^+ is an abbreviation of $\rho; \rho^*$.

Assuming we've been able to define an NMRDP with LDL_f rewards, $\mathcal{N} = \langle L, A, T, \{(\varphi_i, r'_i)_{i=1}^m\} \rangle$, that generates the same rewards as the environment. The equivalent MDP of \mathcal{N} , $\mathcal{M} := \langle S', A, T', R' \rangle$ has a state space $S' := Q_1 \times \dots \times Q_m \times L$. From Theorem 7, the rewards generated by \mathcal{M} are the same as those generated by \mathcal{N} . This also means that the original rewards, produced by the environment, are Markovian with respect to S' . Therefore, by augmenting the observations with the automaton states \vec{q} , we produce a state space that restores the Markov property. This is possible, because these states keep track of the unobservable quantities in the environment state that affect future rewards. This is the important additional information that we need to provide to the agent, we may even not supply the rewards that we generate at all. Figure 3.10 shows this arrangement.

Example 10. We now conclude the Example 9, where we've prepared an NMRDP

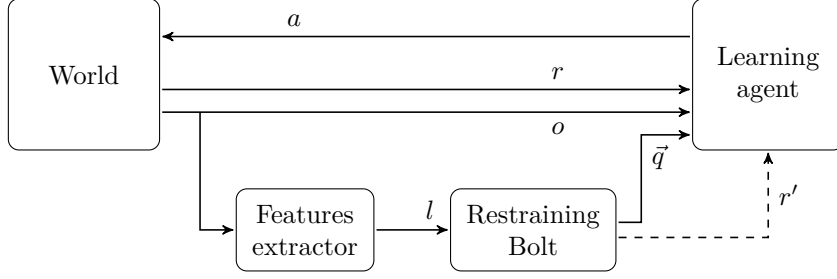


Figure 3.10. Restraining Bolt for partial observations: RL on the state (o, \vec{q}) .

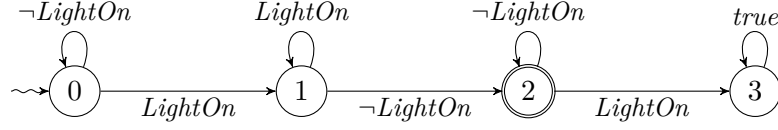


Figure 3.11. The DFA associated to the formula φ_1 , in Example 9.

with a single LDL_f reward associated to the condition φ_1 . The DFA that is associated to this formula is shown in Figure 3.11. The MDP associated to this simple problem is: $\langle Q \times \Omega, A, T, \{(\varphi_1, r')\} \rangle$, where the actions are $A := \{\text{Toggle}, \text{NoOp}\}$, Ω is an image, and $Q := \{0, 1, 2, 3\}$. With this composite state space, the agent has a complete view about the missing steps to achieve the reward; something that it wouldn't know from the current image or the current value of *LightOn*.

We've previously mentioned that this solution may not be feasible for every problem. In fact, we must first exclude all environments in which the observations are not meaningful enough. More precisely, those in which we cannot accurately predict the next reward r_t from the sequence of observations $\langle o_1, \dots, o_t \rangle$. However, these problems would be problematic for any learning algorithm, due to their weak observation function. A second group of environments may define reward functions which are difficult to express in temporal logic. Expressing these goals in LDL_f would generate a large number of fluents and obscure temporal specifications (example: the game of Chess with partial observations of Example 6). However, this last limitation is not as strong as it may seem: often, it is possible to greatly simplify the temporal specification by simply selecting a different set of fluents.

We might think that reproducing the environment's reward function is impossible if it is unknown. This is not necessarily true, because we are those that define the agent's goal and would generate those "environment's" rewards. For an unknown function, we mean that a precise model of that function is not available and cannot be exploited, not that the rewarded goal is obscure. For example, the rewards of Example 9 are unknown, because we don't know the function that maps *images* to rewards.

Conclusion

In this Chapter, we’ve shown that our construction for NMRDP with LDL_f rewards, that we call “Restraining Bolt”, is a valid solution for many problems: temporally-extended tasks, restraining specifications and partial observations. A very interesting aspect is that it can be applied as an additional module, added to the agent’s original design. This is possible, because the extended MDPs only augment the original state spaces with additional informations. As we will see in the next section, in practice, the agent requires few modification in order to properly handle these additional informations. However, the Restraining Bolt is a first important step toward modularity and explainability of (Deep) RL agents designed for complex goals.

3.5 Restrained Deep RL agents

As illustrated in Section 3.2.2, the RL algorithm used in this thesis is Double DQN, a Deep RL method. Double DQN agents contain a Q-Network, which is a function $Q : S \rightarrow \mathbb{R}^{|A|}$, that is parametrized in θ . Given a MDP state $s \in S$, this computes the state-action value for every action $a \in A$. In this section, we will propose an original Q-Network model that properly handles the additional inputs received from the Restraining Bolt.

The Restraining Bolt is an interesting method because we can regard it as a module that, added to the original setup, generates additional rewards and observations. In principle, no structural modifications would be required in the agent’s design: new rewards can be simply summed with the previous ones, and the Restraining Bolt’s states \vec{q} can be stacked with the environment’s observations to produce a composite MDP state (o_t, \vec{q}_t) . Agents can learn from this new state space without modifications⁶.

Deep RL agents, instead, learn approximate value functions and policies. In this case, we should carefully select the agent’s model, a neural network, that has the appropriate expressive power. A network that is suitable to approximate a function $\Omega \rightarrow \mathbb{R}^{|A|}$ is not necessarily appropriate for a function from the new state space, $\Omega \times Q_1 \times \dots \times Q_m$. Overfitting and underfitting are well known issues in Machine Learning.

3.5.1 Q-Network for the Atari games

We will first illustrate the agent’s model that we use in this thesis when the Bolt is not applied. Then, in Section 3.5.2, we’ll propose a modification of this network that accounts for the additional states of the Restraining Bolt. The environments used in this thesis are games from the collection “Atari 2600”. As illustrated in Section 3.2.1, the observations produced are frames of size $(210, 160)$, with an RGB colour depth of 8-bit. Each game defines a different number of actions, 18 at most.

We use the same architecture as [16], which is illustrated here. Slight modifications will be listed in the implementation part, in Section 5.2.1. First, a preprocessing function applies a fixed transformation to each image. Every frame is converted to a gray-scale picture, by computing the luminance value of each pixel. The image is then resized to $(84, 84)$, in order to reduce the input dimensionality. Finally, 4 consecutive images are combined together, producing a tensor of size $(84, 84, 4)$ that can be passed to the network. This last combination allows to create an observation

⁶Extending the size of a table, in order to account for the additional number of states, is not considered a real modification in the agent’s design.

that encodes how the objects in the scene are moving. The lack of this information is one of the causes of non-Markovian rewards that can be easily solved. See Example 7, for an explanation.

Let's define the following abbreviation: $\text{Conv}(n, s, t)$ represents a 2D convolutional layer composed of a number of n filters of size $s \times s$ with a stride of t . Similarly, $\text{Dense}(n)$ represents a fully-connected layer of n units. We can now define the network structure as:

$$\begin{aligned} &\text{Conv}(32, 8, 4), \text{ReLU}, \\ &\text{Conv}(64, 4, 2), \text{ReLU}, \\ &\text{Conv}(64, 3, 1), \text{ReLU}, \\ &\text{Dense}(512), \text{ReLU}, \\ &\text{Dense}(|A|) \end{aligned}$$

where ReLU is the rectifier linear unit applied to each element. In neural networks, images are frequently transformed with a cascade of 2D convolutions, followed by a number of dense layers. The authors of the original paper [16] have shown that this network size generates a model with the appropriate expressive power for our environments.

3.5.2 Q-Network for the Restraining Bolt

We now want to apply the method presented in Section 3.4.3 in those games in which low performances are caused by partial observations. This means that our agent would need to receive the original observation, which is a frame of the game, and the vector of the Bolt's states, \vec{q} . We'll now suppose that our temporally-extended goal can be expressed with a single pair (φ, r') . So, the Restraining Bolt's state is a single scalar identifier q .

As anticipated, we cannot simply stack o and q . Even if the network architecture would allow that, we would assign a very low relative importance to q among the thousands of pixels of which o is composed. Most importantly, the role of q must not be confused with pixels. All these considerations are important because every model introduces some biases, and we want our model's bias to capture the following basic intuition: q is an important index that parametrizes value functions. The state q is a parametrization over value functions because, to different automaton states, there may correspond dramatically different value functions over inputs.

Example 11. Let's consider again the light bulb of Example 10 and the automaton of Figure 3.11. Suppose the initial MDP state is $s_0 = (o_0, 0)$, where o_0 is an image of a dark room. In this case, the model should learn an high state-action value for the action *Toggle*, and a low value for the action *NoOp*. Later on, at some time t ,

the agent may observe the following input: $s_t = (o_0, 2)$. Even though the image is the same, the agent should assign the highest value to *NoOp*. A different automaton state dramatically changes the most promising actions that will lead to the goal.

A very drastic choice would be to maintain a number of $|Q|$ different networks, with the same architecture but different parameters $\theta_1, \dots, \theta_{|Q|}$. At each step, given an input (o, q) the agent may use the network θ_q to predict the actions values for the input o . This strong parametrization would completely separate the value functions. An immediate problem with this approach is space inefficiency (that would be very evident with large Q or vectorial \vec{q}). Most importantly, the networks associated to states that are rarely encountered would be trained on too few input samples.

The model that we propose here is a variant of the network of the previous section. We substitute the last fully-connected layer with one of dimension $|A| \times |Q|$. This means that a number of $|A| \cdot |Q|$ linear units is arranged as a matrix, whose first index is an action and the second index is a Bolt's state. So, for each automaton state, the net will generate a different column of state-action values. The idea behind this choice is that we can safely share the initial layers, whose main goal is to provide an encoding of the observed input. Instead, separating the last layer provides the greatest flexibility among other combinations⁷. This is an intermediate approach between completely shared and completely separate parameters $\theta_1, \dots, \theta_{|Q|}$. For a vectorial \vec{q} , it can be easily extended: the last fully-connected layer would produce tensors of shape $(|A| \times |Q_1| \times \dots \times |Q_m|)$. Since the greatest number of parameters is shared, each combination of automaton states \vec{q} requires a smaller number of training samples to train on.

The resulting Q-Network for the Atari games is:

$$\begin{aligned} &\text{Conv}(32, 8, 4), \text{ReLU}, \\ &\text{Conv}(64, 4, 2), \text{ReLU}, \\ &\text{Conv}(64, 3, 1), \text{ReLU}, \\ &\text{Dense}(512), \text{ReLU}, \\ &\text{Dense}(|A| \times |Q|), \\ &\text{Slice}(\cdot, q) \end{aligned}$$

where $\text{Slice}(\cdot, q)$ indicates that we select the q -th column of the input matrix. This is the agent's model used in this thesis. As we can see, we didn't need to define more than one temporal goal in our experiments.

Some other variants may exist. In fact, we should remember that the automata states are generated from the conversion of LDL_f or LTL_f expressions. Since, this

⁷We didn't motivate why the first layers of the original net should behave as an encoder. However, after the modification, they will be shared and trained with different outputs. So, this role will be encouraged.

translation has a worst case complexity that is doubly exponential in the size of the formula, the state space may be quite large. One possibility would be to investigate whether is it possible to adopt the NFA states, instead of the DFA's, producing a state space that may be exponentially smaller (multiple columns would be active at the same time, in this case). But these variants have not been investigated yet.

Chapter 4

Learning to value fluents in games

In Chapter 3, we’ve presented the problem of Deep Reinforcement Learning for non-Markovian rewards. We’ve seen that a construction based on temporal logics, that we call Restraining Bolt, is an elegant solution that, by producing additional rewards and observations, transforms the original problem to a classic MDP. We report the general scheme here, in Figure 4.1. The two blocks at the bottom are our additions, and part of the solution. We’ve thoroughly addressed the Restraining Bolt in Section 3.4.2, already. In this chapter we want to focus on the other essential component: the features extractor.

The purpose of the features extractor is to receive an observation from the environment and produce a Boolean valuation for some predefined propositional symbols, that we call fluents. We assume that the set of fluents \mathcal{F} has already been defined, and the truth of every atomic proposition in \mathcal{F} can be decided from a single input o ¹.

¹If we did define a symbol that cannot be decided, for example a generic “*GoalReached*”, we need to split that condition into much simpler events, and define *GoalReached* in terms of the new symbols.

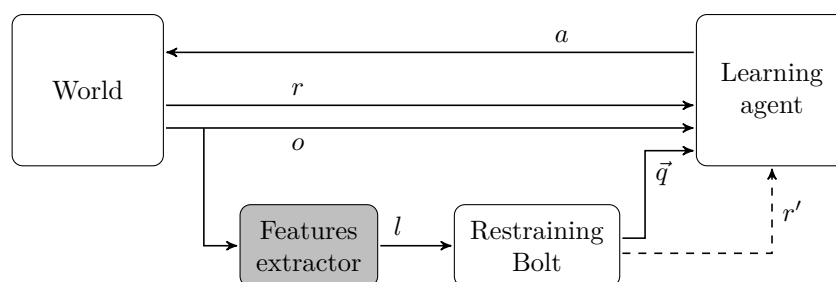


Figure 4.1. In this chapter, we focus on the features extractor.

Usually, the features extractor is not a really interesting component. Once, we've defined a fluent $p \in \mathcal{F}$, we could manually program a function, $f_p : \Omega \rightarrow \mathbb{B}$, that predicts when that event occurs or that condition is verified². This approach is perfectly fine, when applicable. However, the environments used in Deep Reinforcement Learning usually produce high-dimensional or noisy observations. As we may imagine, it becomes really hard to manually classify such inputs in the two classes. So, in order to apply to Deep RL the Restraining Bolt, or any other logic-based method, we must resort to some Machine Learning model that will help us deciding the truth of our atomic propositions.

Any Deep RL agent processes the input observation with a Neural Network. A reasonable choice would be to use a NN also as model for the features extractor. We may use a joint network that predicts the value for every fluent defined: $f : \Omega \rightarrow \mathbb{B}^{|\mathcal{F}|}$. The simplest way to train this model is through supervised learning, where we provide many input-output samples. Supervised learning can generate very accurate models, but, for every image in the training dataset, we would need to manually label the desired outputs, i.e. the fluents that are true in that image. The effort of this manual intervention would completely dominate over the advantages of the high-level, logic approach. If possible, we would certainly like to avoid this manual work.

A very promising alternative is unsupervised learning. These models don't return predictions. Instead, they memorize patterns and features that the training inputs have in common. These models have two representations: the input space, and the latent space. To any input that is presented to the model corresponds a compact representation in the latent space. The purpose of this representation is to distinguish the specific input among all of the training set³. Since the latent space is much more compact, it may be used in other computations in place of the original input. In this case, the latent vector is called an *encoding*.

Unsupervised learning will be a central part of the solution proposed here. However, it may not be the only part, because unsupervised models makes no guarantees about the meaning of the latent representation. This means that we cannot predict what each number in the latent vector represents. So, the proposed model transforms the encodings through a second function, which computes the truth value of the fluents.

² \mathbb{B} is the set $\{0, 1\}$, which represents $\{false, true\}$.

³To emphasize this concept: the purpose of the latent representation is to distinguish the input sample with respect to the training distribution.

4.1 Temporal constraints

In this whole Chapter, we’ll develop an original technique to realize the features extractor. These are the general goals that we want to pursue with this work:

- We choose the set of fluents that should be learnt.
- Learning without manual labelling.
- As few environment specific choices as possible.

In this section, we illustrate the concept of “temporal constraints”. This is the central idea introduced with this work, that will help us achieve the three principles above. As we’ll discuss in Section 4.2 and Limitations and improvements, this method, as realized in this thesis, makes some assumptions that limits its applicability to a specific class of fluents and observations. However, it poses some interesting ideas that certainly needs to be further investigated in future research. This thesis is just an initial study in this direction.

We can start from the following observation: a dataset of labelled samples is a description, by examples, of the desired meaning of the fluents. A good model would interpolate between these samples to inputs that have never been observed. Without these examples, how do we specify the desired meaning of a fluent? Note that by “meaning”, we mean the set of inputs in which the propositional symbol should be valuated to true.

What we propose here is to specify the desired temporal behaviour of these fluents with temporal logics: we can write a temporal formula, in LTL_f or LDL_f , that describes all the possible traces of the fluents we want to define. We don’t talk about *desirable* trajectories. Instead, we define all the *possible* trajectories according to the environment dynamics. For example, suppose that two conditions A and B cannot be true at the same time. Regardless of what we’re trying to achieve, we can write the following temporal constraint: $[true^*](\neg A \vee \neg B)$. This constraint is an invariant because it should hold in every instant, but there are many other interesting constraints that we may specify with temporal logic. We have A and $\langle true^* \rangle (Last \wedge A)$, which respectively mean: every episode starts/ends with A that is *true*. Also, $[true^*; A] \langle true^* \rangle B$ means that every time A becomes true, the event B must follow later on. This is a frequent pattern in request–response behaviours. The automaton associated to this constraint is shown in Figure 4.2.

Example 12. Suppose that an agent should open a door that is closed with a key, and we’ve defined the fluents $\mathcal{F} := \{HaveKey, DoorOpen\}$. We need to train a feature extractor that valuates these two propositions with their intended meaning.

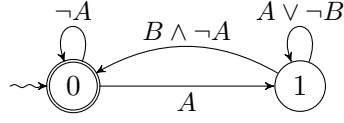


Figure 4.2. The DFA associated to the formula $[true^*; A]\langle true^* \rangle B$.

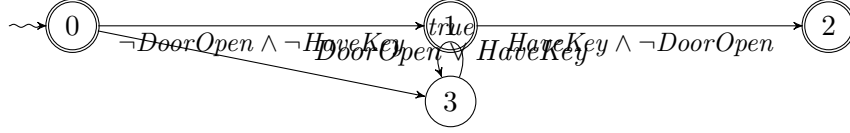


Figure 4.3. The DFA associated to Example 12.

We may write the following constraint:

$$(\neg HaveKey \wedge \neg DoorOpen) \wedge \neg \langle true^*; \neg HaveKey \rangle DoorOpen$$

which says that the door cannot be opened if at the previous instant we don't have a key, and initially the door is closed and the agent has no key. The automaton associated is shown in Figure 4.3. Note that we didn't specify that the door should be eventually opened. It only states what certainly can't happen.

We've just described how temporal constraints work. However, there is one important

4.2 Assumptions

A temporal constraints aren't definitions; they are just minimal constraints. We need additional clues: visual description of fluents. Now follow my assumptions:

- Local properties (with regions I don't have to find elements in a frame).
- The property is visually apparent, inside the region.

Limitations and other ideas for a stronger grounding.

4.3 General structure of the model

Illustration and general description of the model.

4.4 Encoding

Encoder: the model, how it works, what does it learn, size of the encoding.

References: Training Restricted Boltzmann Machines and Deep Belief Networks [23][18].

4.4.1 Model: Deep Belief Network

4.4.2 What does it learn

4.5 Boolean functions

The fluents are true in a set of those configurations.

4.5.1 Learning with genetic algorithms

Ideas from concept learning; genetic algorithm.

References: Genetic Algorithms for Concept learning[14], Genetic Algorithms review[11].

4.5.2 Boolean rules

Representation of boolean functions and training details.

4.6 Limitations and improvements

Chapter 5

AtariEyes package

Intro to the software. What we can do:

- Train a Reinforcement Learning agent.
- Train the features extraction.
- Run a Restraining Bolt while training and playing an agent.

5.1 How to use the software

5.1.1 Tools and setup

5.1.2 Commands

Small user reference.

5.2 Implementation

5.2.1 agent Module

training Module

playing Module

5.2.2 streaming Module

5.2.3 features Module

models Module

genetic Module

temporal Module

Chapter 6

Esperiments

6.1 Breakout

6.1.1 Definitions

6.1.2 Training

6.1.3 Comments

6.2 Montezuma's Revenge

6.2.1 Definitions

6.2.2 Training

6.2.3 Comments

Chapter 7

Conclusions and future work

What I have done (concretely); what I haven't done; how I'd improve the results and how to possibly relax some assumptions.

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