# Reinforcement Learning: A Comprehensive Overview

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# Contents

# Chapter 1

# Introduction

## 1.1 Sequential decision making

**Reinforcement learning** or **RL** is a class of methods for solving various kinds of sequential decision making tasks. In such tasks, we want to design an **agent** that interacts with an external **environment**. The agent maintains an internal state $s_t$, which it passes to its **policy** $\pi$ to choose an action $a_t = \pi(s_t)$. The environment responds by sending back an observation $o_{t+1}$, which the agent uses to update its internal state using the state-update function $s_{t+1} = U(s_t, a_t, o_{t+1})$. See Figure 1.1 for an illustration. There are many real-world applications of these kinds of methods[1], although the methods are more complicated than supervised learning (e.g., training a classifier) or self-supervised learning (e.g., training a language model).

### 1.1.1 Maximizing expected utility

The goal of the agent is to choose a policy $\pi$ so as to maximize the sum of expected rewards:

$$V_\pi(s_0) = \mathbb{E}_{p(a_0,s_1,a_1,\ldots,a_T,s_T|s_0,\pi)}\left[\sum_{t=0}^{T} R(s_t,a_t)|s_0\right] \tag{1.1}$$

where $s_0$ is the agent's initial state, $R(s_t, a_t)$ is the **reward function** that the agent uses to measure the value of performing an action in a given state, $V_\pi(s_0)$ is the **value function** for policy $\pi$ evaluated at $s_0$, and the expectation is wrt

$$\begin{aligned} p(a_0, s_1, a_1, \ldots, a_T, s_T|s_0, \pi) &= \pi(a_0|s_0)p_{\text{env}}(o_1|a_0)\delta(s_1 = U(s_0, a_0, o_1)) && (1.2)\\ &\times \pi(a_1|s_1)p_{\text{env}}(o_2|a_1, o_1)\delta(s_2 = U(s_1, a_1, o_2)) && (1.3)\\ &\times \pi(a_2|s_2)p_{\text{env}}(o_3|a_{1:2}, o_{1:2})\delta(s_3 = U(s_2, a_2, o_3)) \ldots && (1.4) \end{aligned}$$

where $p_{\text{env}}$ is the environment's distribution over observations (which is usually unknown).

We define the optimal policy as

$$\pi^* = \arg\max_\pi \mathbb{E}_{p_0(s_0)}\left[V_\pi(s_0)\right] \tag{1.5}$$

Note that picking a policy to maximize the sum of expected rewards is an instance of the **maximum expected utility** principle. There are various ways to design or learn an optimal policy, depending on the assumptions we make about the environment, and the form of the agent. We will discuss some of these options below.

[1] See e.g., https://bit.ly/42V7dIJ from Csaba szepesvari (2024), https://bit.ly/3EMMYCW from Vitaly Kurin (2022), and https://github.com/montrealrobotics/DeepRLInTheWorld, which seems to be kept up to date.

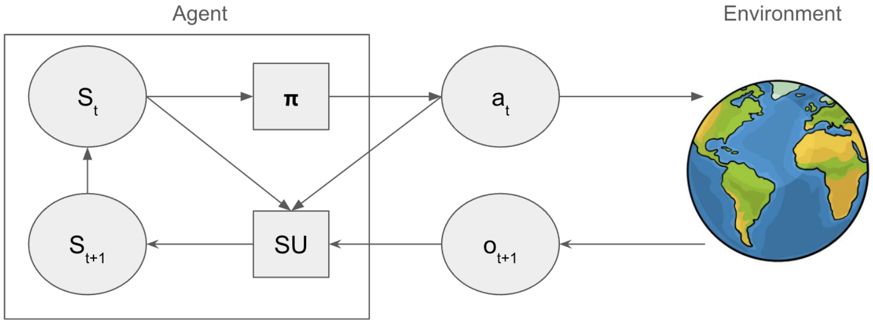


*Figure 1.1: A small agent interacting with a big external world.*

### 1.1.2 Minimizing regret

So far we have defined the RL problem in terms of maximizing the expected reward (utility). However, the upper bound on this is usually unknown, so it can be hard to know how well a given agent is doing. An alternative approach is to try to minimize the **regret**, which is defined as the difference between the expected reward under the agent's policy and the oracle policy $\pi_*$, which knows the true MDP. Specifically, let $\pi_t$ be the agent's policy at time $t$. Then the **per-step regret** at $t$ is defined as

$$l_t \triangleq \mathbb{E}_{s_{1:t}} \left[ R(s_t, \pi_*(s_t)) - \mathbb{E}_{\pi(a_t|s_t)} \left[ R(s_t, a_t) \right] \right] \tag{1.6}$$

Here the expectation is with respect to randomness in choosing actions using the policy $\pi$, as well as earlier observations, actions and rewards, as well as other potential sources of randomness.

### 1.1.3 Episodic vs continual tasks

If the agent can potentially interact with the environment forever, we call it a **continual task** [Nai+21]. In this case, we replace the sum of rewards (when defining the value function) with the **average reward** [WNS21].

Alternatively, we say the agent is in an **episodic task** if its interaction terminates once the system enters a **terminal state** or **absorbing state**, which is a state which transitions to itself with 0 reward. After entering a terminal state, we may start a new **episode** from a new initial world state $z_0 \sim p_0$. (The agent will typically also reinitialize its own internal state $s_0$.) The episode length is in general random. (For example, the length of an interaction with a chatbot may be quite variable, depending on the decisions taken by the chatbot agent and the randomness in the environment (i.e., the responses from the user)). Finally, if the trajectory length $T$ in an episodic task is fixed and known, it is called a **finite horizon problem**.

We define the **return** for a state at time $t$ to be the sum of expected rewards obtained going forwards, where each reward is multiplied by a **discount factor** $\gamma \in [0, 1]$:

$$G_t \triangleq r_t + \gamma r_{t+1} + \gamma^2 r_{t+2} + \cdots + \gamma^{T-t-1} r_{T-1} \tag{1.7}$$

$$= \sum_{k=0}^{T-t-1} \gamma^k r_{t+k} = \sum_{j=t}^{T-1} \gamma^{j-t} r_j \tag{1.8}$$

where $r_t = R(s_t, a_t)$ is the reward, and $G_t$ is the **reward-to-go**. For episodic tasks that terminate at time $T$, we define $G_t = 0$ for $t \geq T$. Clearly, the return satisfies the following recursive relationship:

$$G_t = r_t + \gamma(r_{t+1} + \gamma r_{t+2} + \cdots) = r_t + \gamma G_{t+1} \tag{1.9}$$

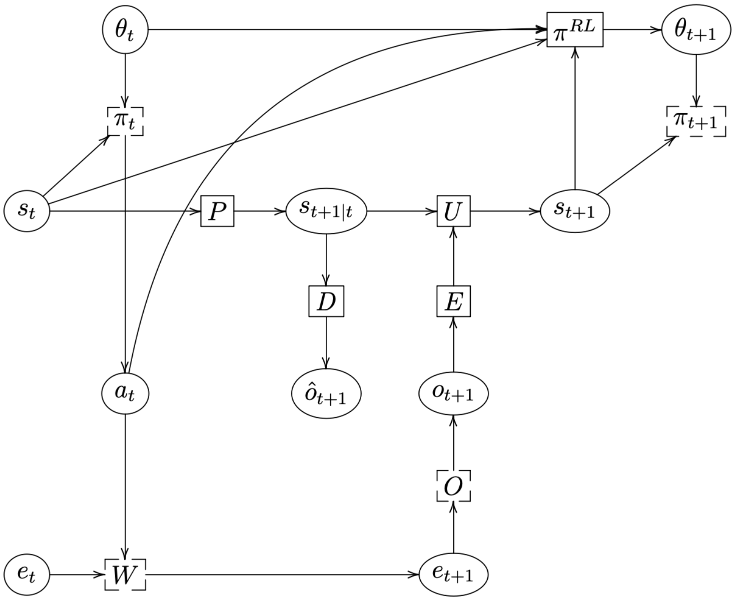


*Figure 1.2: Diagram illustrating the interaction of the agent and environment. The agent has internal state $s_t$, and chooses action $a_t$ based on its policy $\pi_t$. It then predicts its next internal states, $s_{t+1|t}$, via the predict function $P$, and optionally predicts the resulting observation, $\hat{o}_{t+1}$, via the observation decoder $D$. The environment has (hidden) internal state $e_t$, which gets updated by the world model $W$ to give the new state $e_{t+1} = W(e_t, a_t)$ in response to the agent's action. The environment also emits an observation $o_{t+1}$ via the observation model $O$. This gets encoded to $e_{t+1}$ by the agent's observation encoder $E$, which the agent uses to update its internal state using $s_{t+1} = U(s_t, a_t, e_{t+1})$. The policy is parameterized by $\theta_t$, and these parameters may be updated (at a slower time scale) by the RL policy $\pi^{RL}$. Square nodes are functions, circles are variables (either random or deterministic). Dashed square nodes are stochastic functions that take an extra source of randomness (not shown).*

Furthermore, we define the value function to be the expected reward-to-go:

$$V_\pi(s_t) = \mathbb{E}\left[G_t|\pi\right] \tag{1.10}$$

The discount factor $\gamma$ plays two roles. First, it ensures the return is finite even if $T = \infty$ (i.e., infinite horizon), provided we use $\gamma < 1$ and the rewards $r_t$ are bounded. Second, it puts more weight on short-term rewards, which generally has the effect of encouraging the agent to achieve its goals more quickly. (For example, if $\gamma = 0.99$, then an agent that reaches a terminal reward of 1.0 in 15 steps will receive an expected discounted reward of $0.99^{15} = 0.86$, whereas if it takes 17 steps it will only get $0.99^{17} = 0.84$.) However, if $\gamma$ is too small, the agent will become too greedy. In the extreme case where $\gamma = 0$, the agent is completely **myopic**, and only tries to maximize its immediate reward. In general, the discount factor reflects the assumption that there is a probability of $1 - \gamma$ that the interaction will end at the next step. (If $\gamma = 1 - \frac{1}{T}$, the agent expects to live on the order of $T$ steps; for example, if each step is 0.1 seconds, then $\gamma = 0.95$ corresponds to 2 seconds.) For finite horizon problems, where $T$ is known, we can set $\gamma = 1$, since we know the life time of the agent a priori.

### 1.1.4 Universal model

A generic representation for sequential decision making problems (which is an extended version of the "universal modeling framework" proposed in [Pow19; Pow22]) is shown in Figure 1.2. Here we have assumed the environment can be modeled by a controlled **Markov process**[2] with hidden state $e_t$, which gets updated at each step in response to the agent's action $a_t$. To allow for non-deterministic dynamics, we write this as $e_{t+1} = W(e_t, a_t, \epsilon_t^e)$, where $W$ is the environment's state transition function (which is usually not known to the agent) and $\epsilon_t^e$ is random system noise.[3], The agent does not see the world state $e_t$, but instead sees a potentially noisy and/or partial observation $o_{t+1} = O(e_{t+1}, \epsilon_{t+1}^o)$ at each step, where $\epsilon_{t+1}^o$ is random observation noise. For example, when navigating a maze, the agent may only see what is in front of it, rather than seeing everything in the world all at once; furthermore, even the current view may be corrupted by sensor noise. Any given image, such as one containing a door, could correspond to many different locations in the world (this is called **perceptual aliasing**), each of which may require a different action. Thus the agent needs use these observations to incrementally update its own internal **belief state** about the world, using the state update function $s_{t+1} = SU(s_t, a_t, o_{t+1})$; this represents the agent's beliefs about the underlying world state $e_t$, as well as the unknown world model $W$ itself (or some proxy thereof). In the simplest setting, the internal $s_t$ can just store all the past observations, $\boldsymbol{h}_t = (\boldsymbol{o}_{1:t}, \boldsymbol{a}_{1:t-1})$, but such non-parametric models can take a lot of time and space to work with, so we will usually consider parametric approximations. The agent can then pass its state to its policy to pick actions, using $a_{t+1} = \pi_t(s_{t+1})$.

We can further elaborate the behavior of the agent by breaking the state-update function into two parts. First the agent predicts its own next state, $s_{t+1|t} = P(s_t, a_t)$, using a **prediction function** $P$, and then it updates this prediction given the observation using **update function** $U$, to give $s_{t+1} = U(s_{t+1|t}, o_{t+1})$. Thus the $SU$ function is defined as the composition of the predict and update functions: $s_{t+1} = SU(s_t, a_t, o_{t+1}) = U(P(s_t, a_t), o_{t+1})$. If the observations are high dimensional (e.g., images), the agent may choose to encode its observations into a low-dimensional embedding $e_{t+1}$ using an encoder, $e_{t+1} = E(o_{t+1})$; this can encourage the agent to focus on the relevant parts of the sensory signal. (The state update then becomes $s_{t+1} = U(s_{t+1|t}, e_{t+1})$.) Optionally the agent can also learn to invert this encoder by training a decoder to predict the next observation using $\hat{o}_{t+1} = D(s_{t+1|t})$; this can be a useful training signal, as we will discuss in Chapter 4. Finally, the agent needs to learn the action policy $\pi_t$. We parameterize this by $\boldsymbol{\theta}_t$, so $\pi_t(s_t) = \pi(s_t; \boldsymbol{\theta}_t)$. These parameters themselves may need to be learned; we use the notation $\pi^{RL}$ to denote the RL policy which specifies how to update the policy parameters at each step. See Figure 1.2 for an illustration.

We see that, in general, there are three interacting stochastic processes we need to deal with: the environment's states $e_t$ (which are usually affected by the agents actions); the agent's internal states $s_t$ (which reflect its beliefs about the environment based on the observed data); and the the agent's policy parameters $\boldsymbol{\theta}_t$ (which are updated based on the information stored in the belief state). The reason there are so many RL algorithms is that this framework is very general. In the rest of this manuscript we will study special cases, where we make different assumptions about the environment's state $e_t$ and dynamics, the agent's state $s_t$ and dynamics, the form of the action policy $a_t = \pi(s_t, \boldsymbol{\theta}_t)$, and the form of the policy learning method $\boldsymbol{\theta}_{t+1} = \pi^{RL}(\boldsymbol{\theta}_t, s_t, a_t, o_{t+1})$.

### 1.1.5 Further reading

In later chapters, we will describe methods for learning the best policy to maximize $V_\pi(s_0) = \mathbb{E}\left[G_0|s_0, \pi\right])$. More details on RL can be found in textbooks such as [Sze10; SB18; Aga+22a; Pla22; ID19; RJ22; Li23; MMT24], and reviews such as [Aru+17; FL+18; Li18; Wen18a]. For details on how RL relates to **control theory**, see e.g., [Son98; Rec19; Ber19; Mey22], and for connections to operations research, see [Pow22].

## 1.2 Canonical models

In this section, we describe different forms of model for the environment and the agent that have been studied in the literature.

[2] The Markovian assumption is without loss of generality, since we can always condition on the entire past sequence of states by suitably expanding the Markovian state space.

[3] Representing a stochastic function as a deterministic function with some noisy inputs is known as a functional causal model, or structural equation model. This is standard practice in the control theory and causality communities.

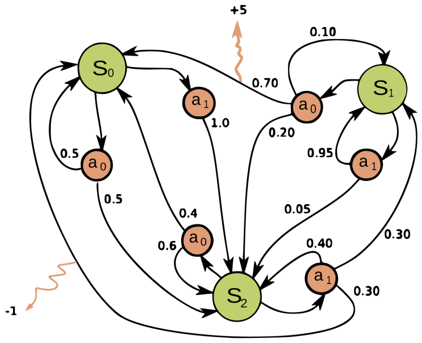


*Figure 1.3: Illustration of an MDP as a finite state machine (FSM). The MDP has three discrete states (green cirlces), two discrete actions (orange circles), and two non-zero rewards (orange arrows). The numbers on the black edges represent state transition probabilities, e.g., $p(s' = s_0|a = a_0, s' = s_0) = 0.7$; most state transitions are impossible (probability 0), so the graph is sparse. The numbers on the yellow wiggly edges represent expected rewards, e.g., $R(s = s_1, a = a_0, s' = s_0) = +5$; state transitions with zero reward are not annotated. From https://en.wikipedia.org/wiki/Markov_decision_process. Used with kind permission of Wikipedia author waldoalvarez.*

### 1.2.1 Partially observed MDPs

The model shown in Figure 1.2 is called a **partially observable Markov decision process** or **POMDP** (pronounced "pom-dee-pee") [KLC98]. Typically the environment's dynamics model is represented by a stochastic transition function, rather than a deterministic function with noise as an input. We can derive this transition function as follows:

$$p(e_{t+1}|e_t, a_t) = \mathbb{E}_{\epsilon_t^e}\left[\mathbb{I}\left(e_{t+1} = W(e_t, a_t, \epsilon_t^e)\right)\right] \tag{1.11}$$

Similarly the stochastic observation function is given by

$$p(o_{t+1}|e_{t+1}) = \mathbb{E}_{\epsilon_{t+1}^o}\left[\mathbb{I}\left(o_{t+1} = O(e_{t+1}, \epsilon_{t+1}^o)\right)\right] \tag{1.12}$$

Note that we can combine these two distributions to derive the joint world model $p_{WO}(e_{t+1}, o_{t+1}|e_t, a_t)$. Also, we can use these distributions to derive the environment's non-Markovian observation distribution, $p_{\text{env}}(o_{t+1}|o_{1:t}, a_{1:t})$, used in Equation (1.4), as follows:

$$p_{\text{env}}(o_{t+1}|o_{1:t}, a_{1:t}) = \sum_{e_{t+1}} p(o_{t+1}|e_{t+1})p(e_{t+1}|a_{1:t}) \tag{1.13}$$

$$p(e_{t+1}|a_{1:t}) = \sum_{e_1} \cdots \sum_{e_t} p(e_1|a_1)p(e_2|e_1, a_1) \dots p(e_{t+1}|e_t, a_t) \tag{1.14}$$

If the world model (both $p(o|z)$ and $p(z'|z, a)$) is known, then we can — in principle — solve for the optimal policy. The method requires that the agent's internal state correspond to the **belief state** $s_t = \boldsymbol{b}_t = p(e_t|\boldsymbol{h}_t)$, where $\boldsymbol{h}_t = (o_{1:t}, a_{1:t-1})$ is the observation history. The belief state can be updated recursively using Bayes rule. See Section 1.2.5 for details. The belief state forms a sufficient statistic for the optimal policy. Unfortunately, computing the belief state and the resulting optimal policy is wildly intractable [PT87; KLC98]. We discuss some approximate methods in Section 1.3.4.

### 1.2.2 Markov decision process (MDPs)

A **Markov decision process** [Put94] is a special case of a POMDP in which the environment states are observed, so $e_t = o_t = s_t$. We usually define an MDP in terms of the state transition matrix induced by the world model:

$$p_S(s_{t+1}|s_t, a_t) = \mathbb{E}_{\epsilon_t^s}\left[\mathbb{I}\left(s_{t+1} = W(s_t, a_t, \epsilon_t^s)\right)\right] \tag{1.15}$$

In lieu of an observation model, we assume the environment (as opposed to the agent) sends out a reward signal, sampled from $p_R(r_t|s_t, a_t, s_{t+1})$. The expected reward is then given by

$$R(s_t, a_t, s_{t+1}) = \sum_r r \;\; p_R(r|s_t, a_t, s_{t+1}) \tag{1.16}$$

$$R(s_t, a_t) = \sum_{s_{t+1}} p_S(s_{t+1}|s_t, a_t) R(s_t, a_t, s_{t+1}) \tag{1.17}$$

Note that the field of control theory uses slightly different terminology and notation when describing the same setup: the environment is called the **plant**, the agent is called the **controller**, States are denoted by $\boldsymbol{x}_t \in \mathcal{X} \subseteq \mathbb{R}^D$, actions are denoted by $\boldsymbol{u}_t \in \mathcal{U} \subseteq \mathbb{R}^K$, and rewards are replaced by costs $c_t \in \mathbb{R}$.

Given a stochastic policy $\pi(a_t|s_t)$, the agent can interact with the environment over many steps. Each step is called a **transition**, and consists of the tuple $(s_t, a_t, r_t, s_{t+1})$, where $a_t \sim \pi(\cdot|s_t)$, $s_{t+1} \sim p_S(s_t, a_t)$, and $r_t \sim p_R(s_t, a_t, s_{t+1})$. Hence, under policy $\pi$, the probability of generating a **trajectory** length $T$, $\boldsymbol{\tau} = (s_0, a_0, r_0, s_1, a_1, r_1, s_2, \ldots, s_T)$, can be written explicitly as

$$p(\boldsymbol{\tau}) = p_0(s_0) \prod_{t=0}^{T-1} \pi(a_t|s_t) p_S(s_{t+1}|s_t, a_t) p_R(r_t|s_t, a_t, s_{t+1}) \tag{1.18}$$

In general, the state and action sets of an MDP can be discrete or continuous. When both sets are finite, we can represent these functions as lookup tables; this is known as a **tabular representation**. In this case, we can represent the MDP as a **finite state machine**, which is a graph where nodes correspond to states, and edges correspond to actions and the resulting rewards and next states. Figure 1.3 gives a simple example of an MDP with 3 states and 2 actions.

If we know the world model $p_S$ and $p_R$, and if the state and action space is tabular, then we can solve for the optimal policy using dynamic programming techniques, as we discuss in Section 2.2. However, typically the world model is unknown, and the states and actions may need complex nonlinear models to represent their transitions. In such cases, we will have to use RL methods to learn a good policy.

### 1.2.3 Contextual MDPs

A **Contextual MDP** [HDCM15] is an MDP where the dynamics and rewards of the environment depend on a hidden static parameter referred to as the context. (This is different to a contextual bandit, discussed in Section 1.2.4, where the context is observed at each step.) A simple example of a contextual MDP is a video game, where each level of the game is **procedurally generated**, that is, it is randomly generated each time the agent starts a new episode. Thus the agent must solve a sequence of related MDPs, which are drawn from a common distribution. This requires the agent to **generalize** across multiple MDPs, rather than overfitting to a specific environment [Cob+19; Kir+21; Tom+22]. (This form of generalization is different from generalization within an MDP, which requires generalizing across states, rather than across environments; both are important.)

A contextual MDP is a special kind of POMDP where the hidden variable corresponds to the unknown parameters of the model. In [Gho+21], they call this an **epistemic POMDP**, which is closely related to the concept of belief state MDP which we discuss in Section 1.2.5.

### 1.2.4 Contextual bandits

A **contextual bandit** is a special case of a POMDP where the world state transition function is independent of the action of the agent and the previous state, i.e., $p(e_t|e_{t-1}, a_t) = p(e_t)$. In this case, we call the world states "contexts"; these are observable by the agent, i.e., $o_t = e_t$. Since the world state distribution is independent of the agents actions, the agent has no effect on the external environment. However, its actions do affect the rewards that it receives. Thus the agent's internal belief state — about the underlying reward function $R(o, a)$ — does change over time, as the agent learns a model of the world (see Section 1.2.5).

A special case of a contextual bandit is a regular bandit, in which there is no context, or equivalently, $s_t$ is some fixed constant that never changes. When there are a finite number of possible actions, $\mathcal{A} = \{a_1, \ldots, a_K\}$, this is called a **multi-armed bandit**.[4] In this case the reward model has the form $R(a) = f(\boldsymbol{w}_a)$, where $\boldsymbol{w}_a$ are the parameters for arm $a$.

Contextual bandits have many applications. For example, consider an **online advertising system**. In this case, the state $s_t$ represents features of the web page that the user is currently looking at, and the action $a_t$ represents the identity of the ad which the system chooses to show. Since the relevance of the ad depends on the page, the reward function has the form $R(s_t, a_t)$, and hence the problem is contextual. The goal is to maximize the expected reward, which is equivalent to the expected number of times people click on ads; this is known as the **click through rate** or **CTR**. (See e.g., [Gra+10; Li+10; McM+13; Aga+14; Du+21; YZ22] for more information about this application.) Another application of contextual bandits arises in **clinical trials** [VBW15]. In this case, the state $s_t$ are features of the current patient we are treating, and the action $a_t$ is the treatment the doctor chooses to give them (e.g., a new drug or a **placebo**).

For more details on bandits, see e.g., [LS19; Sli19].

### 1.2.5 Belief state MDPs

In this section, we describe a kind of MDP where the state represents a probability distribution, known as a **belief state** or **information state**, which is updated by the agent ("in its head") as it receives information from the environment.[5] More precisely, consider a contextual bandit problem, where the agent approximates the unknown reward by a function $R(o, a) = f(o, a; \boldsymbol{w})$. Let us denote the posterior over the unknown parameters by $\boldsymbol{b}_t = p(\boldsymbol{w}|\boldsymbol{h}_t)$, where $\boldsymbol{h}_t = \{o_{1:t}, a_{1:t}, r_{1:t}\}$ is the history of past observations, actions and rewards. This belief state can be updated deterministically using Bayes' rule; we denote this operation by $\boldsymbol{b}_{t+1} = \text{BayesRule}(\boldsymbol{b}_t, o_{t+1}, a_{t+1}, r_{t+1})$. (This corresponds to the state update $SU$ defined earlier.) Using this, we can define the following **belief state MDP**, with deterministic dynamics given by

$$p(\boldsymbol{b}_{t+1}|\boldsymbol{b}_t, o_{t+1}, a_{t+1}, r_{t+1}) = \mathbb{I}\left(\boldsymbol{b}_{t+1} = \text{BayesRule}(\boldsymbol{b}_t, o_{t+1}, a_{t+1}, r_{t+1})\right) \tag{1.19}$$

and reward function given by

$$p(r_t|o_t, a_t, \boldsymbol{b}_t) = \int p_R(r_t|o_t, a_t; \boldsymbol{w}) p(\boldsymbol{w}|\boldsymbol{b}_t) d\boldsymbol{w} \tag{1.20}$$

If we can solve this (PO)MDP, we have the optimal solution to the exploration-exploitation problem (see Section 1.3.5).

As a simple example, consider a context-free **Bernoulli bandit**, where $p_R(r|a) = \text{Ber}(r|\mu_a)$, and $\mu_a = p_R(r = 1|a) = R(a)$ is the expected reward for taking action $a$. The only unknown parameters are $\boldsymbol{w} = \mu_{1:A}$. Suppose we use a factored beta prior

$$p_0(\boldsymbol{w}) = \prod_a \text{Beta}(\mu_a|\alpha_0^a, \beta_0^a) \tag{1.21}$$

where $\boldsymbol{w} = (\mu_1, \ldots, \mu_K)$. We can compute the posterior in closed form to get

$$p(\boldsymbol{w}|\mathcal{D}_t) = \prod_a \text{Beta}(\mu_a|\underbrace{\alpha_0^a + N_t^0(a)}_{\alpha_t^a}, \underbrace{\beta_0^a + N_t^1(a)}_{\beta_t^a}) \tag{1.22}$$

where

$$N_t^r(a) = \sum_{i=1}^{t-1} \mathbb{I}\left(a_i = a, r_i = r\right) \tag{1.23}$$

[4] The terminology arises by analogy to a slot machine (sometimes called a "bandit") in a casino. If there are $K$ slot machines, each with different rewards (payout rates), then the agent (player) must explore the different machines until they have discovered which one is best, and can then stick to exploiting it.

[5] Technically speaking, this is a POMDP, where we assume the states are observed, and the parameters are the unknown hidden random variables. This is in contrast to Section 1.2.1, where the states were not observed, and the parameters were assumed to be known.

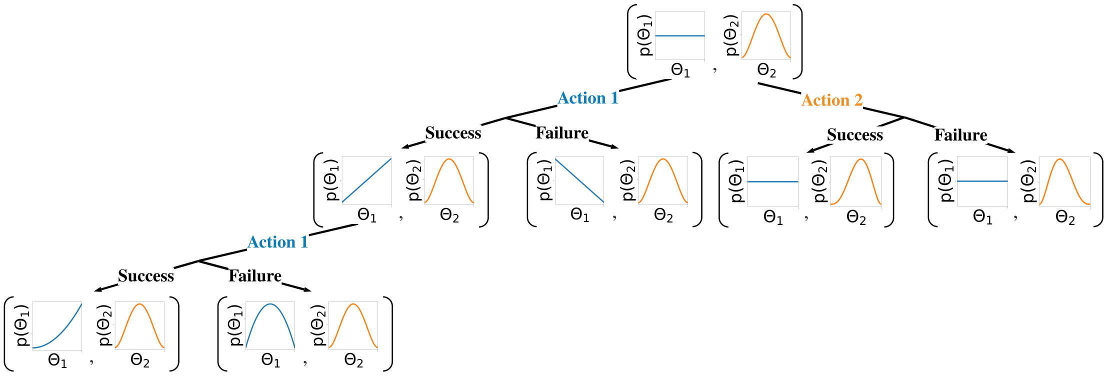


*Figure 1.4: Illustration of sequential belief updating for a two-armed beta-Bernoulli bandit. The prior for the reward for action 1 is the (blue) uniform distribution* Beta(1, 1)*; the prior for the reward for action 2 is the (orange) unimodal distribution* Beta(2, 2)*. We update the parameters of the belief state based on the chosen action, and based on whether the observed reward is success (1) or failure (0).*

This is illustrated in Figure 1.4 for a two-armed Bernoulli bandit. We can use a similar method for a **Gaussian bandit**, where $p_R(r|a) = \mathcal{N}(r|\mu_a, \sigma_a^2)$.

In the case of contextual bandits, the problem is conceptually the same, but becomes more complicated computationally. If we assume a **linear regression bandit**, $p_R(r|s, a; \boldsymbol{w}) = \mathcal{N}(r|\boldsymbol{\phi}(s, a)^\mathsf{T}\boldsymbol{w}, \sigma^2)$, we can use Bayesian linear regression to compute $p(\boldsymbol{w}|\mathcal{D}_t)$ exactly in closed form. If we assume a **logistic regression bandit**, $p_R(r|s, a; \boldsymbol{w}) = \text{Ber}(r|\sigma(\boldsymbol{\phi}(s, a)^\mathsf{T}\boldsymbol{w}))$, we have to use approximate methods for approximate Bayesian logistic regression to compute $p(\boldsymbol{w}|\mathcal{D}_t)$. If we have a **neural bandit** of the form $p_R(r|s, a; \boldsymbol{w}) = \mathcal{N}(r|f(s, a; \boldsymbol{w}))$ for some nonlinear function $f$, then posterior inference is even more challenging (this is equivalent to the problem of inference in Bayesian neural networks, see e.g., [Arb+23] for a review paper for the offline case, and [DMKM22; JCM24] for some recent online methods).

We can generalize the above methods to compute the belief state for the parameters of an MDP in the obvious way, but modeling both the reward function and state transition function.

Once we have computed the belief state, we can derive a policy with optimal regret using the methods like UCB (Section 7.1.2) or Thompson sampling (Section 7.1.3).

### 1.2.6 Optimization problems

The bandit problem is an example of a problem where the agent must interact with the world in order to collect information, but it does not otherwise affect the environment. Thus the agents internal belief state changes over time, but the environment state does not.[6] Such problems commonly arise when we are trying to optimize a fixed but unknown function $R$. We can "query" the function by evaluating it at different points (parameter values), and in some cases, the resulting observation may also include gradient information. The agent's goal is to find the optimum of the function in as few steps as possible.[7] We give some examples of this problem setting below.

[6] In the contextual bandit problem, the environment state (context) does change, but not in response to the agent's actions. Thus $p(o_t)$ is usually assumed to be a static distribution.

[7] If we only care about the final performance of the agent, we can try to minimize the **simple regret**, which is just the regret at the last step, namely $l_T$. This is the difference between the function value we chose and the true optimum. Minimizing simple regret results in a problem known as **pure exploration** [BMS11], where the agent needs to interact with the environment to learn the underlying MDP; at the end, it can then solve for the resulting policy using planning methods (see Section 2.2). However, in general RL problems, it is more common to focus on the **cumulative regret**, also called the **total regret** or just the **regret**, which is defined as $L_T \triangleq \mathbb{E}\left[\sum_{t=1}^T l_t\right]$.

#### 1.2.6.1 Best-arm identification

In the standard multi-armed bandit problem our goal is to maximize the sum of expected rewards. However, in some cases, the goal is to determine the best arm given a fixed budget of $T$ trials; this variant is known as **best-arm identification** [ABM10]. Formally, this corresponds to optimizing the **final reward** criterion:

$$V_{\pi,\pi_T} = \mathbb{E}_{p(a_{1:T},r_{1:T}|s_0,\pi)}\left[R(\hat{a})\right] \tag{1.24}$$

where $\hat{a} = \pi_T(a_{1:T}, r_{1:T})$ is the estimated optimal arm as computed by the **terminal policy** $\pi_T$ applied to the sequence of observations obtained by the exploration policy $\pi$. This can be solved by a simple adaptation of the methods used for standard bandits.

#### 1.2.6.2 Bayesian optimization

Bayesian optimization is a gradient-free approach to optimizing expensive blackbox functions. That is, we want to find

$$\boldsymbol{w}^* = \underset{\boldsymbol{w}}{\operatorname{argmax}}\, R(\boldsymbol{w}) \tag{1.25}$$

for some unknown function $R$, where $\boldsymbol{w} \in \mathbb{R}^N$, using as few actions (function evaluations of $R$) as possible. This is essentially an “infinite arm” version of the best-arm identification problem [Tou14], where we replace the discrete choice of arms $a \in \{1, \ldots, K\}$ with the parameter vector $\boldsymbol{w} \in \mathbb{R}^N$. In this case, the optimal policy can be computed if the agent's state $s_t$ is a belief state over the unknown function, i.e., $s_t = p(R|\boldsymbol{h}_t)$. A common way to represent this distribution is to use Gaussian processes. We can then use heuristics like expected improvement, knowledge gradient or Thompson sampling to implement the corresponding policy, $\boldsymbol{w}_t = \pi(s_t)$. For details, see e.g., [Gar23].

#### 1.2.6.3 Active learning

Active learning is similar to BayesOpt, but instead of trying to find the point at which the function is largest (i.e., $\boldsymbol{w}^*$), we are trying to learn the whole function $R$, again by querying it at different points $\boldsymbol{w}_t$. Once again, the optimal strategy again requires maintaining a belief state over the unknown function, but now the best policy takes a different form, such as choosing query points to reduce the entropy of the belief state. See e.g., [Smi+23].

#### 1.2.6.4 Stochastic Gradient Descent (SGD)

Finally we discuss how to interpret SGD as a sequential decision making process, following [Pow22]. The action space consists of querying the unknown function $R$ at locations $\boldsymbol{a}_t = \boldsymbol{w}_t$, and observing the function value $r_t = R(\boldsymbol{w}_t)$; however, unlike BayesOpt, now we also observe the corresponding gradient $\boldsymbol{g}_t = \nabla_{\boldsymbol{w}} R(\boldsymbol{w})|_{\boldsymbol{w}_t}$, which gives non-local information about the function. The environment state contains the true function $R$ which is used to generate the observations given the agent's actions. The agent state contains the current parameter estimate $\boldsymbol{w}_t$, and may contain other information such as first and second moments $\boldsymbol{m}_t$ and $\boldsymbol{v}_t$, needed by methods such as Adam. The update rule (for vanilla SGD) takes the form $\boldsymbol{w}_{t+1} = \boldsymbol{w}_t + \alpha_t \boldsymbol{g}_t$, where the stepsize $\alpha_t$ is chosen by the policy, $\alpha_t = \pi(s_t)$. The terminal policy has the form $\pi(s_T) = \boldsymbol{w}_T$.

Although in principle it is possible to learn the learning rate (stepsize) policy using RL (see e.g., [Xu+17]), the policy is usually chosen by hand, either using a **learning rate schedule** or some kind of manually designed **adaptive learning rate** policy (e.g., based on second order curvature information).

## 1.3 Reinforcement Learning: a brief overview

In this section, we give a brief overview of how to compute optimal policies when the model of the environment is unknown; this is the core problem tackled by RL. We mostly focus on the MDP case, but discuss the POMDP case in Section 1.3.4.

We can categorize RL methods along mutiple dimensions, such as the following:

| Approach | Method | Functions learned | On/Off | Section |
|---|---|---|---|---|
| Value-based | SARSA | $Q(s, a)$ | On | Section 2.4 |
| Value-based | $Q$-learning | $Q(s, a)$ | Off | Section 2.5 |
| Policy-based | REINFORCE | $\pi(a\|s)$ | On | Section 3.2 |
| Policy-based | A2C | $\pi(a\|s)$, $V(s)$ | On | Section 3.3.1 |
| Policy-based | TRPO/PPO | $\pi(a\|s)$, $\text{Adv}(s, a)$ | On | Section 3.4.3 |
| Policy-based | DDPG | $a = \pi(s)$, $Q(s, a)$ | Off | Section 3.7.1 |
| Policy-based | Soft actor-critic | $\pi(a\|s)$, $Q(s, a)$ | Off | Section 3.6.8 |
| Model-based | MBRL | $p(s'\|s, a)$ | Off | Chapter 4 |

*Table 1.1: Summary of some popular methods for RL. On/off refers to on-policy vs off-policy methods.*

- What does the agent learn? Options include the value function, the policy, the model, or some combination of the above.

- How does the agent represent its unknown functions? The two main choices are to use non-parametric or **tabular representations**, or to use parametric representations based on function approximation. If these functions are based on neural networks, this approach is called "**deep RL**", where the term "deep" refers to the use of neural networks with many layers.

- How are the actions are selected? Options include **on-policy** methods, where actions must be selected by the agent's current policy), and **off-policy** methods, where actions can be select by any kind of policy, including human demonstrations.

Table 1.1 lists a few common examples of RL methods, classified along these lines. More details are given in the subsequent sections.

### 1.3.1 Value-based RL

In this section, we give a brief introduction to **value-based RL**, also called **Approximate Dynamic Programming** or **ADP**; see Chapter 2 for more details.

We introduced the value function $V_\pi(s)$ in Equation (1.1), which we repeat here for convenience:

$$V_\pi(s) \triangleq \mathbb{E}_\pi \left[ G_0 | s_0 = s \right] = \mathbb{E}_\pi \left[ \sum_{t=0}^{\infty} \gamma^t r_t | s_0 = s \right] \tag{1.26}$$

The value function for the optimal policy $\pi^*$ is known to satisfy the following recursive condition, known as **Bellman's equation**:

$$V_*(s) = \max_a R(s, a) + \gamma \mathbb{E}_{p_S(s'|s,a)} \left[ V_*(s') \right] \tag{1.27}$$

This follows from the principle of **dynamic programming**, which computes the optimal solution to a problem (here the value of state $s$) by combining the optimal solution of various subproblems (here the values of the next states $s'$). This can be used to derive the following learning rule:

$$V(s) \leftarrow V(s) + \eta[r + \gamma V(s') - V(s)] \tag{1.28}$$

where $s' \sim p_S(\cdot|s, a)$ is the next state sampled from the environment, and $r = R(s, a)$ is the observed reward. This is called **Temporal Difference** or **TD** learning (see Section 2.3.2 for details). Unfortunately, it is not clear how to derive a policy if all we know is the value function. We now describe a solution to this problem.

We first generalize the notion of value function to assigning a value to a state and action pair, by defining the **Q function** as follows:

$$Q_\pi(s, a) \triangleq \mathbb{E}_\pi \left[ G_0 | s_0 = s, a_0 = a \right] = \mathbb{E}_\pi \left[ \sum_{t=0}^{\infty} \gamma^t r_t | s_0 = s, a_0 = a \right] \tag{1.29}$$

This quantity represents the expected return obtained if we start by taking action $a$ in state $s$, and then follow $\pi$ to choose actions thereafter. The $Q$ function for the optimal policy satisfies a modified Bellman equation

$$Q_*(s, a) = R(s, a) + \gamma \mathbb{E}_{p_S(s'|s,a)} \left[ \max_{a'} Q_*(s', a') \right] \tag{1.30}$$

This gives rise to the following TD update rule:

$$Q(s, a) \leftarrow r + \gamma \max_{a'} Q(s', a') - Q(s, a) \tag{1.31}$$

where we sample $s' \sim p_S(\cdot|s, a)$ from the environment. The action is chosen at each step from the implicit policy

$$a = \operatorname*{argmax}_{a'} Q(s, a') \tag{1.32}$$

This is called **Q learning** (see Section 2.5 for details),

### 1.3.2 Policy-based RL

In this section we give a brief introductin to **Policy-based RL**; for details see Chapter 3.

In policy-based methods, we try to directly maximize $J(\pi_{\boldsymbol{\theta}}) = \mathbb{E}_{p(s_0)} [V_\pi(s_0)]$ wrt the parameter's $\boldsymbol{\theta}$; this is called **policy search**. If $J(\pi_{\boldsymbol{\theta}})$ is differentiable wrt $\boldsymbol{\theta}$, we can use stochastic gradient ascent to optimize $\boldsymbol{\theta}$, which is known as **policy gradient** (see Section 3.1).

Policy gradient methods have the advantage that they provably converge to a local optimum for many common policy classes, whereas $Q$-learning may diverge when approximation is used (Section 2.5.2.4). In addition, policy gradient methods can easily be applied to continuous action spaces, since they do not need to compute $\operatorname{argmax}_a Q(s, a)$. Unfortunately, the score function estimator for $\nabla_{\boldsymbol{\theta}} J(\pi_{\boldsymbol{\theta}})$ can have a very high variance, so the resulting method can converge slowly.

One way to reduce the variance is to learn an approximate value function, $V_{\boldsymbol{w}}(s)$, and to use it as a baseline in the score function estimator. We can learn $V_{\boldsymbol{w}}(s)$ using using TD learning. Alternatively, we can learn an advantage function, $A_{\boldsymbol{w}}(s, a)$, and use it as a baseline. These policy gradient variants are called **actor critic** methods, where the actor refers to the policy $\pi_{\boldsymbol{\theta}}$ and the critic refers to $V_{\boldsymbol{w}}$ or $A_{\boldsymbol{w}}$. See Section 3.3 for details.

### 1.3.3 Model-based RL

In this section, we give a brief introduction to **model-based RL**; for more details, see Chapter 4.

Value-based methods, such as Q-learning, and policy search methods, such as policy gradient, can be very **sample inefficient**, which means they may need to interact with the environment many times before finding a good policy, which can be problematic when real-world interactions are expensive. In model-based RL, we first learn the MDP, including the $p_S(s'|s, a)$ and $R(s, a)$ functions, and then compute the policy, either using approximate dynamic programming on the learned model, or doing lookahead search. In practice, we often interleave the model learning and planning phases, so we can use the partially learned policy to decide what data to collect, to help learn a better model.

### 1.3.4 State uncertainty (partial observability)

In an MDP, we assume that the state of the environment $s_t$ is the same as the observation $o_t$ obtained by the agent. But in many problems, the observation only gives partial information about the underlying state of the world (e.g., a rodent or robot navigating in a maze). This is called **partial observability**. In this case, using a policy of the form $a_t = \pi(o_t)$ is suboptimal, since $o_t$ does not give us complete state information. Instead we need to use a policy of the form $a_t = \pi(\boldsymbol{h}_t)$, where $\boldsymbol{h}_t = (a_1, o_1, \ldots, a_{t-1}, o_t)$ is the entire past history of observations and actions, plus the current observation. Since depending on the entire past is not tractable for a long-lived agent, various approximate solution methods have been developed, as we summarize below.

#### 1.3.4.1 Optimal solution

If we know the true latent structure of the world (i.e., both $p(o|z)$ and $p(z'|z, a)$, to use the notation of Section 1.1.4), then we can use solution methods designed for POMDPs, discussed in Section 1.2.1. This requires using Bayesian inference to compute a belief state, $\boldsymbol{b}_t = p(e_t|\boldsymbol{h}_t)$ (see Section 1.2.5), and then using this belief state to guide our decisions. However, learning the parameters of a POMDP (i.e., the generative latent world model) is very difficult, as is recursively computing and updating the belief state, as is computing the policy given the belief state. Indeed, optimally solving POMDPs is known to be computationally very difficult for any method [PT87; KLC98]. So in practice simpler approximations are used. We discuss some of these below. (For more details, see [Mur00].)

Note that it is possible to marginalize out the POMDP latent state $e_t$, to derive a prediction over the next observable state, $p(\boldsymbol{o}_{t+1}|\boldsymbol{h}_t, \boldsymbol{a}_t)$. This can then become a learning target for a model, that is trained to directly predict future observations, without explicitly invoking the concept of latent state. This is called a **predictive state representation** or **PSR** [LS01]. This is related to the idea of **observable operator models** [Jae00], and to the concept of successor representations which we discuss in Section 4.5.2.

#### 1.3.4.2 Finite observation history

The simplest solution to the partial observability problem is to define the state to be a finite history of the last $k$ observations, $\boldsymbol{s}_t = \boldsymbol{h}_{t-k:t}$; when the observations $\boldsymbol{o}_t$ are images, this is often called **frame stacking**. We can then use standard MDP methods. Unfortunately, this cannot capture long-range dependencies in the data.

#### 1.3.4.3 Stateful (recurrent) policies

A more powerful approach is to use a stateful policy, that can remember the entire past, and not just respond to the current input or last $k$ frames. For example, we can represent the policy by an RNN (recurrent neural network), as proposed in the **R2D2** paper [Kap+18], and used in many other papers. Now the hidden state $e_t$ of the RNN will implicitly summarize the past observations, $\boldsymbol{h}_t$, and can be used in lieu of the state $s_t$ in any standard RL algorithm.

RNNs policies are widely used, and this method is often effective in solving partially observed problems. However, they typically will not plan to perform information-gathering actions, since there is no explicit notion of belief state or uncertainty. However, such behavior can arise via meta-learning [Mik+20].

### 1.3.5 Model uncertainty (exploration-exploitation tradeoff)

In RL problems, we typically assume the underlying transition and reward models are not known. We can either try to explicitly learn these models (as in model-based RL), and then solve for the policy, or just learn the policy directly (as in model-free RL). But in either case, we need to explore the environment in order to collect enough data to figure out what to do. This may involve choosing between actions that the agent knows will yield high reward, vs choosing actions which might not been known to yield high reward but which will be informative about potential future gains. This is called the **exploration-exploitation tradeoff**. In this section, we discuss some simple heuristic solutions to this problem. See Section 7.1 for more sophisticated methods.

If we just want to exploit our current knowledge (without trying to learn new things), we can use the **greedy policy**:

$$a_t = \underset{a}{\operatorname{argmax}}\, Q(s, a) \tag{1.33}$$

We can add exploration to this by sometimes picking some other, non-greedy action, as we discuss below.

One approach is to use an **$\epsilon$-greedy** policy $\pi_\epsilon$, parameterized by $\epsilon \in [0, 1]$. In this case, we pick the greedy action wrt the current model, $a_t = \operatorname{argmax}_a \hat{R}_t(s_t, a)$ with probability $1 - \epsilon$, and a random action with probability $\epsilon$. This rule ensures the agent's continual exploration of all state-action combinations. Unfortunately, this heuristic can be shown to be suboptimal, since it explores every action with at least a

| $\hat{R}(s, a_1)$ | $\hat{R}(s, a_2)$ | $\pi_\epsilon(a\|s_1)$ | $\pi_\epsilon(a\|s_2)$ | $\pi_\tau(a\|s_1)$ | $\pi_\tau(a\|s_2)$ |
|---|---|---|---|---|---|
| 1.00 | 9.00 | 0.05 | 0.95 | 0.00 | 1.00 |
| 4.00 | 6.00 | 0.05 | 0.95 | 0.12 | 0.88 |
| 4.90 | 5.10 | 0.05 | 0.95 | 0.45 | 0.55 |
| 5.05 | 4.95 | 0.95 | 0.05 | 0.53 | 0.48 |
| 7.00 | 3.00 | 0.95 | 0.05 | 0.98 | 0.02 |
| 8.00 | 2.00 | 0.95 | 0.05 | 1.00 | 0.00 |

*Table 1.2: Comparison of $\epsilon$-greedy policy (with $\epsilon = 0.1$) and Boltzmann policy (with $\tau = 1$) for a simple MDP with 6 states and 2 actions. Adapted from Table 4.1 of [GK19].*

constant probability $\epsilon/|\mathcal{A}|$, although this can be solved by annealing $\epsilon$ to 0 over time. Another problem with $\epsilon$-greedy is that it can result in "dithering", in which the agent continually changes its mind about what to do. In [DOB21] they propose a simple solution to this problem, known as **$\epsilon z$-greedy**, that often works well. The idea is that with probability $1 - \epsilon$ the agent exploits, but with with probability $\epsilon$ the agent explores by repeating the sampled action for $n \sim z()$ steps in a row, where $z(n)$ is a distribution over the repeat duration. This can help the agent escape from local minima.

Another simple approach to exploration is to use **Boltzmann exploration**, which assigns higher probabilities to explore more promising actions, taking into account the reward function. That is, we use a policy of the form

$$\pi_\tau(a|s) = \frac{\exp(\hat{R}_t(s_t, a)/\tau)}{\sum_{a'} \exp(\hat{R}_t(s_t, a')/\tau)} \tag{1.34}$$

where $\tau > 0$ is a temperature parameter that controls how entropic the distribution is. As $\tau$ gets close to 0, $\pi_\tau$ becomes close to a greedy policy. On the other hand, higher values of $\tau$ will make $\pi(a|s)$ more uniform, and encourage more exploration. Its action selection probabilities can be much "smoother" with respect to changes in the reward estimates than $\epsilon$-greedy, as illustrated in Table 1.2.

The Boltzmann policy explores equally widely in all states. An alternative approach is to try to explore (state,action) combinations where the consequences of the outcome might be uncertain. This can be achived using an **exploration bonus** $R^b_t(s, a)$, which is large if the number of times we have tried actioon $a$ in state $s$ is small. We can then add $R^b$ to the regular reward, to bias the behavior in a way that will hopefully cause the agent to learn useful information about the world. This is called an **intrinsic reward** function (Section 7.3).

## 1.3.6 Reward functions

Sequential decision making relies on the user to define the reward function in order to encourage the agent to exhibit some desired behavior. In this section, we discuss this crucial aspect of the problem.

### 1.3.6.1 The reward hypothesis

The "**reward hypothesis**" states that "all of what we mean by goals and purposes can be well thought of as maximization of the expected value of the cumulative sum of a received scalar signal (reward)" [Sut04]. (See also the closely related "reward is enough" hypothesis [Sil+21].) Whether this hypothesis is true or not depends on what one means by "goals and purposes". This can be formalized in terms of preference relations over (state,action) trajectories, as discussed in [Bow+23]. In particular, they discuss when a utility function over trajectories can be converted into a Markovian reward of the form $R(s, a, s')$. (See also [Boo+23; BKM24] for some related work on reward function design.)

### 1.3.6.2 Reward hacking

In some cases, the reward function may be misspecified, so even though the agent may maximize the reward, this might turn out not to be what the user desired. For example, suppose the user rewards the agent for making as many paper clips as possible. An optimal agent may convert the whole world into a paper clip factory, because the user forgot to specify various constraints, such as not killing people (which might otherwise be necessary in order to use as many resources as possible for paperclips). In the **AI alignment** community, this example is known as the **paperclip maximizer problem**, and is due to Nick Bostrom [Bos16]. (See e.g., `https://openai.com/index/faulty-reward-functions/` for some examples that have occurred in practice.) This is an example of a more general problem known as **reward hacking** [Ska+22]. For a potential solution, based on the assistance game paradigm, see Section 6.1.4.

#### 1.3.6.3 Sparse reward

Even if the reward function is correct, optimizing it is not always easy. In particular, many problems suffer from **sparse reward**, in which $R(s, a) = 0$ for almost all states and actions, so the agent only every gets feedback (either positive or negative) on the rare occasions when it achieves some unknown goal. This requires **deep exploration** [Osb+19] to find the rewarding states. One approach to this is use to use PSRL (Section 7.1.3.2). However, various other heuristics have been developed, some of which we discuss below.

#### 1.3.6.4 Reward shaping

In **reward shaping**, we add prior knowledge about what we believe good states should look like, as a way to combat the difficulties of learning from sparse reward. That is, we define a new reward function $r' = r + F$, where $F$ is called the shaping function. In general, this can affect the optimal policy. For example, if a soccer playing agent is "artificially" rewarded for making contact with the ball, it might learn to repeatedly touch and untouch the ball (toggling between $s$ and $s'$), rather than trying to win the original game. But in [NHR99], the prove that if the shaping function has the form

$$F(s, a, s') = \gamma\Phi(s') - \Phi(s) \tag{1.35}$$

where $\Phi : \mathcal{S} \to \mathbb{R}$ is a **potential function**, then we can guarantee that the sum of shaped rewards will match the sum of original rewards plus a constant. This is called **Potential-Based Reward Shaping**.

In [Wie03], they prove that (in the tabular case) this approach is equivalent to initializing the value function to $V(s) = \Phi(s)$. In [TMM19], they propose an extension called potential-based advice, where they show that a potential of the form $F(s, a, s', a') = \gamma\Phi(s', a') - \Phi(s, a)$ is also valid (and more expressive). In [Hu+20], they introduce a reward shaping function $z$ which can be used to down-weight or up-weight the shaping function:

$$r'(s, a) = r(s, a) + z_\phi(s, a)F(s, a) \tag{1.36}$$

They use bilevel optimization to optimize $\phi$ wrt the original task performance.

#### 1.3.6.5 Intrinsic reward

In Section 7.3, we discuss **intrinsic reward**, which is a set of methods for encouraging agent behavior without the need for any external reward signal. For example, we might want agents to explore their environment just so they can "figure things out", without any other specific goals in mind. This can be useful even if there is an external reward, but it happens to be sparse.

### 1.3.7 Software

Implementing RL algorithms is much trickier than methods for supervised learning, or generative methods such as language modeling and diffusion, all of which have stable (easy-to-optimize) loss functions. Therefore it is often wise to build on existing software rather than starting from scratch. We list some useful libraries in Section 1.3.7.

In addition, RL experiments can be very high variance, making it hard to draw valid conclusions. See [Aga+21b; Pat+24; Jor+24] for some recommended experimental practices. For example, when reporting performance across different environments, with different intrinsic difficulties (e.g., different kinds of Atari

| URL | Language | Comments |
|---|---|---|
| Stoix | Jax | Mini-library with many methods (including MBRL) |
| PureJaxRL | Jax | Single files with DQN; PPO, DPO |
| JaxRL | Jax | Single files with AWAC, DDPG, SAC, SAC+REDQ |
| Stable Baselines Jax | Jax | Library with DQN, CrossQ, TQC; PPO, DDPG, TD3, SAC |
| Jax Baselines | Jax | Library with many methods |
| Rejax | Jax | Library with DDQN, PPO, (discrete) SAC, DDPG |
| Dopamine | Jax/TF | Library with many methods |
| Rlax | Jax | Library of RL utility functions (used by Acme) |
| Acme | Jax/TF | Library with many methods (uses rlax) |
| CleanRL | PyTorch | Single files with many methods |
| Stable Baselines 3 | PyTorch | Library with DQN; A2C, PPO, DDPG, TD3, SAC, HER |
| TianShou | PyTorch | Library with many methods (including offline RL) |

*Table 1.3: Some open source RL software.*

games), [Aga+21b] recommend reporting the **interquartile mean** (IQM) of the performance metric, which is the mean of the samples between the 0.25 and 0.75 percentiles, (this is a special case of a trimmed mean). Let this estimate be denoted by $\hat{\mu}(\mathcal{D}_i)$, where $\mathcal{D}$ is the empirical data (e.g., reward vs time) from the $i$'th run. We can estimate the uncertainty in this estimate using a nonparametric method, such as bootstrap resampling, or a parametric approximation, such as a Gaussian approximation. (This requires computing the standard error of the mean, $\frac{\hat{\sigma}}{\sqrt{n}}$, where $n$ is the number of trials, and $\hat{\sigma}$ is the estimated standard deviation of the (trimmed) data.)

# Chapter 2

# Value-based RL

## 2.1 Basic concepts

In this section we introduce some definitions and basic concepts.

### 2.1.1 Value functions

Let $\pi$ be a given policy. We define the **state-value function**, or **value function** for short, as follows (with $\mathbb{E}_\pi[\cdot]$ indicating that actions are selected by $\pi$):

$$V_\pi(s) \triangleq \mathbb{E}_\pi [G_0 | s_0 = s] = \mathbb{E}_\pi \left[ \sum_{t=0}^{\infty} \gamma^t r_t | s_0 = s \right] \tag{2.1}$$

This is the expected return obtained if we start in state $s$ and follow $\pi$ to choose actions in a continuing task (i.e., $T = \infty$).

Similarly, we define the **state-action value function**, also known as the $Q$**-function**, as follows:

$$Q_\pi(s, a) \triangleq \mathbb{E}_\pi [G_0 | s_0 = s, a_0 = a] = \mathbb{E}_\pi \left[ \sum_{t=0}^{\infty} \gamma^t r_t | s_0 = s, a_0 = a \right] \tag{2.2}$$

This quantity represents the expected return obtained if we start by taking action $a$ in state $s$, and then follow $\pi$ to choose actions thereafter.

Finally, we define the **advantage function** as follows:

$$\text{Adv}_\pi(s, a) \triangleq Q_\pi(s, a) - V_\pi(s) \tag{2.3}$$

This tells us the benefit of picking action $a$ in state $s$ then switching to policy $\pi$, relative to the baseline return of always following $\pi$. Note that $\text{Adv}_\pi(s, a)$ can be both positive and negative, and $\mathbb{E}_{\pi(a|s)} [\text{Adv}_\pi(s, a)] = 0$ due to a useful equality: $V_\pi(s) = \mathbb{E}_{\pi(a|s)} [Q_\pi(s, a)]$.

### 2.1.2 Bellman's equations

Suppose $\pi_*$ is a policy such that $V_{\pi_*} \geq V_\pi$ for all $s \in \mathcal{S}$ and all policy $\pi$, then it is an **optimal policy**. There can be multiple optimal policies for the same MDP, but by definition their value functions must be the same, and are denoted by $V_*$ and $Q_*$, respectively. We call $V_*$ the **optimal state-value function**, and $Q_*$ the **optimal action-value function**. Furthermore, any finite MDP must have at least one deterministic optimal policy [Put94].

A fundamental result about the optimal value function is **Bellman's optimality equations**:

$$V_*(s) = \max_a R(s,a) + \gamma \mathbb{E}_{p_S(s'|s,a)} \left[ V_*(s') \right] \tag{2.4}$$

$$Q_*(s,a) = R(s,a) + \gamma \mathbb{E}_{p_S(s'|s,a)} \left[ \max_{a'} Q_*(s',a') \right] \tag{2.5}$$

Conversely, the optimal value functions are the only solutions that satisfy the equations. In other words, although the value function is defined as the expectation of a sum of infinitely many rewards, it can be characterized by a recursive equation that involves only one-step transition and reward models of the MDP. Such a recursion play a central role in many RL algorithms we will see later.

Given a value function ($V$ or $Q$), the discrepancy between the right- and left-hand sides of Equations (2.4) and (2.5) are called **Bellman error** or **Bellman residual**. We can define the **Bellman operator** $\mathcal{B}$ given an MDP $M = (R, T)$ and policy $\pi$ as a function that takes a value function $V$ and derives a few value function $V'$ that satisfies

$$V'(s) = \mathcal{B}_M^\pi V(s) \triangleq \mathbb{E}_{\pi(a|s)} \left[ R(s,a) + \gamma \mathbb{E}_{T(s'|s,a)} \left[ V(s') \right] \right] \tag{2.6}$$

This reduces the Bellman error. Applying the Bellman operator to a state is called a **Bellman backup**. If we iterate this process, we will converge to the optimal value function $V_*$, as we discuss in Section 2.2.1.

Given the optimal value function, we can derive an optimal policy using

$$\pi_*(s) = \operatorname*{argmax}_a Q_*(s,a) \tag{2.7}$$

$$= \operatorname*{argmax}_a \left[ R(s,a) + \gamma \mathbb{E}_{p_S(s'|s,a)} \left[ V_*(s') \right] \right] \tag{2.8}$$

Following such an optimal policy ensures the agent achieves maximum expected return starting from any state.

The problem of solving for $V_*$, $Q_*$ or $\pi_*$ is called **policy optimization**. In contrast, solving for $V_\pi$ or $Q_\pi$ for a given policy $\pi$ is called **policy evaluation**, which constitutes an important subclass of RL problems as will be discussed in later sections. For policy evaluation, we have similar Bellman equations, which simply replace $\max_a\{\cdot\}$ in Equations (2.4) and (2.5) with $\mathbb{E}_{\pi(a|s)}\left[\cdot\right]$.

In Equations (2.7) and (2.8), as in the Bellman optimality equations, we must take a maximum over all actions in $\mathcal{A}$, and the maximizing action is called the **greedy action** with respect to the value functions, $Q_*$ or $V_*$. Finding greedy actions is computationally easy if $\mathcal{A}$ is a small finite set. For high dimensional continuous spaces, see Section 2.5.4.1.

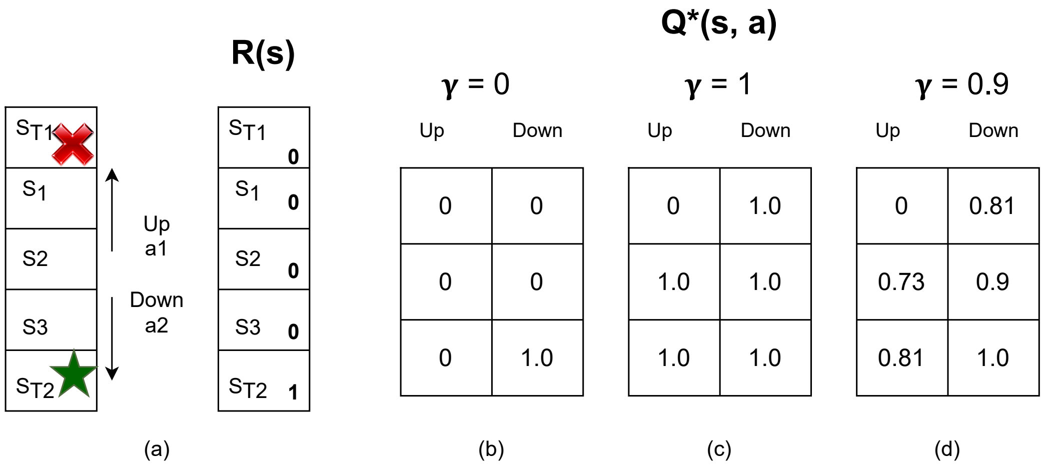
### 2.1.3 Example: 1d grid world

In this section, we show a simple example, to make some of the above concepts more concrete. Consider the 1d **grid world** shown in Figure 2.1(a). There are 5 possible states, among them $S_{T1}$ and $S_{T2}$ are absorbing states, since the interaction ends once the agent enters them. There are 2 actions, ↑ and ↓. The reward function is zero everywhere except at the goal state, $S_{T2}$, which gives a reward of 1 upon entering. Thus the optimal action in every state is to move down.

Figure 2.1(b) shows the $Q_*$ function for $\gamma = 0$. Note that we only show the function for non-absorbing states, as the optimal $Q$-values are 0 in absorbing states by definition. We see that $Q_*(s_3, \downarrow) = 1.0$, since the agent will get a reward of 1.0 on the next step if it moves down from $s_3$; however, $Q_*(s,a) = 0$ for all other state-action pairs, since they do not provide nonzero immediate reward. This optimal $Q$-function reflects the fact that using $\gamma = 0$ is completely myopic, and ignores the future.

Figure 2.1(c) shows $Q_*$ when $\gamma = 1$. In this case, we care about all future rewards equally. Thus $Q_*(s,a) = 1$ for all state-action pairs, since the agent can always reach the goal eventually. This is infinitely far-sighted. However, it does not give the agent any short-term guidance on how to behave. For example, in $s_2$, it is not clear if it is should go up or down, since both actions will eventually reach the goal with identical $Q_*$-values.

Figure 2.1(d) shows $Q_*$ when $\gamma = 0.9$. This reflects a preference for near-term rewards, while also taking future reward into account. This encourages the agent to seek the shortest path to the goal, which is usually



| Up | Down |
|---|---|
| 0 | 0 |
| 0 | 0 |
| 0 | 1.0 |

| Up | Down |
|---|---|
| 0 | 1.0 |
| 1.0 | 1.0 |
| 1.0 | 1.0 |

| Up | Down |
|---|---|
| 0 | 0.81 |
| 0.73 | 0.9 |
| 0.81 | 1.0 |

*Figure 2.1: Left: illustration of a simple MDP corresponding to a 1d grid world of 3 non-absorbing states and 2 actions. Right: optimal Q-functions for different values of $\gamma$. Adapted from Figures 3.1, 3.2, 3.4 of [GK19].*

what we desire. A proper choice of $\gamma$ is up to the agent designer, just like the design of the reward function, and has to reflect the desired behavior of the agent.

## 2.2 Computing the value function and policy given a known world model

In this section, we discuss how to compute the optimal value function (the **prediction problem**) and the optimal policy (the **control problem**) when the MDP model is known. (Sometimes the term **planning** is used to refer to computing the optimal policy, given a known model, but planning can also refer to computing a sequence of actions, rather than a policy.) The algorithms we discuss are based on **dynamic programming** (DP) and **linear programming** (LP).

For simplicity, in this section, we assume discrete state and action sets with $\gamma < 1$. However, exact calculation of optimal policies often depends polynomially on the sizes of $\mathcal{S}$ and $\mathcal{A}$, and is intractable, for example, when the state space is a Cartesian product of several finite sets. This challenge is known as the **curse of dimensionality**. Therefore, approximations are typically needed, such as using parametric or nonparametric representations of the value function or policy, both for computational tractability and for extending the methods to handle MDPs with general state and action sets. This requires the use of **approximate dynamic programming** (ADP) and **approximate linear programming** (ALP) algorithms (see e.g., [Ber19]).

### 2.2.1 Value iteration

A popular and effective DP method for solving an MDP is **value iteration** (VI). Starting from an initial value function estimate $V_0$, the algorithm iteratively updates the estimate by

$$V_{k+1}(s) = \max_a \left[ R(s,a) + \gamma \sum_{s'} p(s'|s,a) V_k(s') \right] \tag{2.9}$$

Note that the update rule, sometimes called a **Bellman backup**, is exactly the right-hand side of the Bellman optimality equation Equation (2.4), with the unknown $V_*$ replaced by the current estimate $V_k$. A fundamental property of Equation (2.9) is that the update is a **contraction**: it can be verified that

$$\max_s |V_{k+1}(s) - V_*(s)| \leq \gamma \max_s |V_k(s) - V_*(s)| \tag{2.10}$$

In other words, every iteration will reduce the maximum value function error by a constant factor.

$V_k$ will converge to $V_*$, after which an optimal policy can be extracted using Equation (2.8). In practice, we can often terminate VI when $V_k$ is close enough to $V_*$, since the resulting greedy policy wrt $V_k$ will be near optimal. Value iteration can be adapted to learn the optimal action-value function $Q_*$.

### 2.2.2 Real-time dynamic programming (RTDP)

In value iteration, we compute $V_*(s)$ and $\pi_*(s)$ for all possible states $s$, averaging over all possible next states $s'$ at each iteration, as illustrated in Figure 2.2(right). However, for some problems, we may only be interested in the value (and policy) for certain special starting states. This is the case, for example, in **shortest path problems** on graphs, where we are trying to find the shortest route from the current state to a goal state. This can be modeled as an episodic MDP by defining a transition matrix $p_S(s'|s,a)$ where taking edge $a$ from node $s$ leads to the neighboring node $s'$ with probability 1. The reward function is defined as $R(s,a) = -1$ for all states $s$ except the goal states, which are modeled as absorbing states.

In problems such as this, we can use a method known as **real-time dynamic programming** or **RTDP** [BBS95], to efficiently compute an **optimal partial policy**, which only specifies what to do for the reachable states. RTDP maintains a value function estimate $V$. At each step, it performs a Bellman backup for the current state $s$ by $V(s) \leftarrow \max_a \mathbb{E}_{p_S(s'|s,a)}\left[R(s,a) + \gamma V(s')\right]$. It picks an action $a$ (often with some exploration), reaches a next state $s'$, and repeats the process. This can be seen as a form of the more general **asynchronous value iteration**, that focuses its computational effort on parts of the state space that are more likely to be reachable from the current state, rather than synchronously updating all states at each iteration.

### 2.2.3 Policy iteration

Another effective DP method for computing $\pi_*$ is **policy iteration**. It is an iterative algorithm that searches in the space of deterministic policies until converging to an optimal policy. Each iteration consists of two steps, **policy evaluation** and **policy improvement**.

The policy evaluation step, as mentioned earlier, computes the value function for the current policy. Let $\pi$ represent the current policy, $\boldsymbol{v}(s) = V_\pi(s)$ represent the value function encoded as a vector indexed by states, $\boldsymbol{r}(s) = \sum_a \pi(a|s)R(s,a)$ represent the reward vector, and $\mathbf{T}(s'|s) = \sum_a \pi(a|s)p(s'|s,a)$ represent the state transition matrix. Bellman's equation for policy evaluation can be written in the matrix-vector form as

$$\boldsymbol{v} = \boldsymbol{r} + \gamma \mathbf{T}\boldsymbol{v} \tag{2.11}$$

This is a linear system of equations in $|\mathcal{S}|$ unknowns. We can solve it using matrix inversion: $\boldsymbol{v} = (\mathbf{I} - \gamma\mathbf{T})^{-1}\boldsymbol{r}$. Alternatively, we can use value iteration by computing $\boldsymbol{v}_{t+1} = \boldsymbol{r} + \gamma\mathbf{T}\boldsymbol{v}_t$ until near convergence, or some form of asynchronous variant that is computationally more efficient.

Once we have evaluated $V_\pi$ for the current policy $\pi$, we can use it to derive a better policy $\pi'$, thus the name policy improvement. To do this, we simply compute a deterministic policy $\pi'$ that acts greedily with respect to $V_\pi$ in every state, using

$$\pi'(s) = \operatorname*{argmax}_a \{R(s,a) + \gamma\mathbb{E}\left[V_\pi(s')\right]\} \tag{2.12}$$

We can guarantee that $V_{\pi'} \geq V_\pi$. This is called the **policy improvement theorem**. To see this, define $\boldsymbol{r}'$, $\mathbf{T}'$ and $\boldsymbol{v}'$ as before, but for the new policy $\pi'$. The definition of $\pi'$ implies $\boldsymbol{r}' + \gamma\mathbf{T}'\boldsymbol{v} \geq \boldsymbol{r} + \gamma\mathbf{T}\boldsymbol{v} = \boldsymbol{v}$, where the equality is due to Bellman's equation. Repeating the same equality, we have

$$\boldsymbol{v} \leq \boldsymbol{r}' + \gamma\mathbf{T}'\boldsymbol{v} \leq \boldsymbol{r}' + \gamma\mathbf{T}'(\boldsymbol{r}' + \gamma\mathbf{T}'\boldsymbol{v}) \leq \boldsymbol{r}' + \gamma\mathbf{T}'(\boldsymbol{r}' + \gamma\mathbf{T}'(\boldsymbol{r}' + \gamma\mathbf{T}'\boldsymbol{v})) \leq \cdots \tag{2.13}$$

$$= (\mathbf{I} + \gamma\mathbf{T}' + \gamma^2\mathbf{T}'^2 + \cdots)\boldsymbol{r}' = (\mathbf{I} - \gamma\mathbf{T}')^{-1}\boldsymbol{r}' = \boldsymbol{v}' \tag{2.14}$$

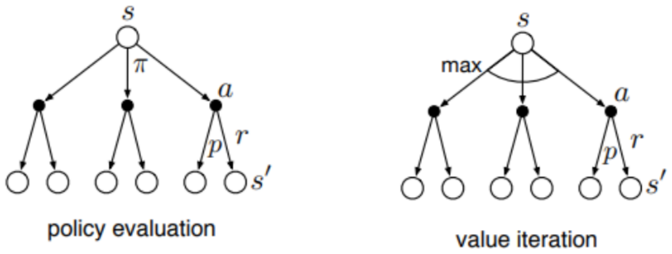


*Figure 2.2: Policy iteration vs value iteration represented as backup diagrams. Empty circles represent states, solid (filled) circles represent states and actions. Adapted from Figure 8.6 of [SB18].*

Starting from an initial policy $\pi_0$, policy iteration alternates between policy evaluation ($E$) and improvement ($I$) steps, as illustrated below:

$$\pi_0 \xrightarrow{E} V_{\pi_0} \xrightarrow{I} \pi_1 \xrightarrow{E} V_{\pi_1} \cdots \xrightarrow{I} \pi_* \xrightarrow{E} V_* \tag{2.15}$$

The algorithm stops at iteration $k$, if the policy $\pi_k$ is greedy with respect to its own value function $V_{\pi_k}$. In this case, the policy is optimal. Since there are at most $|\mathcal{A}|^{|\mathcal{S}|}$ deterministic policies, and every iteration strictly improves the policy, the algorithm must converge after finite iterations.

In PI, we alternate between policy evaluation (which involves multiple iterations, until convergence of $V_\pi$), and policy improvement. In VI, we alternate between one iteration of policy evaluation followed by one iteration of policy improvement (the "max" operator in the update rule). We are in fact free to intermix any number of these steps in any order. The process will converge once the policy is greedy wrt its own value function.

Note that policy evaluation computes $V_\pi$ whereas value iteration computes $V_*$. This difference is illustrated in Figure 2.2, using a **backup diagram**. Here the root node represents any state $s$, nodes at the next level represent state-action combinations (solid circles), and nodes at the leaves representing the set of possible resulting next state $s'$ for each possible action. In PE, we average over all actions according to the policy, whereas in VI, we take the maximum over all actions.

## 2.3 Computing the value function without knowing the world model

In the rest of this chapter, we assume the agent only has access to samples from the environment, $(s', r) \sim p(s', r|s, a)$. We will show how to use these samples to learn optimal value function and $Q$-function, even without knowing the MDP dynamics.

### 2.3.1 Monte Carlo estimation

Recall that $V_\pi(s) = \mathbb{E}[G_t|s_t = s]$ is the sum of expected (discounted) returns from state $s$ if we follow policy $\pi$. A simple way to estimate this is to rollout the policy, and then compute the average sum of discounted rewards. The trajectory ends when we reach a terminal state, if the task is episodic, or when the discount factor $\gamma^t$ becomes negligibly small, whichever occurs first. This is called **Monte Carlo estimation**. We can use this to update our estimate of the value function as follows:

$$V(s_t) \leftarrow V(s_t) + \eta [G_t - V(s_t)] \tag{2.16}$$

where $\eta$ is the learning rate, and the term in brackets is an error term. We can use a similar technique to estimate $Q_\pi(s, a) = \mathbb{E}[G_t|s_t = s, a_t = a]$ by simply starting the rollout with action $a$.

We can use MC estimation of $Q$, together with policy iteration (Section 2.2.3), to learn an optimal policy. Specifically, at iteration $k$, we compute a new, improved policy using $\pi_{k+1}(s) = \operatorname{argmax}_a Q_k(s, a)$, where $Q_k$

is approximated using MC estimation. This update can be applied to all the states visited on the sampled trajectory. This overall technique is called **Monte Carlo control**.

To ensure this method converges to the optimal policy, we need to collect data for every (state, action) pair, at least in the tabular case, since there is no generalization across different values of $Q(s, a)$. One way to achieve this is to use an $\epsilon$-greedy policy (see Section 1.3.5). Since this is an on-policy algorithm, the resulting method will converge to the optimal $\epsilon$-soft policy, as opposed to the optimal policy. It is possible to use importance sampling to estimate the value function for the optimal policy, even if actions are chosen according to the $\epsilon$-greedy policy. However, it is simpler to just gradually reduce $\epsilon$.

### 2.3.2 Temporal difference (TD) learning

The Monte Carlo (MC) method in Section 2.3.1 results in an estimator for $V(s)$ with very high variance, since it has to unroll many trajectories, whose returns are a sum of many random rewards generated by stochastic state transitions. In addition, it is limited to episodic tasks (or finite horizon truncation of continuing tasks), since it must unroll to the end of the episode before each update step, to ensure it reliably estimates the long term return.

In this section, we discuss a more efficient technique called **temporal difference** or **TD** learning [Sut88]. The basic idea is to incrementally reduce the Bellman error for sampled states or state-actions, based on transitions instead of a long trajectory. More precisely, suppose we are to learn the value function $V_\pi$ for a fixed policy $\pi$. Given a state transition $(s_t, a_t, r_t, s_{t+1})$, where $a_t \sim \pi(s_t)$, we change the estimate $V(s_t)$ so that it moves towards the **target value** $y_t = r_t + \gamma V(s_{t+1}) \approx G_{t:t+1}$:

$$V(s_t) \leftarrow V(s_t) + \eta \left[ \underbrace{r_t + \gamma V(s_{t+1}) - V(s_t)}_{\delta_t} \right] \tag{2.17}$$

where $\eta$ is the learning rate. (See [RFP15] for ways to adaptively set the learning rate.) The $\delta_t = y_t - V(s_t)$ term is known as the **TD error**. A more general form of TD update for parametric value function representations is

$$\boldsymbol{w} \leftarrow \boldsymbol{w} + \eta \left[ r_t + \gamma V_{\boldsymbol{w}}(s_{t+1}) - V_{\boldsymbol{w}}(s_t) \right] \nabla_{\boldsymbol{w}} V_{\boldsymbol{w}}(s_t) \tag{2.18}$$

we see that Equation (2.16) is a special case. The TD update rule for evaluating $Q_\pi$ is similar, except we replace states with states and actions.

It can be shown that TD learning in the tabular case, Equation (2.16), converges to the correct value function, under proper conditions [Ber19]. However, it may diverge when using nonlinear function approximators, as we discuss in Section 2.5.2.4. The reason is that this update is a "**semi-gradient**", which refers to the fact that we only take the gradient wrt the value function, $\nabla_{\boldsymbol{w}} V(\boldsymbol{s}_t, \boldsymbol{w}_t)$, treating the target $U_t$ as constant.

The potential divergence of TD is also consistent with the fact that Equation (2.18) does not correspond to a gradient update on any objective function, despite having a very similar form to SGD (stochastic gradient descent). Instead, it is an example of **bootstrapping**, in which the estimate, $V_{\boldsymbol{w}}(s_t)$, is updated to approach a target, $r_t + \gamma V_{\boldsymbol{w}}(s_{t+1})$, which is defined by the value function estimate itself. This idea is shared by DP methods like value iteration, although they rely on the complete MDP model to compute an exact Bellman backup. In contrast, TD learning can be viewed as using sampled transitions to approximate such backups. An example of a non-bootstrapping approach is the Monte Carlo estimation in the previous section. It samples a complete trajectory, rather than individual transitions, to perform an update; this avoids the divergence issue, but is often much less efficient. Figure 2.3 illustrates the difference between MC, TD, and DP.

### 2.3.3 Combining TD and MC learning using TD($\lambda$)

A key difference between TD and MC is the way they estimate returns. Given a trajectory $\boldsymbol{\tau} = (s_0, a_0, r_0, s_1, \ldots, s_T)$, TD estimates the return from state $s_t$ by one-step lookahead, $G_{t:t+1} = r_t + \gamma V(s_{t+1})$, where the return from

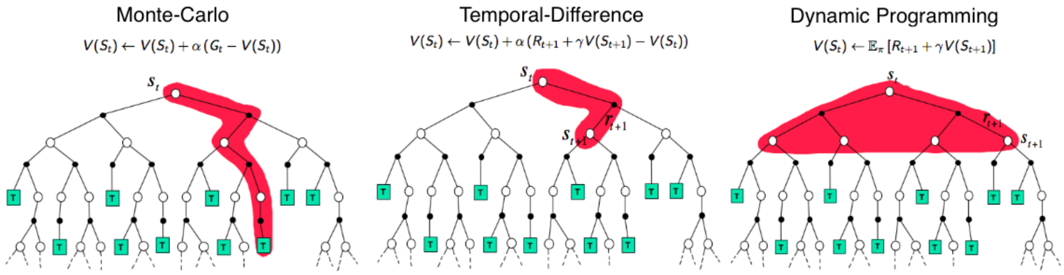

Monte-Carlo
$V(S_t) \leftarrow V(S_t) + \alpha(G_t - V(S_t))$
$s_t$
T
Temporal-Difference
$V(S_t) \leftarrow V(S_t) + \alpha(R_{t+1} + \gamma V(S_{t+1}) - V(S_t))$
$s_t$
$r_{t+1}$
$s_{t+1}$
Dynamic Programming
$V(S_t) \leftarrow \mathbb{E}_\pi[R_{t+1} + \gamma V(S_{t+1})]$
$s_t$
$r_{t+1}$
$s_{t+1}$

*Figure 2.3: Backup diagrams of $V(s_t)$ for Monte Carlo, temporal difference, and dynamic programming updates of the state-value function. Used with kind permission of Andy Barto.*

time $t+1$ is replaced by its value function estimate. In contrast, MC waits until the end of the episode or until $T$ is large enough, then uses the estimate $G_{t:T} = r_t + \gamma r_{t+1} + \cdots + \gamma^{T-t-1} r_{T-1}$. It is possible to interpolate between these by performing an $n$-step rollout, and then using the value function to approximate the return for the rest of the trajectory, similar to heuristic search (Section 4.2.1.4). That is, we can use the **n-step return**

$$G_{t:t+n} = r_t + \gamma r_{t+1} + \cdots + \gamma^{n-1} r_{t+n-1} + \gamma^n V(s_{t+n}) \tag{2.19}$$

For example, the 1-step and 2-step returns are given by

$$G_{t:t+1} = r_t + \gamma v_{t+1} \tag{2.20}$$

$$G_{t:t+2} = r_t + \gamma r_{t+1} + \gamma^2 v_{t+2} \tag{2.21}$$

The corresponding $n$-step version of the TD update becomes

$$\boldsymbol{w} \leftarrow \boldsymbol{w} + \eta \left[G_{t:t+n} - V_{\boldsymbol{w}}(s_t)\right] \nabla_{\boldsymbol{w}} V_{\boldsymbol{w}}(s_t) \tag{2.22}$$

Rather than picking a specific lookahead value, $n$, we can take a weighted average of all possible values, with a single parameter $\lambda \in [0,1]$, by using

$$G_t^\lambda \triangleq (1-\lambda) \sum_{n=1}^{\infty} \lambda^{n-1} G_{t:t+n} \tag{2.23}$$

This is called the **lambda return**. Note that these coefficients sum to one (since $\sum_{t=0}^{\infty}(1-\lambda)\lambda^t = \frac{1-\lambda}{1-\lambda} = 1$, for $\lambda < 1$), so the return is a convex combination of $n$-step returns. See Figure 2.4 for an illustration. We can now use $G_t^\lambda$ inside the TD update instead of $G_{t:t+n}$; this is called **TD**($\lambda$).

Note that, if a terminal state is entered at step $T$ (as happens with episodic tasks), then all subsequent $n$-step returns are equal to the conventional return, $G_t$. Hence we can write

$$G_t^\lambda = (1-\lambda) \sum_{n=1}^{T-t-1} \lambda^{n-1} G_{t:t+n} \; + \lambda^{T-t-1} G_t \tag{2.24}$$

From this we can see that if $\lambda = 1$, the $\lambda$-return becomes equal to the regular MC return $G_t$. If $\lambda = 0$, the $\lambda$-return becomes equal to the one-step return $G_{t:t+1}$ (since $0^{n-1} = 1$ iff $n = 1$), so standard TD learning is often called **TD(0) learning**. This episodic form also gives us the following recursive equation

$$G_t^\lambda = r_t + \gamma[(1-\lambda) v_{t+1} + \lambda G_{t+1}^\lambda] \tag{2.25}$$

which we initialize with $G_T = v_t$.

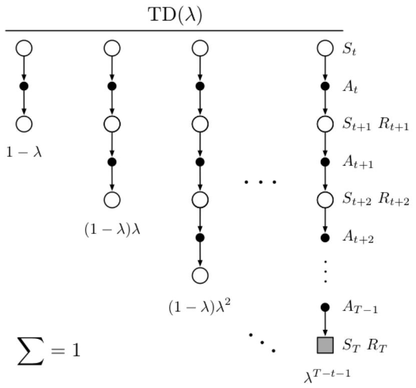


*Figure 2.4: The backup diagram for TD($\lambda$). Standard TD learning corresponds to $\lambda = 0$, and standard MC learning corresponds to $\lambda = 1$. From Figure 12.1 of [SB18]. Used with kind permission of Richard Sutton.*

### 2.3.4 Eligibility traces

An important benefit of using the geometric weighting in Equation (2.23), as opposed to the $n$-step update, is that the corresponding TD learning update can be efficiently implemented through the use of **eligibility traces**, even though $G_t^\lambda$ is a sum of infinitely many terms. The eligibility term is a weighted sum of the gradients of the value function:

$$\boldsymbol{z}_t = \gamma\lambda\boldsymbol{z}_{t-1} + \nabla_{\boldsymbol{w}} V_{\boldsymbol{w}}(s_t) \tag{2.26}$$

(This trace term gets reset to 0 at the start of each episode.) We replace the TD(0) update of $\boldsymbol{w}_{t+1} = \boldsymbol{w}_t + \eta\delta_t\nabla_{\boldsymbol{w}} V_{\boldsymbol{w}}(s_t)$ with the TD($\lambda$) version to get

$$\boldsymbol{w}_{t+1} = \boldsymbol{w}_t + \eta\delta_t\boldsymbol{z}_t \tag{2.27}$$

See [Sei+16] for more details.

## 2.4 SARSA: on-policy TD control

TD learning is for policy evaluation, as it estimates the value function for a fixed policy. In order to find an optimal policy, we may use the algorithm as a building block inside generalized policy iteration (Section 2.2.3). In this case, it is more convenient to work with the action-value function, $Q$, and a policy $\pi$ that is greedy with respect to $Q$. The agent follows $\pi$ in every step to choose actions, and upon a transition $(s, a, r, s')$ the TD update rule is

$$Q(s,a) \leftarrow Q(s,a) + \eta\left[r + \gamma Q(s', a') - Q(s,a)\right] \tag{2.28}$$

where $a' \sim \pi(s')$ is the action the agent will take in state $s'$. After $Q$ is updated (for policy evaluation), $\pi$ also changes accordingly as it is greedy with respect to $Q$ (for policy improvement). This algorithm, first proposed by [RN94], was further studied and renamed to **SARSA** by [Sut96]; the name comes from its update rule that involves an augmented transition $(s, a, r, s', a')$.

In order for SARSA to converge to $Q_*$, every state-action pair must be visited infinitely often, at least in the tabular case, since the algorithm only updates $Q(s,a)$ for $(s,a)$ that it visits. One way to ensure this condition is to use a “greedy in the limit with infinite exploration” (**GLIE**) policy. An example is the $\epsilon$-greedy policy, with $\epsilon$ vanishing to 0 gradually. It can be shown that SARSA with a GLIE policy will converge to $Q_*$ and $\pi_*$ [Sin+00].

## 2.5 Q-learning: off-policy TD control

SARSA is an on-policy algorithm, which means it learns the $Q$-function for the policy it is currently using, which is typically not the optimal policy, because of the need to perform exploration. However, with a simple modification, we can convert this to an off-policy algorithm that learns $Q_*$, even if a suboptimal or exploratory policy is used to choose actions.

### 2.5.1 Tabular Q learning

Suppose we modify SARSA by replacing the sampled next action $a' \sim \pi(s')$ in Equation (2.28) with a greedy action: $a' = \operatorname{argmax}_b Q(s', b)$. This results in the following update when a transition $(s, a, r, s')$ happens

$$Q(s,a) \leftarrow Q(s,a) + \eta \left[ r + \gamma \max_{a'} Q(s', a') - Q(s,a) \right] \tag{2.29}$$

This is the update rule of **Q-learning** for the tabular case [WD92].

Since it is off-policy, the method can use $(s, a, r, s')$ triples coming from any data source, such as older versions of the policy, or log data from an existing (non-RL) system. If every state-action pair is visited infinitely often, the algorithm provably converges to $Q_*$ in the tabular case, with properly decayed learning rates [Ber19]. Algorithm 1 gives a vanilla implementation of Q-learning with $\epsilon$-greedy exploration.

**Algorithm 1:** Tabular Q-learning with $\epsilon$-greedy exploration

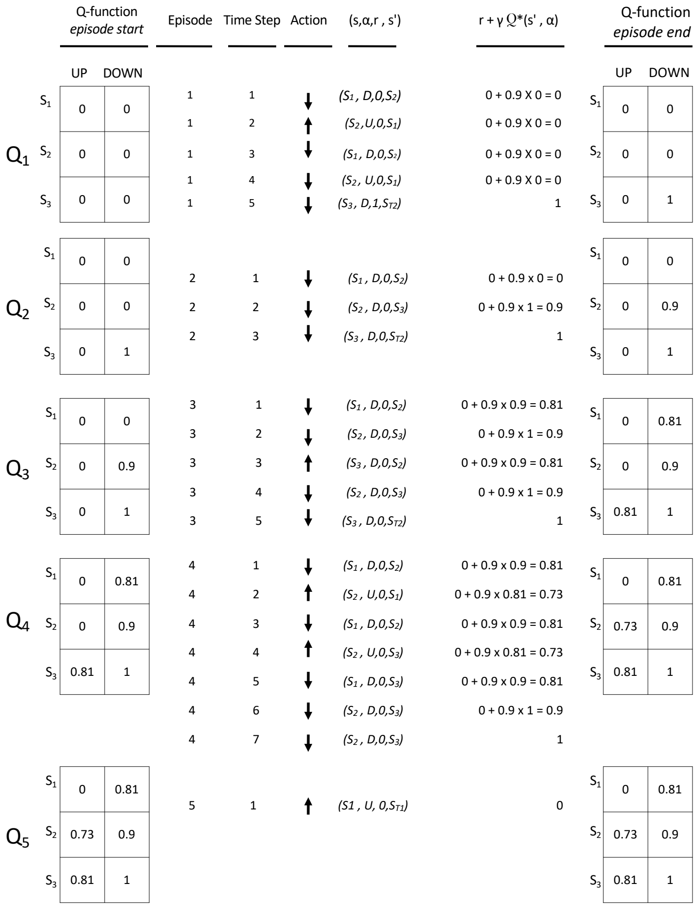
```
Initialize value function $Q$
repeat
    Sample starting state $s$ of new episode
    repeat
        Sample action $a = \begin{cases} \operatorname{argmax}_b Q(s,b), & \text{with probability } 1-\epsilon \\ \text{random action}, & \text{with probability } \epsilon \end{cases}$
        $(s', r) = \text{env.step}(a)$
        Compute the TD error: $\delta = r + \gamma \max_{a'} Q(s', a') - Q(s, a)$
        $Q(s,a) \leftarrow Q(s,a) + \eta\delta$
        $s \leftarrow s'$
    until state $s$ is terminal;
until converged;
```

For terminal states, $s \in \mathcal{S}^+$, we know that $Q(s, a) = 0$ for all actions $a$. Consequently, for the optimal value function, we have $V^*(s) = \max_{a'} Q^*(s, a) = 0$ for all terminal states. When performing online learning, we don't usually know which states are terminal. Therefore we assume that, whenever we take a step in the environment, we get the next state $s'$ and reward $r$, but also a binary indicator done$(s')$ that tells us if $s'$ is terminal. In this case, we set the target value in Q-learning to $V^*(s') = 0$ yielding the modified update rule:

$$Q(s,a) \leftarrow Q(s,a) + \eta \left[ r + (1 - \text{done}(s'))\gamma \max_{a'} Q(s', a') - Q(s,a) \right] \tag{2.30}$$

For brevity, we will usually ignore this factor in the subsequent equations, but it needs to be implemented in the code.

Figure 2.5 gives an example of Q-learning applied to the simple 1d grid world from Figure 2.1, using $\gamma = 0.9$. We show the $Q$-functon at the start and end of each episode, after performing actions chosen by an $\epsilon$-greedy policy. We initialize $Q(s, a) = 0$ for all entries, and use a step size of $\eta = 1$. At convergence, we have $Q_*(s, a) = r + \gamma Q_*(s', a_*)$, where $a_* =\downarrow$ for all states.



| | Q-function *episode start* | | | Episode | Time Step | Action | (s,α,r , s') | r + γ Q*(s' , α) | Q-function *episode end* | | |
|---|---|---|---|---|---|---|---|---|---|---|---|
| | | UP | DOWN | | | | | | | UP | DOWN |
| | $S_1$ | 0 | 0 | 1 | 1 | ↓ | $(S_1, D,0,S_2)$ | 0 + 0.9 X 0 = 0 | $S_1$ | 0 | 0 |
| | | | | 1 | 2 | ↑ | $(S_2,U,0,S_1)$ | 0 + 0.9 X 0 = 0 | | | |
| $Q_1$ | $S_2$ | 0 | 0 | 1 | 3 | ↓ | $(S_1, D,0,S_2)$ | 0 + 0.9 X 0 = 0 | $S_2$ | 0 | 0 |
| | | | | 1 | 4 | ↓ | $(S_2, U,0,S_1)$ | 0 + 0.9 X 0 = 0 | | | |
| | $S_3$ | 0 | 0 | 1 | 5 | ↓ | $(S_3, D,1,S_{T2})$ | 1 | $S_3$ | 0 | 1 |
| | $S_1$ | 0 | 0 | | | | | | $S_1$ | 0 | 0 |
| | | | | 2 | 1 | ↓ | $(S_1, D,0,S_2)$ | 0 + 0.9 x 0 = 0 | | | |
| $Q_2$ | $S_2$ | 0 | 0 | 2 | 2 | ↓ | $(S_2, D,0,S_3)$ | 0 + 0.9 x 1 = 0.9 | $S_2$ | 0 | 0.9 |
| | | | | 2 | 3 | ↓ | $(S_3, D,0,S_{T2})$ | 1 | | | |
| | $S_3$ | 0 | 1 | | | | | | $S_3$ | 0 | 1 |
| | $S_1$ | 0 | 0 | 3 | 1 | ↓ | $(S_1, D,0,S_2)$ | 0 + 0.9 x 0.9 = 0.81 | $S_1$ | 0 | 0.81 |
| | | | | 3 | 2 | ↓ | $(S_2, D,0,S_3)$ | 0 + 0.9 x 1 = 0.9 | | | |
| $Q_3$ | $S_2$ | 0 | 0.9 | 3 | 3 | ↑ | $(S_3, D,0,S_2)$ | 0 + 0.9 x 0.9 = 0.81 | $S_2$ | 0 | 0.9 |
| | | | | 3 | 4 | ↓ | $(S_2, D,0,S_3)$ | 0 + 0.9 x 1 = 0.9 | | | |
| | $S_3$ | 0 | 1 | 3 | 5 | ↓ | $(S_3, D,0,S_{T2})$ | 1 | $S_3$ | 0.81 | 1 |
| | $S_1$ | 0 | 0.81 | 4 | 1 | ↓ | $(S_1, D,0,S_2)$ | 0 + 0.9 x 0.9 = 0.81 | $S_1$ | 0 | 0.81 |
| | | | | 4 | 2 | ↑ | $(S_2, U,0,S_1)$ | 0 + 0.9 x 0.81 = 0.73 | | | |
| $Q_4$ | $S_2$ | 0 | 0.9 | 4 | 3 | ↓ | $(S_1, D,0,S_2)$ | 0 + 0.9 x 0.9 = 0.81 | $S_2$ | 0.73 | 0.9 |
| | | | | 4 | 4 | ↑ | $(S_2, U,0,S_3)$ | 0 + 0.9 x 0.81 = 0.73 | | | |
| | $S_3$ | 0.81 | 1 | 4 | 5 | ↓ | $(S_1, D,0,S_3)$ | 0 + 0.9 x 0.9 = 0.81 | $S_3$ | 0.81 | 1 |
| | | | | 4 | 6 | ↓ | $(S_2, D,0,S_3)$ | 0 + 0.9 x 1 = 0.9 | | | |
| | | | | 4 | 7 | ↓ | $(S_2, D,0,S_3)$ | 1 | | | |
| | $S_1$ | 0 | 0.81 | 5 | 1 | ↑ | $(S1, U, 0,S_{T1})$ | 0 | $S_1$ | 0 | 0.81 |
| $Q_5$ | $S_2$ | 0.73 | 0.9 | | | | | | $S_2$ | 0.73 | 0.9 |
| | $S_3$ | 0.81 | 1 | | | | | | $S_3$ | 0.81 | 1 |

*Figure 2.5: Illustration of Q learning for one random trajectory in the 1d grid world in Figure 2.1 using $\epsilon$-greedy exploration. At the end of episode 1, we make a transition from $S_3$ to $S_{T2}$ and get a reward of $r = 1$, so we estimate $Q(S_3, \downarrow) = 1$. In episode 2, we make a transition from $S_2$ to $S_3$, so $S_2$ gets incremented by $\gamma Q(S_3, \downarrow) = 0.9$. Adapted from Figure 3.3 of [GK19].*

### 2.5.2 Q learning with function approximation

To make Q learning work with high-dimensional state spaces, we have to replace the tabular (non-parametric) representation with a parametric approximation, denoted $Q_{\boldsymbol{w}}(s, a)$. We can update this function using one or more steps of SGD on the following loss function

$$\mathcal{L}(\boldsymbol{w}|\boldsymbol{s}, a, r, \boldsymbol{s}') = \left((r + \gamma \max_{a'} Q_{\boldsymbol{w}}(\boldsymbol{s}', a')) - Q_{\boldsymbol{w}}(\boldsymbol{s}, a)\right)^2 \tag{2.31}$$

Since nonlinear functions need to be trained on minibatches of data, we compute the average loss over multiple randomly sampled experience tuples (see Section 2.5.2.3 for discussion) to get

$$\mathcal{L}(\boldsymbol{w}) = \mathbb{E}_{(\boldsymbol{s},a,r,\boldsymbol{s}')\sim U(\mathcal{D})}\left[\mathcal{L}(\boldsymbol{w}|\boldsymbol{s}, a, r, \boldsymbol{s}')\right] \tag{2.32}$$

See Algorithm 2 for the pseudocode.

**Algorithm 2:** Q learning with function approximation and replay buffers

```
Initialize environment state $\boldsymbol{s}$, network parameters $\boldsymbol{w}_0$, replay buffer $\mathcal{D} = \emptyset$, discount factor $\gamma$, step
  size $\eta$, policy $\pi_0(a|s) = \epsilon \text{Unif}(a) + (1 - \epsilon)\delta(a = \text{argmax}_a Q_{\boldsymbol{w}_0}(s, a))$
for iteration $k = 0, 1, 2, \dots$ do
    for environment step $s = 0, 1, \dots, S - 1$ do
        Sample action: $a \sim \pi_k(a|s)$
        Interact with environment: $(s', r) = \text{env.step}(a)$
        Update buffer: $\mathcal{D} \leftarrow \mathcal{D} \cup \{(s, a, s', r)\}$
    $\boldsymbol{w}_{k,0} \leftarrow \boldsymbol{w}_k$
    for gradient step $g = 0, 1, \dots, G - 1$ do
        Sample batch: $B \subset \mathcal{D}$
        Compute error: $\mathcal{L}(B, \boldsymbol{w}_{k,g}) = \frac{1}{|B|} \sum_{(s,a,r,s') \in B} \left[Q_{\boldsymbol{w}_{k,g}}(s, a) - (r + \gamma \max_{a'} Q_{\boldsymbol{w}_k}(s', a'))\right]^2$
        Update parameters: $\boldsymbol{w}_{k,g} \leftarrow \boldsymbol{w}_{k,g} - \eta \nabla_{\boldsymbol{w}_{k,g}} \mathcal{L}(B, \boldsymbol{w}_{k,g})$
    $\boldsymbol{w}_{k+1} \leftarrow \boldsymbol{w}_{k,G}$
```

#### 2.5.2.1 Neural fitted Q

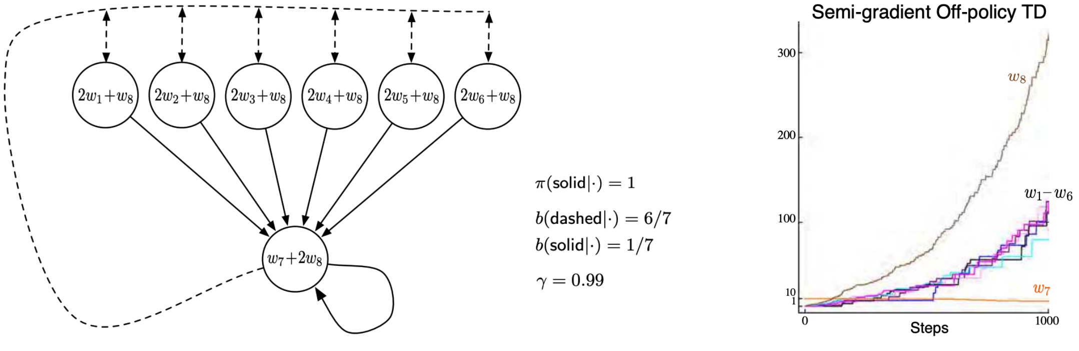
The first approach of this kind is known as **fitted Q evaluation** (or **FQE**) [EGW05], which was extended in [Rie05] to use neural networks. This corresponds to fully optimizing $\mathcal{L}(\boldsymbol{w})$ at each iteration (equivalent to using $G = \infty$ gradient steps).

#### 2.5.2.2 DQN

The influential deep Q-network or DQN paper of [Mni+15] also used neural nets to represent the $Q$ function, but performed a smaller number of gradient updates per iteration. Furthermore, they proposed to modify the target value when fitting the $Q$ function in order to avoid instabilities during training (see Section 2.5.2.4 for details).

The DQN method became famous since it was able to train agents that can outperform humans when playing various Atari games from the **ALE** (Atari Learning Environment) benchmark [Bel+13]. Here the input is a small color image, and the action space corresponds to moving left, right, up or down, plus an optional shoot action.[1]

[1] For more discussion of ALE, see [Mac+18a], and for a recent extension to continuous actions (representing joystick control), see the CALE benchmark of [FC24]. Note that DQN was not the first deep RL method to train an agent from pixel input; that honor goes to [LR10], who trained an autoencoder to embed images into low-dimensional latents, and then used neural fitted Q learning (Section 2.5.2.1) to fit the $Q$ function.



*(a)*

*(b)*

*Figure 2.6: (a) A simple MDP. (b) Parameters of the policy diverge over time. From Figures 11.1 and 11.2 of [SB18]. Used with kind permission of Richard Sutton.*

Since 2015, many more extensions to DQN have been proposed, with the goal of improving performance in various ways, either in terms of peak reward obtained, or sample efficiency (e.g., reward obtained after only 100k steps in the environment, as proposed in the **Atari-100k** benchmark [Kai+19][2]), or training stability, or all of the above. We discuss some of these extensions in Section 2.5.4.

#### 2.5.2.3 Experience replay

Since Q learning is an off-policy method, we can update the Q function using any data source. This is particularly important when we use nonlinear function approximation (see Section 2.5.2), which often needs a lot of data for model fitting. A natural source of data is data collected earlier in the trajectori of the agent; this is called an **experience replay** buffer, which stores $(s, a, r, s')$ transition tuples into a buffer. This can improve the stability and sample efficiency of learning, and was originally proposed in [Lin92].

This modification has two advantages. First, it improves data efficiency as every transition can be used multiple times. Second, it improves stability in training, by reducing the correlation of the data samples that the network is trained on, since the training tuples do not have to come from adjacent moments in time. (Note that experience replay requires the use of off-policy learning methods, such as Q learning, since the training data is sampled from older versions of the policy, not the current policy.)

It is possible to replace the uniform sampling from the buffer with one that favors more important transition tuples that may be more informative about $Q$. This idea is formalized in [Sch+16a], who develop a technique known as **prioritized experience replay**.

#### 2.5.2.4 The deadly triad

The problem with the naive Q learning objective in Equation (2.31) is that it can lead to instability, since the target we are regressing towards uses the same parameters $\boldsymbol{w}$ as the function we are updating. So the network is “chasing its own tail”. Although this is fine for tabular models, it can fail for nonlinear models, as we discuss below.

In general, an RL algorithm can become unstable when it has these three components: function approximation (such as neural networks), bootstrapped value function estimation (i.e., using TD-like methods instead of MC), and off-policy learning (where the actions are sampled from some distribution other than the policy that is being optimized). This combination is known as **the deadly triad** [Sut15; van+18]).

A classic example of this is the simple MDP depicted in Figure 2.6a, due to [Bai95]. (This is known as **Baird’s counter example**.) It has 7 states and 2 actions. Taking the dashed action takes the environment

[2] The Atari-100k benchmark only includes 26 out of 46 games of the ALE that were determined to be “solvable by state-of-the-art model-free deep RL algorithms” at the time of the benchmark’s creation in 2019. This excludes games like Montezuma’s Revenge, which require more exploration and hence more training data.

to the 6 upper states uniformly at random, while the solid action takes it to the bottom state. The reward is 0 in all transitions, and $\gamma = 0.99$. The value function $V_{\boldsymbol{w}}$ uses a linear parameterization indicated by the expressions shown inside the states, with $\boldsymbol{w} \in \mathbb{R}^8$. The target policies $\pi$ always chooses the solid action in every state. Clearly, the true value function, $V_\pi(s) = 0$, can be exactly represented by setting $\boldsymbol{w} = \boldsymbol{0}$.

Suppose we use a behavior policy $b$ to generate a trajectory, which chooses the dashed and solid actions with probabilities 6/7 and 1/7, respectively, in every state. If we apply TD(0) on this trajectory, the parameters diverge to $\infty$ (Figure 2.6b), even though the problem appears simple. In contrast, with on-policy data (that is, when $b$ is the same as $\pi$), TD(0) with linear approximation can be guaranteed to converge to a good value function approximate [TR97]. The difference is that with on-policy learning, as we improve the value function, we also improve the policy, so the two become self-consistent, whereas with off-policy learning, the behavior policy may not match the optimal value function that is being learned, leading to inconsistencies.

The divergence behavior is demonstrated in many value-based bootstrapping methods, including TD, Q-learning, and related approximate dynamic programming algorithms, where the value function is represented either linearly (like the example above) or nonlinearly [Gor95; TVR97; OCD21]. The root cause of these divergence phenomena is that bootstrapping methods typically are not minimizing a fixed objective function. Rather, they create a learning target using their own estimates, thus potentially creating a self-reinforcing loop to push the estimates to infinity. More formally, the problem is that the contraction property in the tabular case (Equation (2.10)) may no longer hold when $V$ is approximated by $V_{\boldsymbol{w}}$.

We discuss some solutions to the deadly triad problem below.

#### 2.5.2.5 Target networks

One heuristic solution to the deadly triad, proposed in the DQN paper, is to use a “frozen” **target network** computed at an earlier iteration to define the target value for the DQN updates, rather than trying to chase a constantly moving target. Specifically, we maintain an extra copy the $Q$-network, $Q_{\boldsymbol{w}^-}$, with the same structure as $Q_{\boldsymbol{w}}$. This new $Q$-network is used to compute bootstrapping targets

$$y(r, \boldsymbol{s}'; \boldsymbol{w}^-) = r + \gamma \max_{a'} Q_{\boldsymbol{w}^-}(\boldsymbol{s}', a') \tag{2.33}$$

for training $Q_{\boldsymbol{w}}$. We can periodically set $\boldsymbol{w}^- \leftarrow \text{sg}(\boldsymbol{w})$, usually after a few episodes, where the stop gradient operator is used to prevent autodiff propagating gradients back to $\boldsymbol{w}$. Alternatively, we can use an exponential moving average (EMA) of the weights, i.e., we use $\overline{\boldsymbol{w}} = \rho \overline{\boldsymbol{w}} + (1-\rho)\text{sg}(\boldsymbol{w})$, where $\rho \ll 1$ ensures that $Q_{\overline{\boldsymbol{w}}}$ slowly catches up with $Q_{\boldsymbol{w}}$. (If $\rho = 0$, we say that this is a **detached target**, since it is just a frozen copy of the current weights.) The final loss has the form

$$\mathcal{L}(\boldsymbol{w}) = \mathbb{E}_{(\boldsymbol{s},a,r,\boldsymbol{s}') \sim U(\mathcal{D})} \left[ \mathcal{L}(\boldsymbol{w}|\boldsymbol{s}, a, r, \boldsymbol{s}') \right] \tag{2.34}$$

$$\mathcal{L}(\boldsymbol{w}|\boldsymbol{s}, a, r, \boldsymbol{s}') = (y(r, \boldsymbol{s}'; \overline{\boldsymbol{w}}) - Q_{\boldsymbol{w}}(\boldsymbol{s}, a))^2 \tag{2.35}$$

Theoretical work justifying this technique is given in [FSW23; Che+24a].

#### 2.5.2.6 Gradient TD methods

A general way to ensure convergence in off-policy learning is to construct an objective function, the minimization of which leads to a good value function approximation. This is the basis of the **gradient TD method** of [SSM08; Mae+09; Ghi+20].

#### 2.5.2.7 Two time-scale methods

Another approach is to update the target value in the TD update more quickly than the value function itself; this is known as a **two timescale optimization** (see e.g., [Yu17; Zha+19; Hon+23]).

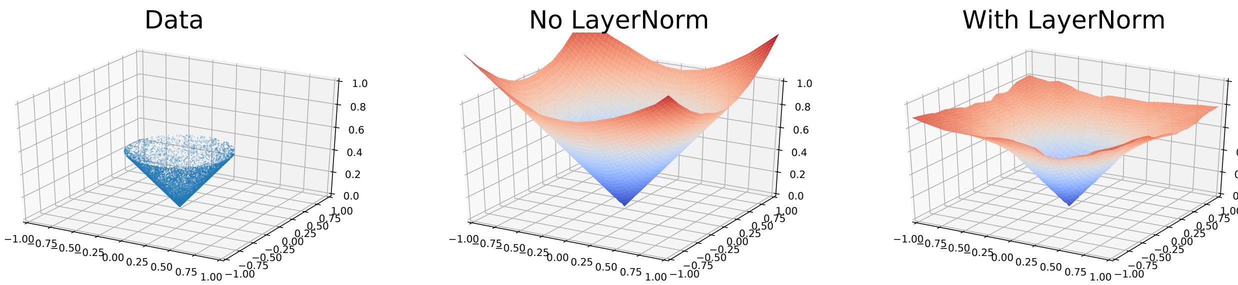


*Figure 2.7: We generate a dataset (left) with inputs $\boldsymbol{x}$ distributed in a circle with radius 0.5 and labels $y = ||\boldsymbol{x}||$. We then fit a two-layer MLP without LayerNorm (center) and with LayerNorm (right). LayerNorm bounds the values and prevents catastrophic overestimation when extrapolating. From Figure 3 of [Bal+23]. Used with kind permission of Philip Ball.*

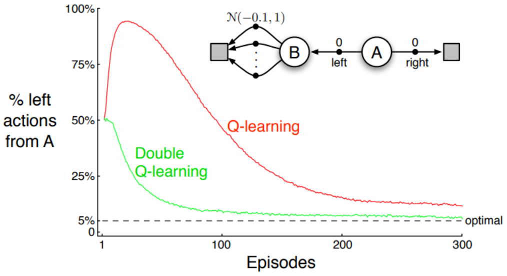


*Figure 2.8: Comparison of Q-learning and double Q-learning on a simple episodic MDP using $\epsilon$-greedy action selection with $\epsilon = 0.1$. The initial state is A, and squares denote absorbing states. The data are averaged over 10,000 runs. From Figure 6.5 of [SB18]. Used with kind permission of Richard Sutton.*

#### 2.5.2.8 Layer norm

More recently, [Gal+24] proved that just adding LayerNorm [BKH16] to the penultimate layer of the critic network, just before the linear head, is sufficient to provably yield convergence of TD learning even in the off-policy setting. In particular, suppose the network has the form $Q(s, a|\boldsymbol{w}, \boldsymbol{\theta}) = \boldsymbol{w}^T \text{ReLU}(\text{LayerNorm}(f(s, a; \boldsymbol{\theta})))$. Since $||\text{LayerNorm}(f(s, a; \boldsymbol{\theta}))|| \leq 1$, we have $||Q(s, a|\boldsymbol{w}, \boldsymbol{\theta}) \leq ||\boldsymbol{w}||$, which means the magnitude of the output is always bounded, as shown in Figure 2.7. In [Gal+24], they prove this (plus $\ell_2$ regularization on $\boldsymbol{w}$, and a sufficiently wide penultimate layer) is sufficient to ensure convergence of the value function estimate.

#### 2.5.2.9 Other methods

A variety of other solutions to the deadly triad have been proposed, including the "chaining value functions" approach of [SSTH22], a combination of target networks and over-parameterized linear function approximation [Che+24a], etc.

### 2.5.3 Maximization bias

Standard Q-learning suffers from a problem known as the **optimizer's curse** [SW06], or the **maximization bias**. The problem refers to the simple statistical inequality: $\mathbb{E}[\max_a X_a] \geq \max_a \mathbb{E}[X_a]$, for a set of random variables $\{X_a\}$. Thus, if we pick actions greedily according to their random scores $\{X_a\}$, we might pick a wrong action just because random noise makes it appealing.

Figure 2.8 gives a simple example of how this can happen in an MDP. The start state is A. The right action gives a reward 0 and terminates the episode. The left action also gives a reward of 0, but then enters state B, from which there are many possible actions, with rewards drawn from $\mathcal{N}(-0.1, 1.0)$. Thus the expected return for any trajectory starting with the left action is $-0.1$, making it suboptimal. Nevertheless, the RL algorithm may pick the left action due to the maximization bias making B appear to have a positive value.

#### 2.5.3.1 Double Q-learning

One solution to avoid the maximization bias is to use two separate $Q$-functions, $Q_1$ and $Q_2$, one for selecting the greedy action, and the other for estimating the corresponding $Q$-value. In particular, upon seeing a transition $(s, a, r, s')$, we perform the following update for $i = 1 : 2$:

$$Q_i(s,a) \leftarrow Q_i(s,a) + \eta(y_i(s,a) - Q_i(s,a)) \tag{2.36}$$

$$y_i(s,a) = r + \gamma Q_i(s', \operatorname*{argmax}_{a'} Q_{-i}(s',a')) \tag{2.37}$$

So we see that $Q_1$ uses $Q_2$ to choose the best action but uses $Q_1$ to evaluate it, and vice versa. This technique is called **double Q-learning** [Has10]. Figure 2.8 shows the benefits of the algorithm over standard Q-learning in a toy problem.

#### 2.5.3.2 Double DQN

In [HGS16], they combine double Q learning with deep Q networks (Section 2.5.2.2) to get **double DQN**. This modifies Equation (2.37) to its gradient form, and then the current network for action proposals, but the target network for action evaluation. Thus the training target becomes

$$y(r, \boldsymbol{s}'; \boldsymbol{w}, \overline{\boldsymbol{w}}) = r + \gamma Q_{\overline{\boldsymbol{w}}}(\boldsymbol{s}', \operatorname*{argmax}_{a'} Q_{\boldsymbol{w}}(\boldsymbol{s}', a')) \tag{2.38}$$

In Section 3.7.2 we discuss an extension called **clipped double DQN** which uses two Q networks and their frozen copies to define the following target:

$$y(r, \boldsymbol{s}'; \boldsymbol{w}_{1:2}, \overline{\boldsymbol{w}}_{1:2}) = r + \gamma \min_{i=1,2} Q_{\overline{\boldsymbol{w}}_i}(\boldsymbol{s}', \operatorname*{argmax}_{a'} Q_{\boldsymbol{w}_i}(\boldsymbol{s}', a')) \tag{2.39}$$

where $Q_{\overline{\boldsymbol{w}}_i}$ is the target network for $Q_{\boldsymbol{w}_i}$.

#### 2.5.3.3 Randomized ensemble DQN

The double DQN method is extended in the **REDQ** (randomized ensembled double Q learning) method of [Che+20], which uses an ensemble of $N > 2$ Q-networks. Furthermore, at each step, it draws a random sample of $M \leq N$ networks, and takes the minimum over them when computing the target value. That is, it uses the following update (see Algorithm 2 in appendix of [Che+20]):

$$y(r, \boldsymbol{s}'; \boldsymbol{w}_{1:N}, \overline{\boldsymbol{w}}_{1:N}) = r + \gamma \max_{a'} \min_{i \in \mathcal{M}} Q_{\overline{\boldsymbol{w}}_i}(\boldsymbol{s}', a') \tag{2.40}$$

where $\mathcal{M}$ is a random subset from the $N$ value functions. The ensemble reduces the variance, and the minimum reduces the overestimation bias.[3] If we set $N = M = 2$, we get a method similar to clipped double Q learning. (Note that REDQ is very similiar to the **Random Ensemble Mixture** method of [ASN20], which was designed for offline RL.)

### 2.5.4 DQN extensions

In this section, we discuss various extensions of DQN.

[3] In addition, REDQ performs $G \gg 1$ updates of the value functions for each environment step; this high **Update-To-Data** (UTD) ratio (also called **Replay Ratio**) is critical for sample efficiency, and is commonly used in model-based RL.

#### 2.5.4.1 Q learning for continuous actions

Q learning is not directly applicable to continuous actions due to the need to compute the argmax over actions. An early solution to this problem, based on neural fitted Q learning (see Section 2.5.2.1), is proposed in [HR11]. This became the basis of the DDPG algorithm of Section 3.7.1, which learns a policy to predict the argmax.

An alternative approach is to use gradient-free optimizers such as the cross-entropy method to approximate the argmax. The **QT-Opt** method of [Kal+18] treats the action vector $\boldsymbol{a}$ as a sequence of actions, and optimizes one dimension at a time [Met+17]. The **CAQL** (continuous action $Q$-learning) method of [Ryu+20]) uses mixed integer programming to solve the argmax problem, leveraging the ReLU structure of the $Q$-network. The method of [Sey+22] quantizes each action dimension separately, and then solves the argmax problem using methods inspired by multi-agent RL.

#### 2.5.4.2 Dueling DQN

The **dueling DQN** method of [Wan+16], learns a value function and an advantage function, and derives the Q function, rather than learning it directly. This is helpful when there are many actions with similar $Q$-values, since the advantage $A(s,a) = Q(s,a) - V(s)$ focuses on the differences in value relative to a shared baseline.

In more detail, we define a network with $|A|+1$ output heads, which computes $A_{\boldsymbol{w}}(\boldsymbol{s},a)$ for $a = 1:A$ and $V_{\boldsymbol{w}}(\boldsymbol{s})$. We can then derive

$$Q_{\boldsymbol{w}}(\boldsymbol{s},a) = V_{\boldsymbol{w}}(\boldsymbol{s}) + A_{\boldsymbol{w}}(\boldsymbol{s},a) \tag{2.41}$$

However, this naive approach ignores the following constraint that holds for any policy $\pi$:

$$\begin{aligned} \mathbb{E}_{\pi(a|s)}\left[A^\pi(s,a)\right] &= \mathbb{E}_{\pi(a|s)}\left[Q^\pi(s,a) - V^\pi(s)\right] && (2.42) \\ &= V^\pi(s) - V^\pi(s) = 0 && (2.43) \end{aligned}$$

Fortunately, for the optimal policy $\pi^*(s) = \operatorname{argmax}_{a'} Q^*(s,a')$ we have

$$\begin{aligned} 0 &= \mathbb{E}_{\pi^*(a|s)}\left[Q^*(s,a)\right] - V^*(s) && (2.44) \\ &= Q^*(s, \operatorname*{argmax}_{a'} Q^*(s,a')) - V^*(s) && (2.45) \\ &= \max_{a'} Q^*(s,a') - V^*(s) && (2.46) \\ &= \max_{a'} A^*(s,a') && (2.47) \end{aligned}$$

Thus we can satisfy the constraint for the optimal policy by subtracting off $\max_a A(s,a)$ from the advantage head. Equivalently we can compute the Q function using

$$Q_{\boldsymbol{w}}(\boldsymbol{s},a) = V_{\boldsymbol{w}}(\boldsymbol{s}) + A_{\boldsymbol{w}}(\boldsymbol{s},a) - \max_{a'} A_{\boldsymbol{w}}(\boldsymbol{s},a') \tag{2.48}$$

In practice, the max is replaced by an average, which seems to work better empirically.

#### 2.5.4.3 Noisy nets and exploration

Standard DQN relies on the epsilon-greedy strategy to perform exploration. However, this will explore equally in all states, whereas we would like to the amount of exploration to be state dependent, to reflect the amount of uncertainty in the outcomes of trying each action in that state due to lack of knowledge (i.e., **epistemic uncertainty** rather than aleatoric or irreducile uncertainty). An early approach to this, known as **noisy nets** [For+18], added random noise to the network weights to encourage exploration which is temporally consistent within episodes. More recent methods for exploration are discussed in Section 1.3.5.

#### 2.5.4.4 Multi-step DQN

As we discussed in Section 2.3.3, we can reduce the bias introduced by bootstrapping by replacing TD(1) updates with TD($n$) updates, where we unroll the value computation for $n$ MC steps, and then plug in the value function at the end. We can apply this to the DQN context by defining the target

$$y(s_0, a_0) = \sum_{t=1}^{n} \gamma^{t-1} r_t + \gamma^n \max_{a_n} Q_{\boldsymbol{w}}(s_n, a_n) \tag{2.49}$$

This can be implemented for episodic environments by storing experience tuples of the form

$$\tau = (s, a, \sum_{k=1}^{n} \gamma^{k-1} r_k, s_n, \text{done}) \tag{2.50}$$

where done $= 1$ if the trajectory ended at any point during the $n$-step rollout.

Theoretically this method is only valid if all the intermediate actions, $a_{2:n-1}$, are sampled from the current optimal policy derived from $Q_{\boldsymbol{w}}$, as opposed to some behavior policy, such as epsilon greedy or some samples from the replay buffer from an old policy. In practice, we can just restrict sampling to recent samples from the replay buffer, making the resulting method approximately on-policy.

Instead of using a fixed $n$, it is possible to use a weighted combination of returns; this is known as the $Q(\lambda)$ algorithm [PW94; Koz+21].

#### 2.5.4.5 Rainbow

The **Rainbow** method of [Hes+18] combined 6 improvements to the vanilla DQN method, as listed below. (The paper is called “Rainbow” due to the color coding of their results plot, a modified version of which is shown in Figure 2.9.) At the time it was published (2018), this produced SOTA results on the Atari-200M benchmark. The 6 improvements are as follows:

- Use double DQN, as in Section 2.5.3.2.
- Use prioritized experience replay, as in Section 2.5.2.3.
- Use the categorical DQN (C51) (Section 7.2.2) distributional RL method.
- Use n-step returns (with $n = 3$), as in Section 2.5.4.4.
- Use dueling DQN, as in Section 2.5.4.2.
- Use noisy nets, as in Section 2.5.4.3.

Each improvement gives diminishing returns, as can be see in Figure 2.9.

Recently the “Beyond the Rainbow” paper [Unk24] proposed several more extensions:

- Use a larger CNN with residual connections, namely the Impala network from [Esp+18] with the modifications (including the use of spectral normalization) proposed in [SS21].
- Replace C51 with Implicit Quantile Networks [Dab+18].
- Use **Munchausen RL** [VPG20], which modifies the Q learning update rule by adding an entropy-like penalty.
- Collect 1 environment step from 64 parallel workers for each minibatch update (rather than taking many steps from a smaller number of workers).

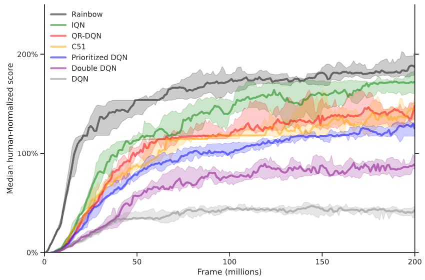


*Figure 2.9: Plot of median human-normalized score over all 57 Atari games for various DQN agents. The yellow, red and green curves are distributional RL methods (Section 7.2), namely categorical DQN (C51) (Section 7.2.2) Quantile Regression DQN (Section 7.2.1), and Implicit Quantile Networks [Dab+18]. Figure from `https://github.com/google-deepmind/dqn_zoo`.*

#### 2.5.4.6 Bigger, Better, Faster

At the time of writing this document (2024), the SOTA on the 100k sample-efficient Atari benchmark [Kai+19] is obtained by the **BBF** algorithm of [Sch+23b]. (BBF stands for “Bigger, Better, Faster”.) It uses the following tricks, in order of decreasing importance:

- Use a larger CNN with residual connections, namely a modified version of the Impala network from [Esp+18].
- Increase the **update-to-data** (UTD) ratio (number of times we update the Q function for every observation that is observed), in order to increase sample efficiency [HHA19].
- Use a periodic soft reset of (some of) the network weights to avoid loss of elasticity due to increased network updates, following the **SR-SPR** method of [D’O+22].
- Use n-step returns, as in Section 2.5.4.4, and then gradually decrease (anneal) the n-step return from $n = 10$ to $n = 3$, to reduce the bias over time.
- Add weight decay.
- Add a self-predictive representation loss (Section 4.4.2.4) to increase sample efficiency.
- Gradually increase the discount factor from $\gamma = 0.97$ to $\gamma = 0.997$, to encourage longer term planning once the model starts to be trained.[4]
- Drop noisy nets (which requires multiple network copies and thus slows down training due to increased memory use), since it does not help.
- Use dueling DQN (see Section 2.5.4.2).
- Use distributional DQN (see Section 7.2).

#### 2.5.4.7 Other methods

Many other methods have been proposed to reduce the sample complexity of value-based RL while maintaining performance, see e.g., the **MEME** paper of [Kap+22].

[4] The **Agent 57** method of [Bad+20] automatically learns the exploration rate and discount factor using a multi-armed bandit stratey, which lets it be more exploratory or more exploitative, depending on the game. This resulted in super human performance on all 57 Atari games in ALE. However, it required 80 billion frames (environment steps)! This was subsequently reduced to the “standard” 200M frames in the **MEME** method of [Kap+22].

# Chapter 3

# Policy-based RL

In the previous section, we considered methods that estimate the action-value function, $Q(s, a)$, from which we derive a policy. However, these methods have several disadvantages: (1) they can be difficult to apply to continuous action spaces; (2) they may diverge if function approximation is used (see Section 2.5.2.4); (3) the training of $Q$, often based on TD-style updates, is not directly related to the expected return garnered by the learned policy; (4) they learn deterministic policies, whereas in stochastic and partially observed environments, stochastic policies are provably better [JSJ94].

In this section, we discuss **policy search** methods, which directly optimize the parameters of the policy so as to maximize its expected return. We mostly focus on **policy gradient** methods, that use the gradient of the loss to guide the search. As we will see, these policy methods often benefit from estimating a value or advantage function to reduce the variance in the policy search process, so we will also use techniques from Chapter 2.

The parametric policy will be denoted by $\pi_{\boldsymbol{\theta}}(a|s)$, which is usually some form of neural network. For discrete actions, the final layer is usually passed through a softmax function and then into a categorical distribution. For continuous actions, we typically use a Gaussian output layer (potentially clipped to a suitable range, such as $[-1, 1]$), although it is also possible to use more expressive (multi-modal) distributions, such as diffusion models [Ren+24].

There are many implementation details one needs to get right to get good performance when designing such neural networks. For example, [Fur+21] recommends using ELU instead of RELU activations, and using LayerNorm. (In [Gal+24] they recently proved that adding layer norm to the final layer of a DQN model is sufficient to guarantee that value learning is stable, even in the nonlinear setting.) However, we do not discuss these details in this manuscript.

For more details on policy gradient methods, see [Wen18b; Leh24].

## 3.1 The policy gradient theorem

We start by defining the objective function for policy learning, and then derive its gradient. The objective, which we aim to maximize, is defined as

$$\begin{aligned} J(\pi) &\triangleq \mathbb{E}_\pi\left[\sum_{t=0}^{\infty}\gamma^t R_{t+1}\right] && (3.1)\\ &= \sum_{t=0}^{\infty}\gamma^t \sum_s \left(\sum_{s_0} p_0(s_0)p^\pi(s_0 \to s, t)\right)\sum_a \pi(a|s)R(s,a) && (3.2)\\ &= \sum_s \left(\sum_{s_0}\sum_{t=0}^{\infty}\gamma^t p_0(s_0)p^\pi(s_0 \to s, t)\right)\sum_a \pi(a|s)R(s,a) && (3.3)\\ &= \sum_s \rho_\pi^\gamma(s)\sum_a \pi(a|s)R(s,a) && (3.4)\end{aligned}$$

where we have defined the discounted state visitation measure

$$\rho_\pi^\gamma(s) \triangleq \sum_{t=0}^{\infty}\gamma^t \underbrace{\sum_{s_0} p_0(s_0)p^\pi(s_0 \to s, t)}_{p_t^\pi(s)} \tag{3.5}$$

where $p^\pi(s_0 \to s, t)$ is the probability of going from $s_0$ to $s$ in $t$ steps, and $p_t^\pi(s)$ is the marginal probability of being in state $s$ at time $t$ (after each episodic reset). Note that $\rho_\pi^\gamma$ is a measure of time spent in non-terminal states, but it is not a probability measure, since it is not normalized, i.e., $\sum_s \rho_\pi^\gamma(s) \neq 1$. However, we may abuse notation and still treat it like a probability, so we can write things like

$$\mathbb{E}_{\rho_\pi^\gamma(s)}\left[f(s)\right] = \sum_s \rho_\pi^\gamma(s)f(s) \tag{3.6}$$

Using this notation, we can define the objective as

$$J(\pi) = \mathbb{E}_{\rho_\pi^\gamma(s),\pi(a|s)}\left[R(s,a)\right] \tag{3.7}$$

We can also define a normalized version of the measure $\rho$ by noting that $\sum_{t=0}^{\infty}\gamma^t = \frac{1}{1-\gamma}$ for $\gamma < 1$. Hence the normalized discounted state visitation distribution is given by

$$p_\pi^\gamma(s) = (1-\gamma)\rho_\pi^\gamma(s) = (1-\gamma)\sum_{t=0}^{\infty}\gamma^t p_t(s) \tag{3.8}$$

(Note the change from $\rho$ to $p$.)

Note that in [SB18, Sec 13.2], they use slightly different notation. In particular, they assume $\gamma = 1$, and define the non-discounted state visitation measure as $\eta(s)$ and the corresponding normalized version by $\mu(s)$. This is equivalent to ignoring the discount factor $\gamma^t$ when defining $\rho_\pi(s)$. This is standard practice in many implementations, since we can just average over (unweighted) trajectories when estimating the objective and its gradient, even though it results in a biased estimate [NT20; CVRM23].

By using the **log derivative trick** (which is the simple observation that $\nabla \log \pi = \frac{\nabla \pi}{\pi}$), plus some other algebraic tricks, one can show that the gradient of the above objective is given by

$$\begin{aligned} \nabla_{\boldsymbol{\theta}} J(\boldsymbol{\theta}) &= \sum_s \rho_\pi^\gamma(s)\sum_a Q^\pi(s,a)\nabla_{\boldsymbol{\theta}}\pi_{\boldsymbol{\theta}}(a|s) && (3.9)\\ &= \sum_s \rho_\pi^\gamma(s)\sum_a Q^{\pi_{\boldsymbol{\theta}}}(s,a)\pi_{\boldsymbol{\theta}}(a|s)\nabla_{\boldsymbol{\theta}}\log\pi_{\boldsymbol{\theta}}(a|s) && (3.10)\\ &= \mathbb{E}_{\rho_\pi^\gamma(s)\pi_{\boldsymbol{\theta}}(a|s)}\left[Q^{\pi_{\boldsymbol{\theta}}}(s,a)\nabla_{\boldsymbol{\theta}}\log\pi_{\boldsymbol{\theta}}(a|s)\right] && (3.11)\end{aligned}$$

This is known as the **policy gradient theorem** [Sut+99]. In statistics, the term $\nabla_{\boldsymbol{\theta}} \log \pi_{\boldsymbol{\theta}}(\boldsymbol{a}|\boldsymbol{s})$ is called the (Fisher) **score function**[1], so sometimes Equation (3.11) is called the **score function estimator** or **SFE** [Fu15; Moh+20].

## 3.2 REINFORCE

One way to apply the policy gradient theorem to optimize a policy is to use stochastic gradient ascent. Theoretical results concerning the convergence and sample complexity of such methods can be found in [Aga+21a].

To implement such a method, let $\boldsymbol{\tau} = (s_0, a_0, r_0, s_1, \ldots, s_T)$ be a trajectory created by sampling from $s_0 \sim p_0$ and then following $\pi_{\boldsymbol{\theta}}$. Then we have

$$\nabla_{\boldsymbol{\theta}} J(\pi_{\boldsymbol{\theta}}) = \sum_{t=0}^{\infty} \gamma^t \mathbb{E}_{p_t(s)\pi_{\boldsymbol{\theta}}(a_t|s_t)} \left[ \nabla_{\boldsymbol{\theta}} \log \pi_{\boldsymbol{\theta}}(a_t|s_t) Q_{\pi_{\boldsymbol{\theta}}}(s_t, a_t) \right] \tag{3.12}$$

$$\approx \sum_{t=0}^{T-1} \gamma^t G_t \nabla_{\boldsymbol{\theta}} \log \pi_{\boldsymbol{\theta}}(a_t|s_t) \tag{3.13}$$

where the return is defined as follows

$$G_t \triangleq r_t + \gamma r_{t+1} + \gamma^2 r_{t+2} + \cdots + \gamma^{T-t-1} r_{T-1} = \sum_{k=0}^{T-t-1} \gamma^k r_{t+k} = \sum_{j=t}^{T-1} \gamma^{j-t} r_j \tag{3.14}$$

See Algorithm 3 for the pseudocode.

**Algorithm 3:** REINFORCE (episodic version)

```
Initialize policy parameters $\boldsymbol{\theta}$
repeat
    Sample an episode $\boldsymbol{\tau} = (s_0, a_0, r_0, s_1, \ldots, s_T)$ using $\pi_{\boldsymbol{\theta}}$
    for $t = 0, 1, \ldots, T-1$ do
        $G_t = \sum_{k=t+1}^{T} \gamma^{k-t-1} R_k$
        $\boldsymbol{\theta} \leftarrow \boldsymbol{\theta} + \eta_{\boldsymbol{\theta}} \gamma^t G_t \nabla_{\boldsymbol{\theta}} \log \pi_{\boldsymbol{\theta}}(a_t|s_t)$
until converged;
```

In practice, estimating the policy gradient using Equation (3.11) can have a high variance. A **baseline** function $b(s)$ can be used for variance reduction to get

$$\nabla_{\boldsymbol{\theta}} J(\pi_{\boldsymbol{\theta}}) = \mathbb{E}_{\rho_{\boldsymbol{\theta}}(s)\pi_{\boldsymbol{\theta}}(a|s)} \left[ \nabla_{\boldsymbol{\theta}} \log \pi_{\boldsymbol{\theta}}(a|s)(Q_{\pi_{\boldsymbol{\theta}}}(s,a) - b(s)) \right] \tag{3.15}$$

Any function that satisfies $\mathbb{E}\left[\nabla_{\boldsymbol{\theta}} b(s)\right] = 0$ is a valid baseline. This follows since

$$\sum_a \nabla_{\boldsymbol{\theta}} \pi_{\boldsymbol{\theta}}(a|s)(Q(s,a) - b(s)) = \nabla_{\boldsymbol{\theta}} \sum_a \pi_{\boldsymbol{\theta}}(a|s) Q(s,a) - \nabla_{\boldsymbol{\theta}} [\sum_a \pi_{\boldsymbol{\theta}}(a|s)] b(s) = \nabla_{\boldsymbol{\theta}} \sum_a \pi_{\boldsymbol{\theta}}(a|s) Q(s,a) - 0 \tag{3.16}$$

A common choice for the baseline is $b(s) = V_{\pi_{\boldsymbol{\theta}}}(s)$. This is a good choice since $V_{\pi_{\boldsymbol{\theta}}}(s)$ and $Q(s,a)$ are correlated and have similar magnitudes, so the scaling factor in front of the gradient term will be small.

Using this we get an update of the following form

$$\boldsymbol{\theta} \leftarrow \boldsymbol{\theta} + \eta \sum_{t=0}^{T-1} \gamma^t (G_t - b(s_t)) \nabla_{\boldsymbol{\theta}} \log \pi_{\boldsymbol{\theta}}(a_t|s_t) \tag{3.17}$$

[1] This is distinct from the Stein score, which is the gradient wrt the argument of the log probability, $\nabla_{\boldsymbol{a}} \log \pi_{\boldsymbol{\theta}}(\boldsymbol{a}|\boldsymbol{s})$, as used in diffusion.

This is is called the **REINFORCE** estimator [Wil92].[2] The update equation can be interpreted as follows: we compute the sum of discounted future rewards induced by a trajectory, compared to a baseline, and if this is positive, we increase $\boldsymbol{\theta}$ so as to make this trajectory more likely, otherwise we decrease $\boldsymbol{\theta}$. Thus, we reinforce good behaviors, and reduce the chances of generating bad ones.

## 3.3 Actor-critic methods

An **actor-critic** method [BSA83] uses the policy gradient method, but where the expected return $G_t$ is estimated using temporal difference learning of a value function instead of MC rollouts. (The term "actor" refers to the policy, and the term "critic" refers to the value function.) The use of bootstrapping in TD updates allows more efficient learning of the value function compared to MC, and further reduces the variance. In addition, it allows us to develop a fully online, incremental algorithm, that does not need to wait until the end of the trajectory before updating the parameters.

### 3.3.1 Advantage actor critic (A2C)

Concretely, consider the use of the one-step TD method to estimate the return in the episodic case, i.e., we replace $G_t$ with $G_{t:t+1} = r_t + \gamma V_{\boldsymbol{w}}(s_{t+1})$. If we use $V_{\boldsymbol{w}}(s_t)$ as a baseline, the REINFORCE update in Equation (3.17) becomes

$$\boldsymbol{\theta} \leftarrow \boldsymbol{\theta} + \eta \sum_{t=0}^{T-1} \gamma^t \left(G_{t:t+1} - V_{\boldsymbol{w}}(s_t)\right) \nabla_{\boldsymbol{\theta}} \log \pi_{\boldsymbol{\theta}}(a_t|s_t) \tag{3.18}$$

$$= \boldsymbol{\theta} + \eta \sum_{t=0}^{T-1} \gamma^t \big(r_t + \gamma V_{\boldsymbol{w}}(s_{t+1}) - V_{\boldsymbol{w}}(s_t)\big) \nabla_{\boldsymbol{\theta}} \log \pi_{\boldsymbol{\theta}}(a_t|s_t) \tag{3.19}$$

Note that $\delta_t = r_{t+1} + \gamma V_{\boldsymbol{w}}(s_{t+1}) - V_{\boldsymbol{w}}(s_t)$ is a single sample approximation to the advantage function $\text{Adv}(s_t, a_t) = Q(s_t, a_t) - V(s_t)$. This method is therefore called **advantage actor critic** or **A2C**. See Algorithm 4 for the pseudo-code.[3] (Note that $V_{\boldsymbol{w}}(s_{t+1}) = 0$ if $s_t$ is a done state, representing the end of an episode.) Note that this is an on-policy algorithm, where we update the value function $V_{\boldsymbol{w}}^{\pi}$ to reflect the value of the current policy $\pi$. See Section 3.3.3 for further discussion of this point.

In practice, we should use a stop-gradient operator on the target value for the TD update, for reasons explained in Section 2.5.2.4. Furthermore, it is common to add an entropy term to the policy, to act as a regularizer (to ensure the policy remains stochastic, which smoothens the loss function — see Section 3.6.8). If we use a shared network with separate value and policy heads, we need to use a single loss function for training all the parameters $\boldsymbol{\phi}$. Thus we get the following loss, for each trajectory, where we want to minimize TD loss, maximize the policy gradient (expected reward) term, and maximize the entropy term.

$$\mathcal{L}(\boldsymbol{\phi}; \tau) = \frac{1}{T} \sum_{t=1}^{T} \left[\lambda_{TD} \mathcal{L}_{TD}(s_t, a_t, r_t, s_{t+1}) - \lambda_{PG} J_{PG}(s_t, a_t, r_t, s_{t+1}) - \lambda_{ent} J_{ent}(s_t)\right] \tag{3.20}$$

$$y_t = r_t + \gamma(1 - \text{done}(s_t)) V_{\boldsymbol{\phi}}(s_{t+1}) \tag{3.21}$$

$$\mathcal{L}_{TD}(s_t, a_t, r_t, s_{t+1}) = (\text{sg}(y_t) - V_\phi(s))^2 \tag{3.22}$$

$$J_{PG}(s_t, a_t, r_t, s_{t+1}) = (\text{sg}(y_t - V_\phi(s_t)) \log \pi_{\boldsymbol{\phi}}(a_t|s_t) \tag{3.23}$$

$$J_{ent}(s_t) = -\sum_a \pi_{\boldsymbol{\phi}}(a|s_t) \log \pi_{\boldsymbol{\phi}}(a|s_t) \tag{3.24}$$

[2] The term "REINFORCE" is an acronym for "REward Increment = nonnegative Factor x Offset Reinforcement x Characteristic Eligibility". The phrase "characteristic eligibility" refers to the $\nabla \log \pi_{\boldsymbol{\theta}}(a_t|s_t)$ term; the phrase "offset reinforcement" refers to the $G_t - b(s_t)$ term; and the phrase "nonnegative factor" refers to the learning rate $\eta$ of SGD.

[3] In [Mni+16], they proposed a distributed version of A2C known as **A3C** which stands for "asynchrononous advantage actor critic".

**Algorithm 4:** Advantage actor critic (A2C) algorithm (episodic)

```
Initialize actor parameters $\boldsymbol{\theta}$, critic parameters $\boldsymbol{w}$
repeat
    Sample starting state $s_0$ of a new episode
    for $t = 0, 1, 2, \ldots$ do
        Sample action $a_t \sim \pi_{\boldsymbol{\theta}}(\cdot|s_t)$
        $(s_{t+1}, r_t, \text{done}_t) = \text{env.step}(s_t, a_t)$
        $y_t = r_t + \gamma(1 - \text{done}_t)V_{\boldsymbol{w}}(s_{t+1})$ // Target
        $\delta_t = y_t - V_{\boldsymbol{w}}(s_t)$ // Advantage
        $\boldsymbol{w} \leftarrow \boldsymbol{w} + \eta_{\boldsymbol{w}} \delta_t \nabla_{\boldsymbol{w}} V_{\boldsymbol{w}}(s_t)$ // Critic
        $\boldsymbol{\theta} \leftarrow \boldsymbol{\theta} + \eta_{\boldsymbol{\theta}} \gamma^t \delta_t \nabla_{\boldsymbol{\theta}} \log \pi_{\boldsymbol{\theta}}(a_t|s_t)$ // Actor
        if $done_t = 1$ then
            break
until converged;
```

To handle the dynamically varying scales of the different loss functions, we can use the **PopArt** method of [Has+16; Hes+19] to allow for a fixed set of hyper-parameter values for $\lambda_i$. (PopArt stands for "Preserving Outputs Precisely, while Adaptively Rescaling Targets".)

### 3.3.2 Generalized advantage estimation (GAE)

In A2C, we replaced the high variance, but unbiased, MC return $G_t$ with the low variance, but biased, one-step bootstrap return $G_{t:t+1} = r_t + \gamma V_{\boldsymbol{w}}(s_{t+1})$. More generally, we can compute the $n$-step estimate

$$G_{t:t+n} = r_t + \gamma r_{t+1} + \gamma^2 r_{t+2} + \cdots + \gamma^{n-1} r_{t+n-1} + \gamma^n V_{\boldsymbol{w}}(s_{t+n}) \tag{3.25}$$

and thus obtain the (truncated) $n$-step advantage estimate as follows:

$$A_{\boldsymbol{w}}^{(n)}(s_t, a_t) = G_{t:t+n} - V_{\boldsymbol{w}}(s_t) \tag{3.26}$$

Unrolling to infinity, we get

$$\begin{aligned} A_t^{(1)} &= r_t + \gamma v_{t+1} - v_t \tag{3.27} \\ A_t^{(2)} &= r_t + \gamma r_{t+1} + \gamma^2 v_{t+2} - v_t \tag{3.28} \\ &\vdots \tag{3.29} \\ A_t^{(\infty)} &= r_t + \gamma r_{t+1} + \gamma^2 r_{t+2} + \cdots - v_t \tag{3.30} \end{aligned}$$

$A_t^{(1)}$ is high bias but low variance, and $A_t^{(\infty)}$ is unbiased but high variance.

Instead of using a single value of $n$, we can take a weighted average. That is, we define

$$A_t = \frac{\sum_{n=1}^T w_n A_t^{(n)}}{\sum_{n=1}^T w_n} \tag{3.31}$$

If we set $w_n = \lambda^{n-1}$ we get the following simple recursive calculation:

$$\begin{aligned} \delta_t &= r_t + \gamma v_{t+1} - v_t \tag{3.32} \\ A_t &= \delta_t + \gamma\lambda\delta_{t+1} + \cdots + (\gamma\lambda)^{T-(t+1)}\delta_{T-1} = \delta_t + \gamma\lambda A_{t+1} \tag{3.33} \end{aligned}$$

**Algorithm 5:** Generalized Advantage Estimation

```
def GAE($r_{1:T}, v_{1:T}, \gamma, \lambda$)
$A' = 0$
for $t = T : 1$ do
    $\delta_t = r_t + \gamma v_{t+1} - v_t$
    $A' = \delta_t + \gamma \lambda A'$
    $A_t = A'$ // advantage
    $y_t = A_t + v_t$ // TD target
Return $(A_{1:T}), y_{1:T})$
```

**Algorithm 6:** Actor critic with GAE

```
Initialize parameters $\boldsymbol{\phi}$, environment state $s$
repeat
    $(s_1, a_1, r_1, \ldots, s_T) = \text{rollout}(s, \pi_{\boldsymbol{\phi}})$
    $v_{1:T} = V_{\boldsymbol{\phi}}(s_{1:T})$
    $(A_{1:T}, y_{1:T}) = \text{sg}(\text{GAE}(r_{1:T}, v_{1:T}, \gamma, \lambda))$
    $\mathcal{L}(\boldsymbol{\phi}) = \frac{1}{T} \sum_{t=1}^{T} \left[ \lambda_{TD} (V_{\boldsymbol{\phi}}(s_t) - y_t)^2 - \lambda_{PG} A_t \log \pi_{\boldsymbol{\phi}}(a_t|s_t) - \lambda_{ent} \mathbb{H}(\pi_{\boldsymbol{\phi}}(\cdot|s_t)) \right]$
    $\boldsymbol{\phi} := \boldsymbol{\phi} - \eta \nabla \mathcal{L}(\boldsymbol{\phi})$
until *converged*;
```

Here $\lambda \in [0, 1]$ is a parameter that controls the bias-variance tradeoff: larger values decrease the bias but increase the variance. This is called **generalized advantage estimation** (**GAE**) [Sch+16b]. See Algorithm 5 for some pseudocode. Using this, we can define a general actor-critic method, as shown in Algorithm 6.

We can generalize this approach even further, by using gradient estimators of the form

$$\nabla J(\boldsymbol{\theta}) = \mathbb{E}\left[ \sum_{t=0}^{\infty} \Psi_t \nabla \log \pi_{\boldsymbol{\theta}}(a_t|s_t) \right] \tag{3.34}$$

where $\Psi_t$ may be any of the following:

$$\Psi_t = \sum_{i=t}^{\infty} \gamma^i r_i \qquad \text{Monte Carlo target} \tag{3.35}$$

$$\Psi_t = \sum_{i=t}^{\infty} \gamma^i r_i - V_{\boldsymbol{w}}(s_t) \qquad \text{MC with baseline} \tag{3.36}$$

$$\Psi_t = A_{\boldsymbol{w}}(s_t, a_t) \qquad \text{advantage function} \tag{3.37}$$

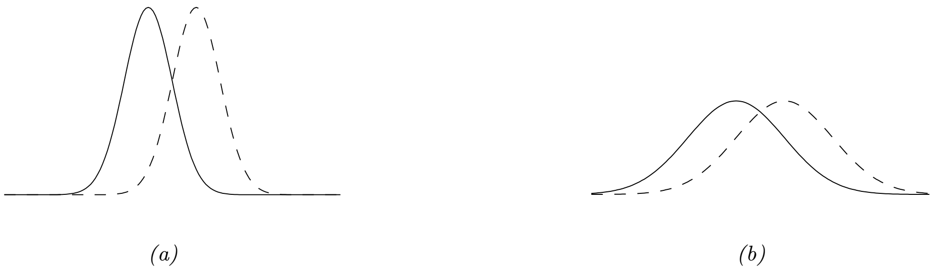
$$\Psi_t = Q_{\boldsymbol{w}}(s_t, a_t) \qquad \text{Q function} \tag{3.38}$$

$$\Psi_t = r_t + V_{\boldsymbol{w}}(s_{t+1}) - V_{\boldsymbol{w}}(s_t) \qquad \text{TD residual} \tag{3.39}$$

See [Sch+16b] for details.

### 3.3.3 Two-time scale actor critic algorithms

In standard AC, we update the actor and critic in parallel. However, it is better to let critic $V_{\boldsymbol{w}}$ learn using a faster learning rate (or more updates), so that it reflects the value of the current policy $\pi_{\boldsymbol{\theta}}$ more accurately, in order to get better gradient estimates for the policy update. This is known as two timescale learning or **bilevel optimization** [Yu17; Zha+19; Hon+23; Zhe+22a; Lor24]. (See also Section 4.3.1, where we discuss RL from a game theoretic perspective.)



*(a)*

*(b)*

*Figure 3.1: Changing the mean of a Gaussian by a fixed amount (from solid to dotted curve) can have more impact when the (shared) variance is small (as in a) compared to when the variance is large (as in b). Hence the impact (in terms of prediction accuracy) of a change to $\mu$ depends on where the optimizer is in $(\mu, \sigma)$ space. From Figure 3 of [Hon+10], reproduced from [Val00]. Used with kind permission of Antti Honkela.*

### 3.3.4 Natural policy gradient methods

In this section, we discuss an improvement to policy gradient methods that uses preconditioning to speedup convergence. In particular, we replace gradient descent with **natural gradient descent** (**NGD**) [Ama98; Mar20], which we explain below. We then show how to combine it with actor-critic.

#### 3.3.4.1 Natural gradient descent

NGD is a second order method for optimizing the parameters of (conditional) probability distributions, such as policies, $\pi_{\boldsymbol{\theta}}(\boldsymbol{a}|\boldsymbol{s})$. It typically converges faster and more robustly than SGD, but is computationally more expensive.

Before we explain NGD, let us review standard SGD, which is an update of the following form

$$\boldsymbol{\theta}_{k+1} = \boldsymbol{\theta}_k - \eta_k \boldsymbol{g}_k \tag{3.40}$$

where $\boldsymbol{g}_k = \nabla_{\boldsymbol{\theta}} \mathcal{L}(\boldsymbol{\theta}_k)$ is the gradient of the loss at the previous parameter values, and $\eta_k$ is the learning rate. It can be shown that the above update is equivalent to minimizing a locally linear approximation to the loss, $\hat{\mathcal{L}}_k$, subject to the constraint that the new parameters do not move too far (in Euclidean distance) from the previous parameters:

$$\boldsymbol{\theta}_{k+1} = \underset{\boldsymbol{\theta}}{\operatorname{argmin}}\, \hat{\mathcal{L}}_k(\boldsymbol{\theta}) \;\text{ s.t. }\; ||\boldsymbol{\theta} - \boldsymbol{\theta}_k||_2^2 \leq \epsilon \tag{3.41}$$

$$\hat{\mathcal{L}}_k(\boldsymbol{\theta}) = \mathcal{L}(\boldsymbol{\theta}_k) + \boldsymbol{g}_k^{\mathsf{T}}(\boldsymbol{\theta} - \boldsymbol{\theta}_k) \tag{3.42}$$

where the step size $\eta_k$ is proportional to $\epsilon$. This is called a **proximal update** [PB+14].

One problem with the SGD update is that Euclidean distance in parameter space does not make sense for probabilistic models. For example, consider comparing two Gaussians, $p_{\boldsymbol{\theta}} = p(y|\mu, \sigma)$ and $p_{\boldsymbol{\theta}'} = p(y|\mu', \sigma')$. The (squared) Euclidean distance between the parameter vectors decomposes as $||\boldsymbol{\theta} - \boldsymbol{\theta}'||_2^2 = (\mu - \mu')^2 + (\sigma - \sigma')^2$. However, the predictive distribution has the form $\exp(-\frac{1}{2\sigma^2}(y - \mu)^2)$, so changes in $\mu$ need to be measured relative to $\sigma$. This is illustrated in Figure 3.1(a-b), which shows two univariate Gaussian distributions (dotted and solid lines) whose means differ by $\epsilon$. In Figure 3.1(a), they share the same small variance $\sigma^2$, whereas in Figure 3.1(b), they share the same large variance. It is clear that the difference in $\mu$ matters much more (in terms of the effect on the distribution) when the variance is small. Thus we see that the two parameters interact with each other, which the Euclidean distance cannot capture.

The key to NGD is to measure the notion of distance between two probability distributions in terms of the KL divergence. This can be approximated in terms of the **Fisher information matrix** (FIM). In particular, for any given input $\boldsymbol{x}$, we have

$$D_{\mathbb{KL}}\left(p_{\boldsymbol{\theta}}(\boldsymbol{y}|\boldsymbol{x}) \parallel p_{\boldsymbol{\theta}+\boldsymbol{\delta}}(\boldsymbol{y}|\boldsymbol{x})\right) \approx \frac{1}{2}\boldsymbol{\delta}^{\mathsf{T}}\mathbf{F}_{\boldsymbol{x}}\boldsymbol{\delta} \tag{3.43}$$

where $\mathbf{F}_{\boldsymbol{x}}$ is the FIM

$$\mathbf{F}_{\boldsymbol{x}}(\boldsymbol{\theta}) = -\mathbb{E}_{p_{\boldsymbol{\theta}}(\boldsymbol{y}|\boldsymbol{x})}\left[\nabla^2 \log p_{\boldsymbol{\theta}}(\boldsymbol{y}|\boldsymbol{x})\right] = \mathbb{E}_{p_{\boldsymbol{\theta}}(\boldsymbol{y}|\boldsymbol{x})}\left[(\nabla \log p_{\boldsymbol{\theta}}(\boldsymbol{y}|\boldsymbol{x}))(\nabla \log p_{\boldsymbol{\theta}}(\boldsymbol{y}|\boldsymbol{x}))^{\mathsf{T}}\right] \tag{3.44}$$

We now replace the Euclidean distance between the parameters, $d(\boldsymbol{\theta}_k, \boldsymbol{\theta}_{k+1}) = ||\boldsymbol{\delta}||_2^2$, with

$$d(\boldsymbol{\theta}_k, \boldsymbol{\theta}_{k+1}) = \boldsymbol{\delta}^{\mathsf{T}} \mathbf{F}_k \boldsymbol{\delta}_k \tag{3.45}$$

where $\boldsymbol{\delta} = \boldsymbol{\theta}_{k+1} - \boldsymbol{\theta}_k$ and $\mathbf{F}_k = \mathbf{F}_{\boldsymbol{x}}(\boldsymbol{\theta}_k)$ for a randomly chosen input $\boldsymbol{x}$. This gives rise to the following constrained optimization problem:

$$\boldsymbol{\delta}_k = \underset{\boldsymbol{\delta}}{\operatorname{argmin}}\, \hat{\mathcal{L}}_k(\boldsymbol{\theta}_k + \boldsymbol{\delta}) \;\; \text{s.t.} \;\; \boldsymbol{\delta}^{\mathsf{T}} \mathbf{F}_k \boldsymbol{\delta} \le \epsilon \tag{3.46}$$

If we replace the constraint with a Lagrange multiplier, we get the unconstrained objective:

$$J_k(\boldsymbol{\delta}) = \mathcal{L}(\boldsymbol{\theta}_k) + \boldsymbol{g}_k^{\mathsf{T}} \boldsymbol{\delta} + \eta_k \boldsymbol{\delta}^{\mathsf{T}} \mathbf{F}_k \boldsymbol{\delta} \tag{3.47}$$

Solving $J_k(\boldsymbol{\delta}) = 0$ gives the update

$$\boldsymbol{\delta} = -\eta_k \mathbf{F}_k^{-1} \boldsymbol{g}_k \tag{3.48}$$

The term $\mathbf{F}^{-1}\boldsymbol{g}$ is called the **natural gradient**. This is equivalent to a preconditioned gradient update, where we use the inverse FIM as a preconditioning matrix. We can compute the (adaptive) learning rate using

$$\eta_k = \sqrt{\frac{\epsilon}{\boldsymbol{g}_k^{\mathsf{T}} \mathbf{F}_k^{-1} \boldsymbol{g}_k}} \tag{3.49}$$

Computing the FIM can be hard. A simple approximation is to replace the model's distribution with the empirical distribution. In particular, define $p_{\mathcal{D}}(\boldsymbol{x}, \boldsymbol{y}) = \frac{1}{N}\sum_{n=1}^N \delta_{\boldsymbol{x}_n}(\boldsymbol{x})\delta_{\boldsymbol{y}_n}(\boldsymbol{y})$, $p_{\mathcal{D}}(\boldsymbol{x}) = \frac{1}{N}\sum_{n=1}^N \delta_{\boldsymbol{x}_n}(\boldsymbol{x})$ and $p_{\boldsymbol{\theta}}(\boldsymbol{x}, \boldsymbol{y}) = p_{\mathcal{D}}(\boldsymbol{x}) p(\boldsymbol{y}|\boldsymbol{x}, \boldsymbol{\theta})$. Then we can compute the **empirical Fisher** [Mar16] as follows:

$$\begin{aligned}
\mathbf{F}(\boldsymbol{\theta}) &= \mathbb{E}_{p_{\boldsymbol{\theta}}(\boldsymbol{x},\boldsymbol{y})}\left[\nabla \log p(\boldsymbol{y}|\boldsymbol{x}, \boldsymbol{\theta}) \nabla \log p(\boldsymbol{y}|\boldsymbol{x}, \boldsymbol{\theta})^{\mathsf{T}}\right] && (3.50)\\
&\approx \mathbb{E}_{p_{\mathcal{D}}(\boldsymbol{x},\boldsymbol{y})}\left[\nabla \log p(\boldsymbol{y}|\boldsymbol{x}, \boldsymbol{\theta}) \nabla \log p(\boldsymbol{y}|\boldsymbol{x}, \boldsymbol{\theta})^{\mathsf{T}}\right] && (3.51)\\
&= \frac{1}{|\mathcal{D}|} \sum_{(\boldsymbol{x},\boldsymbol{y}) \in \mathcal{D}} \nabla \log p(\boldsymbol{y}|\boldsymbol{x}, \boldsymbol{\theta}) \nabla \log p(\boldsymbol{y}|\boldsymbol{x}, \boldsymbol{\theta})^{\mathsf{T}} && (3.52)
\end{aligned}$$

#### 3.3.4.2 Natural actor critic

To apply NGD to RL, we can adapt the A2C algorithm in Algorithm 6. In particular, define

$$\boldsymbol{g}_{kt} = \nabla_{\boldsymbol{\theta}_k} A_t \log \pi_{\boldsymbol{\theta}}(\boldsymbol{a}_t | \boldsymbol{s}_t) \tag{3.53}$$

where $A_t$ is the advantage function at step $t$ of the random trajectory generated by the policy at iteration $k$. Now we compute

$$\boldsymbol{g}_k = \frac{1}{T}\sum_{t=1}^T \boldsymbol{g}_{kt}, \;\; \mathbf{F}_k = \frac{1}{T}\sum_{t=1}^T \boldsymbol{g}_{kt} \boldsymbol{g}_{kt}^{\mathsf{T}} \tag{3.54}$$

and compute $\boldsymbol{\delta}_{k+1} = -\eta_k \mathbf{F}_k^{-1} \boldsymbol{g}_k$. This approach is called **natural policy gradient** [Kak01; Raj+17].

We can compute $\mathbf{F}_k^{-1}\boldsymbol{g}_k$ without having to invert $\mathbf{F}_k$ by using the conjugate gradient method, where each CG step uses efficient methods for Hessian-vector products [Pea94]. This is called **Hessian free optimization** [Mar10]. Similarly, we can efficiently compute $\boldsymbol{g}_k^{\mathsf{T}}(\mathbf{F}_k^{-1}\boldsymbol{g}_k)$.

As a more accurate alternative to the empirical Fisher, [MG15] propose the **KFAC** method, which stands for "Kronecker factored approximate curvature"; this approximates the FIM of a DNN as a block diagonal matrix, where each block is a Kronecker product of two small matrices. This was applied to policy gradient learning in [Wu+17].

### 3.3.5 Architectural issues

It is common to use a single neural network for both the actor and critic, but using different output heads: a scalar output for the value function, and a vector output for the policy. For example, the **Amago** method [GFZ24], t uses a transformer backbone. To train the shared model, they construct a unified objective $\mathcal{L} = E[\lambda_0 \mathcal{L}_{TD} + \lambda_1 \mathcal{L}_{PG}]$, where the TD and policy gradient losses are dynamically normalized using the **PopArt** method of [Has+16; Hes+19] to allow for a fixed set of hyper-parameter values for $\lambda_i$, even as the range of the losses change over time. (PopArt stands for "Preserving Outputs Precisely, while Adaptively Rescaling Targets".)

## 3.4 Policy improvement methods

In this section, we discuss methods that try to monotonically improve performance of the policy at each step, rather than just following the gradient, which can result in a high variance estimate where performance can increase or decrease at each step. These are called **policy improvement** methods. Our presentation is based on [QPC24].

### 3.4.1 Policy improvement lower bound

We start by stating a useful result from [Ach+17]. Let $\pi_k$ be the current policy at step $k$, and let $\pi$ be any other policy (e.g., a candidate new one). Let $p^{\gamma}_{\pi_k}$ be the normalized discounted state visitation distribution for $\pi_k$, defined in Equation (3.8). Let $A^{\pi_k}(s,a) = Q^{\pi_k}(s,a) - V^{\pi_k}(s)$ be the advantage function. Finally, let the total variation distance between two distributions be given by

$$\text{TV}(p,q) \triangleq \frac{1}{2}||\boldsymbol{p} - \boldsymbol{q}||_1 = \frac{1}{2}\sum_s |p(s) - q(s)| \tag{3.55}$$

Then one can show [Ach+17] that

$$J(\pi) - J(\pi_k) \geq \underbrace{\frac{1}{1-\gamma}\mathbb{E}_{p^{\gamma}_{\pi_k}(s)\pi_k(a|s)}\left[\frac{\pi(a|s)}{\pi_k(a|s)}A^{\pi_k}(s,a)\right]}_{L(\pi,\pi_k)} - \frac{2\gamma C^{\pi,\pi_k}}{(1-\gamma)^2}\mathbb{E}_{p^{\gamma}_{\pi_k}(s)}\left[\text{TV}(\pi(\cdot|s),\pi_k(\cdot|s))\right] \tag{3.56}$$

where $C^{\pi,\pi_k} = \max_s |\mathbb{E}_{\pi(a|s)}\left[A^{\pi_k}(s,a)\right]|$. In the above, $L(\pi,\pi_k)$ is a surrogate objective, and the second term is a penalty term.

If we can optimize this lower bound (or a stochastic approximation, based on samples from the current policy $\pi_k$), we can guarantee monotonic policy improvement (in expectation) at each step. We will replace this objective with a trust-region update that is easier to optimize:

$$\pi_{k+1} = \underset{\pi}{\text{argmax}}\, L(\pi,\pi_k) \;\; \text{s.t.} \;\; \mathbb{E}_{p^{\gamma}_{\pi_k}(s)}\left[\text{TV}(\pi,\pi_k)(s)\right] \leq \epsilon \tag{3.57}$$

The constraint bounds the worst-case performance decline at each update. The overall procedure becomes an approximate policy improvement method. There are various ways of implementing the above method in practice, some of which we discuss below. (See also [GDWF22], who propose a framework called **mirror learning**, that justifies these "approximations" as in fact being the optimal thing to do for a different kind of objective; see also [Vas+21].)

### 3.4.2 Trust region policy optimization (TRPO)

In this section, we describe the **trust region policy optimization** (**TRPO**) method of [Sch+15b]. This implements an approximation to Equation (3.57). First, it leverages the fact that if

$$\mathbb{E}_{p^{\gamma}_{\pi_k}(s)}\left[D_{\mathbb{KL}}\left(\pi_k \parallel \pi\right)(s)\right] \leq \delta \tag{3.58}$$

then $\pi$ also satisfies the TV constraint with $\delta = \frac{\epsilon^2}{2}$. Next it considers a first-order expansion of the surrogate objective to get

$$L(\pi, \pi_k) = \mathbb{E}_{p^\gamma_{\pi_k}(s)\pi_k(a|s)}\left[\frac{\pi(a|s)}{\pi_k(a|s)} A^{\pi_k}(s,a)\right] \approx \boldsymbol{g}_k^\mathsf{T}(\boldsymbol{\theta} - \boldsymbol{\theta}_k) \tag{3.59}$$

where $\boldsymbol{g}_k = \nabla_{\boldsymbol{\theta}} L(\pi_{\boldsymbol{\theta}}, \pi_k)|_{\boldsymbol{\theta}_k}$. Finally it considers a second-order expansion of the KL term to get the approximate constraint

$$\mathbb{E}_{p^\gamma_{\pi_k}(s)}\left[D_{\mathbb{KL}}\left(\pi_k \parallel \pi\right)(s)\right] \approx \frac{1}{2}(\boldsymbol{\theta} - \boldsymbol{\theta}_k)^\mathsf{T}\mathbf{F}_k(\boldsymbol{\theta} - \boldsymbol{\theta}_k) \tag{3.60}$$

where $\mathbf{F}_k = \boldsymbol{g}_k\boldsymbol{g}_k^\mathsf{T}$ is an approximation to the Fisher information matrix (see Equation (3.54)). We then use the update

$$\boldsymbol{\theta}_{k+1} = \boldsymbol{\theta}_k + \eta_k \boldsymbol{v}_k \tag{3.61}$$

where $\boldsymbol{v}_k = \mathbf{F}_k^{-1}\boldsymbol{g}_k$ is the natural gradient, and the step size is initialized to $\eta_k = \sqrt{\frac{2\delta}{\boldsymbol{v}_k^\mathsf{T}\mathbf{F}_k\boldsymbol{v}_k}}$. (In practice we compute $\boldsymbol{v}_k$ by approximately solving the linear system $\mathbf{F}_k\boldsymbol{v} = \boldsymbol{g}_k$ using conjugate gradient methods, which just require matrix vector multiplies.) We then use a backtracking line search procedure to ensure the trust region is satisfied.

### 3.4.3 Proximal Policy Optimization (PPO)

In this section, we describe the the **proximal policy optimization** or **PPO** method of [Sch+17], which is a simplification of TRPO.

We start by noting the following result:

$$\mathbb{E}_{p^\gamma_{\pi_k}(s)}\left[\mathrm{TV}(\pi, \pi_k)(s)\right] = \frac{1}{2}\mathbb{E}_{(s,a)\sim p^\gamma_{\pi_k}}\left[|\frac{\pi(a|s)}{\pi_k(a|s)} - 1|\right] \tag{3.62}$$

This holds provided the support of $\pi$ is contained in the support of $\pi_k$ at every state. We then use the following update:

$$\pi_{k+1} = \underset{\pi}{\operatorname{argmax}}\, \mathbb{E}_{(s,a)\sim p^\gamma_{\pi_k}}\left[\min\left(\rho_k(s,a)A^{\pi_k}(s,a), \tilde{\rho}_k(s,a)A^{\pi_k}(s,a)\right)\right] \tag{3.63}$$

where $\rho_k(s,a) = \frac{\pi(a|s)}{\pi_k(a|s)}$ is the likelihood ratio, and $\tilde{\rho}_k(s,a) = \mathrm{clip}(\rho_k(s,a), 1-\epsilon, 1+\epsilon)$, where $\mathrm{clip}(x,l,u) = \min(\max(x,l),u)$. See [GDWF22] for a theoretical justification for these simplifications. Furthermore, this can be modified to ensure monotonic improvement as discussed in [WHT19], making it a true bound optimization method.

Some pseudocode for PPO (with GAE) is given in Algorithm 7. It is basically identical to the AC code in Algorithm 6, except the policy loss has the form $\min(\rho_t A_t, \tilde{\rho}_t A_t)$ instead of $A_t \log \pi_{\boldsymbol{\phi}}(a_t|s_t)$, and we perform multiple policy updates per rollout, for increased sample efficiency. For all the implementation details, see https://iclr-blog-track.github.io/2022/03/25/ppo-implementation-details/.

### 3.4.4 Variational Maximum a Posteriori Policy Optimization (VMPO)

In this section, we discuss the **VMPO** algorithm of [FS+19], which is an on-policy extension of the earlier off-policy MPO (MAP policy optimization) algorithm that we discuss in Section 3.6.5. VMPO was originally explained in terms of the "control as inference" framework (see Section 3.6), but we can also view it as a constrained policy improvement method, based on Equation (3.57). In particular, VMPO leverages the fact that if

$$\mathbb{E}_{p^\gamma_{\pi_k}(s)}\left[D_{\mathbb{KL}}\left(\pi \parallel \pi_k\right)(s)\right] \le \delta \tag{3.64}$$

then $\pi$ also satisfies the TV constraint with $\delta = \frac{\epsilon^2}{2}$.

Note that here the KL is reversed compared to TRPO in Section 3.4.2. This new version will encourage $\pi$ to be mode-covering, so it will naturally have high entropy, which can result in improved robustness.

**Algorithm 7:** PPO with GAE

```
Initialize parameters $\boldsymbol{\phi}$, environment state $s$
for iteration $k = 1, 2, \ldots$ do
    $\boldsymbol{\phi}_{\text{old}} \leftarrow \boldsymbol{\phi}$
    $(\tau, s) = \text{rollout}(s, \pi_{\boldsymbol{\phi}_{\text{old}}})$
    $(s_1, a_1, r_1, \ldots, s_T) = \tau$
    $v_t = V_{\boldsymbol{\phi}}(s_t)$ for $t = 1 : T$
    $(A_{1:T}, y_{1:T}) = \text{GAE}(r_{1:T}, v_{1:T}, \gamma, \lambda)$
    for $m = 1 : M$ do
        $\rho_t = \frac{\pi_{\boldsymbol{\phi}}(a_t|s_t)}{\pi_{\boldsymbol{\phi}_{\text{old}}}(a_t|s_t)}$ for $t = 1 : T$
        $\tilde{\rho}_t = \text{clip}(\rho_t)$ for $t = 1 : T$
        $\mathcal{L}(\boldsymbol{\phi}) = \frac{1}{T} \sum_{t=1}^{T} \left[ \lambda_{TD} (V_{\boldsymbol{\phi}}(s_t) - y_t)^2 - \lambda_{PG} \min(\rho_t A_t, \tilde{\rho}_t A_t) - \lambda_{ent} \, \mathbb{H}(\pi_{\boldsymbol{\phi}}(\cdot|s_t)) \right]$
        $\boldsymbol{\phi} := \boldsymbol{\phi} - \eta \nabla_{\boldsymbol{\phi}} \mathcal{L}(\boldsymbol{\phi})$
```

Unfortunately, this kind of KL is harder to compute, since we are taking expectations wrt the unknown distribution $\pi$.

To solve this problem, VMPO adopts an EM-type approach. In the E step, we compute a non-parametric version of the state-action distribution given by the unknown new policy:

$$\psi(s, a) = \pi(a|s) p^{\gamma}_{\pi_k}(s) \tag{3.65}$$

The optimal new distribution is given by

$$\psi_{k+1} = \underset{\psi}{\text{argmax}}\, \mathbb{E}_{\psi(s,a)} \left[ A^{\pi_k}(s, a) \right] \quad \text{s.t.} \quad D_{\mathbb{KL}} \left( \psi \parallel \psi_k \right) \leq \delta \tag{3.66}$$

where $\psi_k(s, a) = \pi_k(a|s) p^{\gamma}_{\pi_k}(s)$. The solution to this is

$$\psi_{k+1}(s, a) = p^{\gamma}_{\pi_k}(s) \pi_k(a|s) w(s, a) \tag{3.67}$$

$$w(s, a) = \frac{\exp(A^{\pi_k}(s, a)/\lambda^*)}{Z(\lambda^*)} \tag{3.68}$$

$$Z(\lambda) = \mathbb{E}_{(s,a) \sim p^{\gamma}_{\pi_k}} \left[ \exp(A^{\pi_k}(s, a)/\lambda) \right] \tag{3.69}$$

$$\lambda^* = \underset{\lambda \geq 0}{\text{argmin}}\, \lambda\delta + \lambda \log Z(\lambda) \tag{3.70}$$

In the M step, we project this target distribution back onto the space of parametric policies, while satisfying the KL trust region constraint:

$$\pi_{k+1} = \underset{\pi}{\text{argmax}}\, \mathbb{E}_{(s,a) \sim p^{\gamma}_{\pi_k}} \left[ w(s, a) \log \pi(a|s) \right] \quad \text{s.t.} \quad \mathbb{E}_{p^{\gamma}_{\pi_k}} \left[ D_{\mathbb{KL}} \left( \psi_k \parallel \psi \right)(s) \right] \leq \delta \tag{3.71}$$

## 3.5 Off-policy methods

In many cases, it is useful to train a policy using data collected from a distinct **behavior policy** $\pi_b(a|s)$ that is not the same as the **target policy** $\pi(a|s)$ that is being learned. For example, this could be data collected from earlier trials or parallel workers (with different parameters $\boldsymbol{\theta}'$) and stored in a **replay buffer**, or it could be **demonstration data** from human experts. This is known as **off-policy RL**, and can be much more sample efficient than the on-policy methods we have discussed so far, since these methods can use data from multiple sources. However, off-policy methods are more complicated, as we will explain below.

The basic difficulty is that the target policy that we want to learn may want to try an action in a state that has not been experienced before in the existing data, so there is no way to predict the outcome of this new $(s, a)$ pair. In this section, we tackle this problem by assuming that the target policy is not too different from the behavior policy, so that the ratio $\pi(a|s)/\pi_b(a|s)$ is bounded, which allows us to use methods based on importance sampling. In the online learning setting, we can ensure this property by using conservative incremental updates to the policy. Alternatively we can use policy gradient methods with various regularization methods, as we discuss below.

In Section 7.6, we discuss offline RL, which is an extreme instance of off-policy RL where we have a fixed behavioral dataset, possibly generated from an unknown behavior policy, and can never collect any new data.

### 3.5.1 Policy evaluation using importance sampling

Assume we have a dataset of the form $\mathcal{D} = \{\boldsymbol{\tau}^{(i)}\}_{1 \leq i \leq n}$, where each trajectory is a sequence $\boldsymbol{\tau}^{(i)} = (s_0^{(i)}, a_0^{(i)}, r_0^{(i)}, s_1^{(i)} \ldots)$, where the actions are sampled according to a behavior policy $\pi_b$, and the reward and next states are sampled according to the reward and transition models. We want to use this offline dataset to evaluate the performance of some target policy $\pi$; this is called **off-policy policy evaluation** or **OPE**. If the trajectories $\boldsymbol{\tau}^{(i)}$ were sampled from $\pi$. we could use the standard Monte Carlo estimate:

$$\hat{J}(\pi) \triangleq \frac{1}{n} \sum_{i=1}^{n} \sum_{t=0}^{T-1} \gamma^t r_t^{(i)} \tag{3.72}$$

However, since the trajectories are sampled from $\pi_b$, we use **importance sampling** (IS) to correct for the distributional mismatch, as first proposed in [PSS00]. This gives

$$\hat{J}_{\text{IS}}(\pi) \triangleq \frac{1}{n} \sum_{i=1}^{n} \frac{p(\boldsymbol{\tau}^{(i)}|\pi)}{p(\boldsymbol{\tau}^{(i)}|\pi_b)} \sum_{t=0}^{T-1} \gamma^t r_t^{(i)} \tag{3.73}$$

It can be verified that $\mathbb{E}_{\pi_b}\left[\hat{J}_{\text{IS}}(\pi)\right] = J(\pi)$, that is, $\hat{J}_{\text{IS}}(\pi)$ is **unbiased**, provided that $p(\boldsymbol{\tau}|\pi_b) > 0$ whenever $p(\boldsymbol{\tau}|\pi) > 0$. The **importance ratio**, $\frac{p(\boldsymbol{\tau}^{(i)}|\pi)}{p(\boldsymbol{\tau}^{(i)}|\pi_b)}$, is used to compensate for the fact that the data is sampled from $\pi_b$ and not $\pi$. It can be simplified as follows:

$$\frac{p(\boldsymbol{\tau}|\pi)}{p(\boldsymbol{\tau}|\pi_b)} = \frac{p(s_0)\prod_{t=0}^{T-1} \pi(a_t|s_t) p_S(s_{t+1}|s_t, a_t) p_R(r_t|s_t, a_t, s_{t+1})}{p(s_0)\prod_{t=0}^{T-1} \pi_b(a_t|s_t) p_S(s_{t+1}|s_t, a_t) p_R(r_t|s_t, a_t, s_{t+1})} = \prod_{t=0}^{T-1} \frac{\pi(a_t|s_t)}{\pi_b(a_t|s_t)} \tag{3.74}$$

This simplification makes it easy to apply IS, as long as the target and behavior policies are known. (If the behavior policy is unknown, we can estimate it from $\mathcal{D}$, and replace $\pi_b$ by its estimate $\hat{\pi}_b$. For convenience, define the **per-step importance ratio** at time $t$ by

$$\rho_t(\boldsymbol{\tau}) \triangleq \pi(a_t|s_t)/\pi_b(a_t|s_t) \tag{3.75}$$

We can reduce the variance of the estimator by noting that the reward $r_t$ is independent of the trajectory beyond time $t$. This leads to a **per-decision importance sampling** variant:

$$\hat{J}_{\text{PDIS}}(\pi) \triangleq \frac{1}{n} \sum_{i=1}^{n} \sum_{t=0}^{T-1} \prod_{t' \leq t} \rho_{t'}(\boldsymbol{\tau}^{(i)}) \gamma^t r_t^{(i)} \tag{3.76}$$

### 3.5.2 Off-policy actor critic methods

In this section, we discuss how to extend actor-critic methods to work with off-policy data.

#### 3.5.2.1 Learning the critic using V-trace

In this section we build on Section 3.5.1 to develop a practical method, known as **V-trace** [Esp+18], to estimate the value function for a target policy using off-policy data. (This is an extension of the earlier **Retrace** algorithm [Mun+16], which estimates the $Q$ function using off-policy data.)

First consider the $n$-step target value for $V(s_i)$ in the on-policy case:

$$V_i = V(s_i) + \sum_{t=i}^{i+n-1} \gamma^{t-i} r_t + \gamma^n V(s_{i+n}) \tag{3.77}$$

$$= V(s_i) + \sum_{t=i}^{i+n-1} \gamma^{t-i} \underbrace{(r_t + \gamma V(s_{t+1}) - V(s_t))}_{\delta_t} \tag{3.78}$$

where we define $\delta_t = (r_t + \gamma V(s_{t+1}) - V(s_t))$ as the TD error at time $t$. To extend this to the off-policy case, we use the per-step importance ratio trick. However, to bound the variance of the estimator, we truncate the IS weights. In particular, we define

$$c_t = \min\left(\overline{c}, \frac{\pi(a_t|s_t)}{\pi_b(a_t|s_t)}\right), \; \rho_t = \min\left(\overline{\rho}, \frac{\pi(a_t|s_t)}{\pi_b(a_t|s_t)}\right) \tag{3.79}$$

where $\overline{c}$ and $\overline{\rho}$ are hyperparameters. We then define the V-trace target value for $V(s_i)$ as

$$v_i = V(s_i) + \sum_{t=i}^{i+n-1} \gamma^{t-i} \left(\prod_{t'=i}^{t-1} c_{t'}\right) \rho_t \delta_t \tag{3.80}$$

Note that we can compute these targets recursively using

$$v_i = V(s_i) + \rho_i \delta_i + \gamma c_i (v_{i+1} - V(s_{i+1})) \tag{3.81}$$

The product of the weights $c_i \ldots c_{t-1}$ (known as the "trace") measures how much a temporal difference $\delta_t$ at time $t$ impacts the update of the value function at earlier time $i$. If the policies are very different, the variance of this product will be large. So the truncation parameter $\overline{c}$ is used to reduce the variance. In [Esp+18], they find $\overline{c} = 1$ works best.

The use of the target $\rho_t \delta_t$ rather than $\delta_t$ means we are evaluating the value function for a policy that is somewhere between $\pi_b$ and $\pi$. For $\overline{\rho} = \infty$ (i.e., no truncation), we converge to the value function $V^{\pi}$, and for $\overline{\rho} \to 0$, we converge to the value function $V^{\pi_b}$. In [Esp+18], they find $\overline{\rho} = 1$ works best. (An alternative to clipping the importance weights is to use a resampling technique, and then use unweighted samples to estimate the value function [Sch+19].)

Note that if $\overline{c} = \overline{\rho}$, then $c_i = \rho_i$. This gives rise to the simplified form

$$v_t = V(s_t) + \sum_{j=0}^{n-1} \gamma^j \left(\prod_{m=0}^{j} c_{t+m}\right) \delta_{t+j} \tag{3.82}$$

We can use the above V-trace targets to learn an approximate value function by minimizing the usual $\ell_2$ loss:

$$\mathcal{L}(\boldsymbol{w}) = \mathbb{E}_{t\sim\mathcal{D}}\left[(v_t - V_{\boldsymbol{w}}(s_t))^2\right] \tag{3.83}$$

the gradient of which has the form

$$\nabla\mathcal{L}(\boldsymbol{w}) = 2\mathbb{E}_{t\sim\mathcal{D}}\left[(v_t - V_{\boldsymbol{w}}(s_t))\nabla_{\boldsymbol{w}} V_{\boldsymbol{w}}(s_t)\right] \tag{3.84}$$

#### 3.5.2.2 Learning the actor

We now discuss how to update the actor using an off-policy estimate of the policy gradient. We start by defining the objective to be the expected value of the new policy, where the states are drawn from the behavior policy's state distribution, but the actions are drawn from the target policy:

$$J_{\pi_b}(\pi_{\boldsymbol{\theta}}) = \sum_s p^{\gamma}_{\pi_b}(s) V_\pi(s) = \sum_s p^{\gamma}_{\pi_b}(s) \sum_a \pi_{\boldsymbol{\theta}}(a|s) Q_\pi(s,a) \tag{3.85}$$

Differentiating this and ignoring the term $\nabla_{\boldsymbol{\theta}} Q_\pi(s,a)$, as suggested by [DWS12], gives a way to (approximately) estimate the **off-policy policy-gradient** using a one-step IS correction ratio:

$$\nabla_{\boldsymbol{\theta}} J_{\pi_b}(\pi_{\boldsymbol{\theta}}) \approx \sum_s \sum_a p^{\gamma}_{\pi_b}(s) \nabla_{\boldsymbol{\theta}} \pi_{\boldsymbol{\theta}}(a|s) Q_\pi(s,a) \tag{3.86}$$

$$= \mathbb{E}_{p^{\gamma}_{\pi_b}(s), \pi_b(a|s)} \left[ \frac{\pi_{\boldsymbol{\theta}}(a|s)}{\pi_b(a|s)} \nabla_{\boldsymbol{\theta}} \log \pi_{\boldsymbol{\theta}}(a|s) Q_\pi(s,a) \right] \tag{3.87}$$

In practice, we can approximate $Q_\pi(s_t, a_t)$ by $q_t = r_t + \gamma v_{t+1}$, where $v_{t+1}$ is the V-trace estimate for state $s_{t+1}$. If we use $V(s_t)$ as a baseline, to reduce the variance, we get the following gradient estimate for the policy:

$$\nabla J(\boldsymbol{\theta}) = \mathbb{E}_{t \sim \mathcal{D}} \left[ \rho_t \nabla_{\boldsymbol{\theta}} \log \pi_{\boldsymbol{\theta}}(a_t|s_t)(r_t + \gamma v_t - V_{\boldsymbol{w}}(s_t)) \right] \tag{3.88}$$

We can also replace the 1-step IS-weighted TD error $\rho_t(r_t + \gamma v_t - V_{\boldsymbol{w}}(s_t))$ with an IS-weighted GAE value by modifying the generalized advantage estimation method in Section 3.3.2. In particular, we just need to define $\lambda_t = \lambda \min(1, \rho_t)$. We denote the IS-weighted GAE estimate as $A^\rho_t$.[4]

#### 3.5.2.3 Example: IMPALA

As an example of an off-policy AC method, we consider **IMPALA**, which stands for "Importance Weighted Actor-Learning Architecture". [Esp+18]. This uses shared parameters for the policy and value function (with different output heads), and adds an entropy bonus to ensure the policy remains stochastic. Thus we end up with the following objective, which is very similar to on-policy actor-critic shown in Algorithm 6:

$$\mathcal{L}(\boldsymbol{\phi}) = \mathbb{E}_{t \sim \mathcal{D}} \left[ \lambda_{TD} (V_{\boldsymbol{\phi}}(s_t) - v_t)^2 - \lambda_{PG} A^\rho_t \log \pi_{\boldsymbol{\phi}}(a_t|s_t) - \lambda_{ent} \mathbb{H}(\pi_{\boldsymbol{\phi}}(\cdot|s_t)) \right] \tag{3.89}$$

The only difference from standard A2C is that we need to store the probabilities of each action, $\pi_b(a_t|s_t)$, in addition to $(s_t, a_t, r_t, s_{t+1})$ in the dataset $\mathcal{D}$, which can be used to compute the importance ratio $\rho_t$ in Equation (3.79). [Esp+18] was able to use this method to train a single agent (using a shared CNN and LSTM for both value and policy) to play all 57 games at a high level. Furthermore, they showed that their method — thanks to its off-policy corrections — outperformed the A3C method (a parallel version of A2C) in Section 3.3.1.

In [SHS20], they analyse te variance of the V-trace estimator, used to compute $\rho_t$ in Equation (3.79). They show that to keep this bounded, it is necessary to mix some off-policy data (from the replay buffer) with some fresh online data from the current policy.

### 3.5.3 Off-policy policy improvement methods

So far we have focused on actor-critic methods. However, policy improvement methods, such as PPO, are often preferred to AC methods, since they monotonically improve the objective. In [QPC21] they propose one way to extend PPO to the off-policy case. This method was generalized in [QPC24] to cover a variety of policy improvement algorithms, including TRPO and VMPO. We give a brief summary below.

[4] For an implementation, see https://github.com/google-deepmind/rlax/blob/master/rlax/_src/multistep.py#L39

The key insight is to realize that we can generalize the lower bound in Equation (3.56) to any reference policy

$$J(\pi) - J(\pi_k) \geq \frac{1}{1-\gamma}\mathbb{E}_{p^{\gamma}_{\pi_{\text{ref}}}(s)\pi_k(a|s)}\left[\frac{\pi(a|s)}{\pi_{\text{ref}}(a|s)}A^{\pi_k}(s,a)\right] - \frac{2\gamma C^{\pi,\pi_k}}{(1-\gamma)^2}\mathbb{E}_{p^{\gamma}_{\pi_{\text{ref}}}(s)}\left[\text{TV}(\pi(\cdot|s), \pi_{\text{ref}}(\cdot|s))\right] \tag{3.90}$$

The reference policy can be any previous policy, or a convex combination of them. In particular, if $\pi_k$ is the current policy, we can consider the reference policy to be $\pi_{\text{ref}} = \sum_{i=1}^{M} \nu_i \pi_{k-i}$, where $0 \leq \nu_i \leq 1$ and $\sum_i \nu_i = 1$ are mixture weights. We can approximate the expectation by sampling from the replay buffer, which contains samples from older policies. That is, $(s,a) \sim p^{\gamma}_{\pi_{\text{ref}}}$ can be implemented by $i \sim \nu$ and $(s,a) \sim p^{\gamma}_{\pi_{k-i}}$.

To compute the advantage function $A^{\pi_k}$ from off policy data, we can adapt the V-trace method of Equation (3.82) to get

$$A^{\pi_k}_{\text{trace}}(s_t, a_t) = \delta_t + \sum_{j=0}^{n-1} \gamma^j \left(\prod_{m=1}^{j} c_{t+m}\right)\delta_{t+j} \tag{3.91}$$

where $\delta_t = r_t + \gamma V(s_{t+1}) - V(s_t)$, and $c_t = \min\left(\bar{c}, \frac{\pi_k(a_t|s_t)}{\pi_{k-i}(a_t|s_t)}\right)$ is the truncated importance sampling ratio.

To compute the TV penalty term from off policy data, we need to choose between the PPO (Section 3.4.3), VMPO (Section 3.4.4) and TRPO (Section 3.4.2) approach. We discuss each of these cases below.

#### 3.5.3.1 Off-policy PPO

We can derive an off-policy version of PPO using an update of the following form (known as **Generalized PPO**):

$$\pi_{k+1} = \underset{\pi}{\text{argmax}}\, \mathbb{E}_{i\sim\nu}\left[\mathbb{E}_{(s,a)\sim p^{\gamma}_{\pi_{k-i}}}\left[\min(\rho_{k-i}(s,a)A^{\pi_k}(s,a), \tilde{\rho}_{k-i}(s,a)A^{\pi_k}(s,a))\right]\right] \tag{3.92}$$

where $\rho_{k-i}(s,a) = \frac{\pi(a|s)}{\pi_{k-i}(a|s)}$ and $\tilde{\rho}_{k-i}(s,a) = \text{clip}(\frac{\pi(a|s)}{\pi_{k-i}(a|s)}, l, u)$, where $l = \frac{\pi_k(a|s)}{\pi_{k-i}(a|s)} - \epsilon$ and $u = \frac{\pi_k(a|s)}{\pi_{k-i}(a|s)} + \epsilon$. (For other off-policy variants of PPO, see e.g., [Men+23; LMW24].)

#### 3.5.3.2 Off-policy TRPO

For details on the off-policy version of TRPO, see [QPC24].

#### 3.5.3.3 Off-policy VMPO

For an off-policy version of VMPO, see the discussion of MPO in Section 3.6.5.

## 3.6 RL as inference

In this section, we discuss an approach to policy optimization that reduces it to probabilistic inference. This is called **RL as inference**, and has been discussed in numerous works (see e.g., [Att03; TS06; Tou09; ZABD10; RTV12; BT12; KGO12; HR17; Lev18; Fur+21; Zha+24]). The primary advantage of this approach is that it enables policy learning using off-policy data, while avoiding the need to use (potentially high variance) importance sampling corrections. (This is because the inference approach takes expectations wrt $d_q(s)$ instead of $d_\pi(s)$, where $q$ is an auxiliary distribution, $\pi$ is the policy which is being optimized, and $d$ is the state visitation measure.) A secondary advantage is that it enables us to use the large toolkit of methods for probabilistic modeling and inference to solve RL problems. The resulting framework forms the foundation of the the MPO discussed in Section 3.6.5, the SAC method discussed in Section 3.6.8, as well as the SMC planning method discussed in Section 4.2.3.

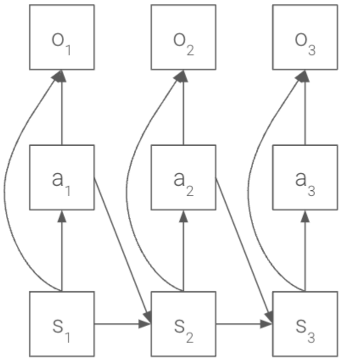


*Figure 3.2: A graphical model for optimal control.*

The core of these methods is based on the probabilistic model shown in Figure 3.2. This shows an MDP augmented with new variables, $\mathcal{O}_t$. These are called **optimality variables**, and indicating whether the action at time $t$ is optimal or not. We assume these have the following probability distribution:

$$p(\mathcal{O}_t = 1|s_t, a_t) \propto \exp(\eta^{-1} G(s_t, a_t)) \tag{3.93}$$

where $\eta > 0$ is a temperature parameter, and $G(s, a)$ is some quality function, such as $G(s, a) = R(s, a)$, or $G(s, a) = Q(s, a)$ or $G(s, a) = A(s, a)$. For brevity, we will just write $p(\mathcal{O} = 1|\cdot)$ to denote the probability of the event that $\mathcal{O}_t = 1$ for all time steps. (Note that the specific value of 1 is arbitrary; this likelihood function is really just a non-negative weighting term that biases the action trajectory, as we show below.)

### 3.6.1 Deterministic case (planning/control as inference)

Our goal is to find trajectories that are optimal. That is, we would like to find the mode (or posterior samples) from the following distribution:

$$p(\boldsymbol{\tau}|\mathcal{O} = 1, \pi) \propto p(\boldsymbol{\tau}, \mathcal{O} = 1|\pi) \propto \left[ p(s_1) \prod_{t=1}^{T-1} \pi(a_t|s_t) p(s_{t+1}|s_t, a_t) \right] \left[ \prod_{t=1}^{T} p(\mathcal{O}_t = 1|s_t, a_t) \right] \tag{3.94}$$

where $\pi$ is the policy.

Let us start by considering the deterministic case, where $p(s_{t+1}|s_t, a_t)$ is either 1 or 0, depending on whether the transition is feasible or not. In this case, rather than learning a policy $\pi$ that maps states to actions we just need to learn a plan (a specific sequence of action $\boldsymbol{a}_{1:T}$) for each starting state $s_1$. This is equivalent to a **shortest path** problem, i.e., we want to maximize

$$p(\boldsymbol{\tau}|\mathcal{O} = 1, \boldsymbol{a}_{1:T}) \propto p(s_1) \left[ \prod_{t=1}^{T-1} p(s_{t+1}|s_t, a_t) \right] \left[ \exp(\sum_{t=1}^{T} R(s_t, a_t)) \right] \tag{3.95}$$

(Typically the initial state $s_1$ is known, in which case $p(s_1)$ is a delta function.)

The MAP sequence of actions, which we denote by $\hat{\boldsymbol{a}}_{1:T}(s_1)$, is the optimal **open loop plan**. (It is called "open loop" since the agent does not need to observe the state, since $s_t$ is uniquely determined by $s_1$ and $\boldsymbol{a}_{1:t}$, both of which are known.) Computing this trajectory is known as the **control as inference** problem [Wat+21]. Such open loop planning problems can be solved using model predictive control methods, discussed in Section 4.2.4.

### 3.6.2 Stochastic case (policy learning as variational inference)

In the stochastic case, we want to learn a policy $\pi$ which maps states to actions, and which generates a distribution over trajectories which are optimal. Thus we define the objective as

$$\log p(\mathcal{O}=1|\pi) = \log \int p_\pi(\boldsymbol{\tau}) p(\mathcal{O}=1|\boldsymbol{\tau}) d\boldsymbol{\tau} \tag{3.96}$$

where we define

$$p_\pi(\boldsymbol{\tau}) = p(s_1) \prod_t p(s_{t+1}|s_t, a_t)\pi(a_t|s_t) \tag{3.97}$$

Since marginalizing over trajectories is difficult, we introduce a variational distribution $q(\boldsymbol{\tau})$ to simplify the computations. We assume $q$ factors in the same way:

$$q(\boldsymbol{\tau}) = p(s_1) \prod_t p(s_{t+1}|s_t, a_t)\pi_q(a_t|s_t) \tag{3.98}$$

Now note the following identity

$$\begin{aligned} D_{\mathbb{KL}}\left(q(\boldsymbol{\tau}) \parallel p_\pi(\boldsymbol{\tau}|\mathcal{O}=1)\right) &= \mathbb{E}_q\left[\log q(\boldsymbol{\tau}) - \log \frac{p_\pi(\mathcal{O}=1|\boldsymbol{\tau})p_\pi(\boldsymbol{\tau})}{p_\pi(\mathcal{O}=1)}\right] && (3.99) \\ &= \mathbb{E}_q\left[\log q(\boldsymbol{\tau}) - \log p_\pi(\mathcal{O}=1|\boldsymbol{\tau}) - \log p_\pi(\boldsymbol{\tau})\right] + \log p_\pi(\mathcal{O}=1) && (3.100) \end{aligned}$$

Hence

$$\begin{aligned} \log p(\mathcal{O}=1|\pi) &= \mathbb{E}_q\left[\log p(\mathcal{O}=1|\boldsymbol{\tau}) - \log \frac{q(\boldsymbol{\tau})}{p(\boldsymbol{\tau})} + \log \frac{q(\boldsymbol{\tau})}{p(\boldsymbol{\tau}|\mathcal{O}=1)}\right] && (3.101) \\ &= J(p_\pi, q) + D_{\mathbb{KL}}\left(q(\boldsymbol{\tau}) \parallel p_\pi(\boldsymbol{\tau}|\mathcal{O}=1)\right) && (3.102) \end{aligned}$$

where $J$ is defined by

$$\begin{aligned} J(\pi_p, \pi_q) &= \mathbb{E}_q\left[\log p_\pi(\mathcal{O}=1|\boldsymbol{\tau})\right] - D_{\mathbb{KL}}\left(q(\boldsymbol{\tau}) \parallel p_\pi(\boldsymbol{\tau})\right) && (3.103) \\ &= \sum_{t=1}^{T} \mathbb{E}_q\left[\eta^{-1}G(s_t, a_t) - D_{\mathbb{KL}}\left(\pi_q(\cdot|s_t) \parallel \pi_p(\cdot|s_t)\right)\right] && (3.104) \end{aligned}$$

Since $D_{\mathbb{KL}}\left(q(\boldsymbol{\tau}) \parallel p_\pi(\boldsymbol{\tau}|\mathcal{O}=1)\right) \geq 0$, we see that $\log p(\mathcal{O}=1|\pi) \geq J(p_\pi, q)$; hence $J$ is called the **evidence lower bound** or **ELBO**. We can define the policy learning task as maximizing the ELBO, subject to the constraints that $\pi_p$ and $\pi_q$ are distributions that integrate to 1 across actions for all states.

To extend to the infinite time discounted case, we define $d_\pi(s)$ as the unnormalized discounted distribution over states

$$d_\pi(s) = \sum_{t=1}^{\infty} \gamma^t p(s_t = s|\pi) \tag{3.105}$$

We now replace the $\sum_t E_{q(s)}$ with $E_{d_q(s)}$ to get the constrained objective

$$\max_{\pi_p, \pi_q} J(\pi_p, \pi_q) \;\; \text{s.t.} \;\; \int d_q(s) \int \pi_p(a|s) da ds = 1, \;\; \int d_q(s) \int \pi_q(a|s) da ds = 1 \tag{3.106}$$

There are two main ways to solve this optimization problem, which we call “EM control” and “KL control”, following [Fur+21]. We describe these below.

### 3.6.3 EM control

In this section, we discuss ways to optimize **??** using the **Expectation Maximization** or **EM** algorithm, which is a widely used **bound optimization** method, also called a **MM** (majorize / maximize) method, that mononotonically increases a lower bound on its objective (see [HL04] for a tutorial). In the E step, we maximize $J$ wrt a non-parametric representation of the variational posterior $\pi_q$, while holding the parametric prior $\pi_p = \pi_{\boldsymbol{\theta}_p}^{k-1}$ fixed at the value from the previous ($k-1$'th) iteration, to get $\pi_q^k$. In the M step, we then maximize $J$ wrt $\pi_p$, holding the variational posterior fixed at $\pi_q^k$, to get the updated policy $\pi_{\boldsymbol{\theta}_p}^k$.

In more detail, in the E step we maximize the following wrt $\pi_q$:

$$\begin{aligned} J(\pi_{\theta_p}^{k-1}, \pi_q) = & \int d_q(s) \int \pi_q(s|a) \eta^{-1} G(s,a) da ds \\ & - \int d_q(s) \int \pi_q(a|s) \log \frac{\pi_q(a|s)}{\pi_{\theta_p^{k-1}}(a|s)} da ds + \lambda \left( 1 - \int d_{\pi(s)} \int \pi_q(a|s) da ds \right) \end{aligned} \tag{3.107}$$

where $\lambda$ is a Lagrange multiplier. The optimal (non-parametric) solution to this is

$$\pi_q^k(a|s) = Z(s)^{-1} \pi_{\theta_p^{k-1}}(a|s) \exp(\eta^{-1} G(s,a)) \tag{3.108}$$

where $Z$ is the partition function

$$Z(s) = \int \pi_{\theta_P^{k-1}}(a|s) \exp(\eta^{-1} G(s,a)) da \tag{3.109}$$

In the M step, we maximize the following wrt $\pi_{\theta_p}$:

$$J(\pi_q^k, \pi_p) = \mathbb{E}_{d_q(s) \pi_q^k(a|s)} \left[ \log \pi_{\theta_p}(a|s) \right] \tag{3.110}$$

which we recognize as a weighted maximum likelihood problem.

### 3.6.4 KL control (maximum entropy RL)

In KL control, we only optimize the variational posterior $\pi_q$, holding the prior $\pi_p$ fixed. Thus we only have an E step. In addition, we represent $\pi_q$ parameterically, as $\pi_{\theta_q}$, instead of the non-parametric approach used by EM. Thus we can drop the Lagrange multipler term and just maximize

$$J(\pi_p, \pi_{\theta_q}) = \mathbb{E}_{d_q(s) \pi_{\theta_q}(a|s)} \left[ \eta^{-1} G(s,a) - \log \frac{\pi_{\theta_q}(a|s)}{\pi_p}(a|s) \right] \tag{3.111}$$

If the prior is uniform, then the (rescaled) objective becomes

$$J(\pi_p, \pi_q) = \sum_{t=1}^{T} \mathbb{E}_q \left[ R(s_t, a_t) - \eta H(\pi_q(\cdot|s_t)) \right] \tag{3.112}$$

where $-H(q) = D_{\mathbb{KL}}(q \parallel \text{unif}) = \sum_a q(a) \log \frac{q(a)}{c}$ is the negative entropy function and $c$ is a constant. This is called the **maximum entropy RL** objective [ZABD10; Haa+18a; Haa+18b]. This differs from the standard objective used in RL training (namely a lower bound on sum of expected rewards) by virtue of the addition of the entropy regularizer. See Section 3.6.8 for further discussion.

### 3.6.5 Maximum a Posteriori Policy Optimization (MPO)

In this section, we discuss the **MPO** method of [Abd+18]. This is an instance of EM control, where $G(s,a) = Q(s,a)$, which is estimated using the retrace algorithm (see Section 3.5.2.1) or a single-step Bellman update.

It implements the E step using Equation (3.108), where we approximate $Z(s)$ with Monte Carlo:

$$q^k(a|s) = \frac{1}{\hat{Z}(s)} \pi_{\theta_p^{k-1}}(a|s) \exp(\eta^{-1} G(s,a)) \tag{3.113}$$

$$Z(s) \approx \frac{1}{M} \sum_{j=1}^{M} \exp(\eta^{-1} G(s,a_j)),\ a_j \sim \pi_{\theta_p^{k-1}}(\cdot|s) \tag{3.114}$$

In addition, the (inverse) temperature parameter $\eta$ is solved for by minimizing the dual of Equation (3.108), which is given by

$$g(\eta) = \eta\epsilon + \eta \log \mathbb{E}_{d_q(s)\pi_{\theta_p^{k-1}}(a|s)} \left[ \exp\left( \eta^{-1} Q^{\pi_{\theta_p}^{k-1}}(s,a) \right) \right] \tag{3.115}$$

In the M step, MPO augments the objective in Equation (3.110) with a log prior at the $k$'th step of the form $\log p_k(\theta_p)$ to create a MAP estimate. That is, it optimizes the following wrt $\theta_p$:

$$J(q^k, \pi_{\theta_p}) = \mathbb{E}_{d_q(s)q(a|s)} \left[ \log \pi_{\theta_p}(a|s) \right] + \log p_k(\theta_p) \tag{3.116}$$

We can think of this step as projecting the non-parametric policy $q$ back to the space of parameterizable policies $\Pi_\theta$.

We assume the prior is a Gaussian centered at the previous parameters,

$$p_k(\boldsymbol{\theta}) = \mathcal{N}(\boldsymbol{\theta}|\boldsymbol{\theta}_k, \lambda \mathbf{F}_k) = c \exp\left( -\lambda (\boldsymbol{\theta} - \boldsymbol{\theta}_k)^{\mathsf{T}} \mathbf{F}_k^{-1} (\boldsymbol{\theta} - \boldsymbol{\theta}_k) \right) \tag{3.117}$$

where $F_k$ is the Fisher information matrix. If we view this as a second order approximation to the KL, we can rewrite the objective as

$$\max_{\theta_p} E_{d_q(s)} \left[ E_{q(a|s)} \log \pi(a|s,\theta_p) - \lambda D_{\mathbb{KL}} \left( \pi(a|s,\boldsymbol{\theta}_k) \parallel \pi(a|s,\theta_p) \right) \right] \tag{3.118}$$

We can approximate the expectation wrt $d_q(s)$ by sampling states from a replay buffer, and the expectaton wrt $q(a|s)$ by sampling from the policy. The KL term can be computed analytically for Gaussian policies. We can then optimize this objective using SGD.

Note that we can also rewrite this as a constrained optimization problem

$$\max_{\theta_p} E_{d_q(s)} \left[ E_{q(a|s)} \log \pi(a|s,\theta_p) \right] \quad \text{s.t.} \quad E_{d_q(s)} \left[ D_{\mathbb{KL}} \left( \pi(a|s,\theta_k) \parallel \pi(a|s,\theta_p) \right) \right] \leq \epsilon_m \tag{3.119}$$

This can be optimized using a trust region method.

### 3.6.6 Sequential Monte Carlo Policy Optimisation (SPO)

In this section, we discuss **SPO** method of [Mac+24]. This is a model-based version of MPO, which uses Sequential Monte Carlo (SMC) to perform approximate inference in the E step. In particular, it samples from a distribution over optimal future trajectories starting from the current state, $s_t$, and using the current policy $\pi_{\theta_p}$ and dynamics model $\mathcal{T}(s'|s,a)$. From this it derives a non-parametric distribution over the optimal actions to take at the next step, $q(a_t|s_t)$. (see Section 4.2.3 for details). This becomes a target for the parametric policy update in the M step, which is the same weighted maximum likelihood method used by MPO.

### 3.6.7 AWR and AWAC

The **Advantage Weighted Regression** or **AWR** method of [Pen+19] and the **Advantage Weighted Actor Critic** or **AWAC** method of [Nai+20] are both EM control methods. AWR uses $G(s,a) = A(s,a)$, where the advantage function is estimated using GAE. The value function $V(s)$ is estimated using TD($\lambda$), and is the value for the average of all previous policies, $\tilde{\pi}_{p^k} = \frac{1}{k} \sum_{j=0}^{j-1} \pi_{\theta_p^j}$. In contrast, AWAC uses $G(s,a) = Q(s,a)$, which is estimated by TD(0).

The (non-parametric) E step is closed form, as in other EM control methods, where the temperate $\eta$ is treated as a hyper-paraemter. The (parametric) M step is a weighted maximum likelihood step that is solved with SGD.

### 3.6.8 Soft Actor Critic (SAC)

The **soft actor-critic** (**SAC**) algorithm [Haa+18a; Haa+18b] is an off-policy actor-critic method based on the maximum entropy RL method we discussed in Section 3.6.4. This is an instance of the KL control scheme where the variational posterior policy $\pi_q = \pi_{\theta_q}$ is parameterized, but the prior policy $\pi_p$ is fixed to the uniform distribution. (Thus SAC only has an E step (implemented with SGD), but no M step.)

SAC uses $G(s,a) = Q^{\text{soft}}(s,a)$, where the soft-Q function is defined below. This is estimated using a TD(0)-like method, as we discuss below.

Crucially, even though SAC is off-policy and utilizes a replay buffer to sample past experiences, the policy update is done using the actor's own probability distribution, eliminating the need to use importance sampling to correct for discrepancies between the behavior policy (used to collect data) and the target policy (used for updating), as we will see below.

#### 3.6.8.1 SAC objective

We can write the maxent RL objective for the E step as follows: Equation (3.112) using modified notation:

$$J^{\text{SAC}}(\boldsymbol{\theta}) \triangleq \mathbb{E}_{p^{\gamma}_{\pi_{\boldsymbol{\theta}}}(s)\pi_{\boldsymbol{\theta}}(a|s)}\left[R(s,a) + \alpha\,\mathbb{H}(\pi_{\boldsymbol{\theta}}(\cdot|s))\right] \tag{3.120}$$

Note that the entropy term makes the objective easier to optimize, and encourages exploration. To optimize this, we can perform a policy evaluation step, and then a policy improvement step.

#### 3.6.8.2 Policy evaluation

In the tabular case, we can perform policy evaluation by repeatedly applying a modified Bellman backup operator $\mathcal{T}^{\pi}$ defined as

$$\mathcal{T}^{\pi}Q(\boldsymbol{s}_t, \boldsymbol{a}_t) = r(\boldsymbol{s}_t, \boldsymbol{a}_t) + \gamma\mathbb{E}_{\boldsymbol{s}_{t+1}\sim p}\left[V(\boldsymbol{s}_{t+1})\right] \tag{3.121}$$

where

$$V(\boldsymbol{s}_t) = \mathbb{E}_{\boldsymbol{a}_t\sim\pi}\left[Q(\boldsymbol{s}_t, \boldsymbol{a}_t) - \alpha\log\pi(\boldsymbol{a}_t|\boldsymbol{s}_t)\right] \tag{3.122}$$

is the **soft value function**. If we iterate $Q^{k+1} = \mathcal{T}^{\pi}Q^{k}$,, this will converge to the soft $Q$ function for $\pi$.

We now generalize this to the non-tabular case. We hold the policy parameters $\pi$ fixed and optimize the parameters $\boldsymbol{w}$ of the $Q$ function by minimizing

$$J_Q(\boldsymbol{w}) = \mathbb{E}_{(\boldsymbol{s}_t,\boldsymbol{a}_t,r_{t+1},\boldsymbol{s}_{t+1})\sim\mathcal{D}}\left[\frac{1}{2}\left(Q_{\boldsymbol{w}}(\boldsymbol{s}_t,\boldsymbol{a}_t) - y(r_{t+1},\boldsymbol{s}_{t+1})\right)^2\right] \tag{3.123}$$

where $\mathcal{D}$ is a replay buffer,

$$y(r_{t+1}, \boldsymbol{s}_{t+1}) = r_{t+1} + \gamma V_{\overline{\boldsymbol{w}}}(\boldsymbol{s}_{t+1}) \tag{3.124}$$

is the frozen target value, and and $V_{\overline{\boldsymbol{w}}}(\boldsymbol{s})$ is a frozen version of the soft value function from Equation (3.122):

$$V_{\overline{\boldsymbol{w}}}(\boldsymbol{s}_t) = \mathbb{E}_{\pi(\boldsymbol{a}_t|\boldsymbol{s}_t)}\left[Q_{\overline{\boldsymbol{w}}}(\boldsymbol{s}_t,\boldsymbol{a}_t) - \alpha\log\pi(\boldsymbol{a}_t|\boldsymbol{s}_t)\right] \tag{3.125}$$

where $\overline{\boldsymbol{w}}$ is the EMA version of $\boldsymbol{w}$. (The use of a frozen target is to avoid bootstrapping instabililities discussed in Section 2.5.2.4.)

To avoid the positive overestimation bias that can occur with actor-critic methods, [Haa+18a], suggest fitting two soft $Q$ functions, by optimizing $J_Q(\boldsymbol{w}_i)$, for $i = 1, 2$, independently. Inspired by clipped double $Q$ learning, used in TD3 (Section 3.7.2), the targets are defined as

$$y(r_{t+1}, \boldsymbol{s}_{t+1}; \overline{\boldsymbol{w}}_{1:2}, \boldsymbol{\theta}) = r_{t+1} + \gamma\left[\min_{i=1,2} Q_{\overline{\boldsymbol{w}}_i}(\boldsymbol{s}_{t+1}, \tilde{\boldsymbol{a}}_{t+1}) - \alpha\log\pi_{\boldsymbol{\theta}}(\tilde{\boldsymbol{a}}_{t+1}|\boldsymbol{s}_{t+1})\right] \tag{3.126}$$

where $\tilde{\boldsymbol{a}}_{t+1} \sim \pi_{\boldsymbol{\theta}}(\boldsymbol{s}_{t+1})$ is a sampled next action. In [Che+20], they propose the REDQ method (Section 2.5.3.3) which uses a random ensemble of $N \geq 2$ networks instead of just 2.

#### 3.6.8.3 Policy improvement

In the policy improvement step, we derive the new policy based on the soft $Q$ function by softmaxing over the possible actions for each state. We then project the update back on to the policy class $\Pi$:

$$\pi_{\text{new}} = \arg\min_{\pi' \in \Pi} D_{\mathbb{KL}} \left( \pi'(\cdot|\boldsymbol{s}_t) \parallel \frac{\exp(\frac{1}{\alpha} Q^{\pi_{\text{old}}}(\boldsymbol{s}_t, \cdot))}{Z^{\pi_{\text{old}}}(\boldsymbol{s}_t)} \right) \tag{3.127}$$

(The partition function $Z^{\pi_{\text{old}}}(\boldsymbol{s}_t)$ may be intractable to compute for a continuous action space, but it cancels out when we take the derivative of the objective, so this is not a problem, as we show below.) After solving the above optimization problem, we are guaranteed to satisfy the soft policy improvement theorem, i.e., $Q^{\pi_{\text{new}}}(\boldsymbol{s}_t, \boldsymbol{a}_t) \geq Q^{\pi_{\text{old}}}(\boldsymbol{s}_t, \boldsymbol{a}_t)$ for all $\boldsymbol{s}_t$ and $\boldsymbol{a}_t$.

We now generalize this to the non-tabular case. For policy improvement, we hold the value function parameters $\boldsymbol{w}$ fixed and optimize the parameters $\boldsymbol{\theta}$ of the policy by minimizing the objective below, which is derived from the KL term by multiplying by $\alpha$ and dropping the constant $Z$ term:

$$J_\pi(\boldsymbol{\theta}) = \mathbb{E}_{\boldsymbol{s}_t \sim \mathcal{D}} \left[ \mathbb{E}_{\boldsymbol{a}_t \sim \pi_{\boldsymbol{\theta}}} \left[ \alpha \log \pi_{\boldsymbol{\theta}}(\boldsymbol{a}_t|\boldsymbol{s}_t) - Q_{\boldsymbol{w}}(\boldsymbol{s}_t, \boldsymbol{a}_t) \right] \right] \tag{3.128}$$

Since we are taking gradients wrt $\boldsymbol{\theta}$, which affects the inner expectation term, we need to either use the REINFORCE estimator from Equation (3.15) or the **reparameterization trick** (see e.g., [Moh+20]). The latter is much lower variance, so is preferable.

To explain this in more detail, let us assume the policy distribution has the form $\pi_{\boldsymbol{\theta}}(\boldsymbol{a}_t|\boldsymbol{s}_t) = \mathcal{N}(\boldsymbol{\mu}_{\boldsymbol{\theta}}(\boldsymbol{s}_t), \sigma^2 \mathbf{I})$. We can write the random action as $\boldsymbol{a}_t = f_{\boldsymbol{\theta}}(\boldsymbol{s}_t, \boldsymbol{\epsilon}_t)$, where $f$ is a deterministic function of the state and a noise variable $\boldsymbol{\epsilon}_t$, since $\boldsymbol{a}_t = \boldsymbol{\mu}(\boldsymbol{s}_t) + \sigma^2 \boldsymbol{\epsilon}_t$, where $\boldsymbol{\epsilon}_t \sim \mathcal{N}(\mathbf{0}, \mathbf{I})$. The objective now becomes

$$J_\pi(\boldsymbol{\theta}) = \mathbb{E}_{\boldsymbol{s}_t \sim \mathcal{D}, \boldsymbol{\epsilon}_t \sim \mathcal{N}} \left[ \alpha \log \pi_{\boldsymbol{\theta}}(f_{\boldsymbol{\theta}}(\boldsymbol{s}_t, \boldsymbol{\epsilon}_t)|\boldsymbol{s}_t) - Q_{\boldsymbol{w}}(\boldsymbol{s}_t, f_{\boldsymbol{\theta}}(\boldsymbol{s}_t, \boldsymbol{\epsilon}_t)) \right] \tag{3.129}$$

where we have replaced the expectation of $\boldsymbol{a}_t$ wrt $\pi_{\boldsymbol{\theta}}$ with an expectation of $\boldsymbol{\epsilon}_t$ wrt its noise distribution $\mathcal{N}$. Hence we can now safely take stochastic gradients. See Algorithm 8 for the pseudocode.

For discrete actions, we can replace the Gaussian reparameterization with the gumbel-softmax reparameterization [JGP16; MMT17]. Alternatively, we can eschew sampling and compute the expectations over the actions explicitly, to derive lower variance versions of the equations; this is known as **SAC-Discrete** [Chr19].

#### 3.6.8.4 Adjusting the temperature

In [Haa+18b] they propose to automatically adjust the temperature parameter $\alpha$ by optimizing

$$J(\alpha) = \mathbb{E}_{\boldsymbol{s}_t \sim \mathcal{D}, \boldsymbol{a}_t \sim \pi_{\boldsymbol{\theta}}} \left[ -\alpha(\log \pi_{\boldsymbol{\theta}}(\boldsymbol{a}_t|\boldsymbol{s}_t) + \overline{H}) \right]$$

where $\overline{H}$ is the target entropy (a hyper-parameter). This objective is approximated by sampling actions from the replay buffer.

## 3.7 Deterministic policy gradient methods

In this section, we consider the case of a deterministic policy, that predicts a unique action for each state, so $a_t = \mu_{\boldsymbol{\theta}}(s_t)$, rather than $a_t \sim \pi_{\boldsymbol{\theta}}(s_t)$. (We require that the actions are continuous, because we will take the Jacobian of the $Q$ function wrt the actions; if the actions are discrete, we can just use DQN.) The advantage of using a deterministic policy is that we can modify the policy gradient method so that it can work off policy without needing importance sampling, as we will see.

Following Equation (3.7), we define the value of a policy as the expected discounted reward per state:

$$J(\mu_{\boldsymbol{\theta}}) \triangleq \mathbb{E}_{\rho_{\mu_{\boldsymbol{\theta}}}(s)} \left[ R(s, \mu_{\boldsymbol{\theta}}(s)) \right] \tag{3.130}$$

**Algorithm 8:** SAC

```
Initialize environment state $\boldsymbol{s}$, policy parameters $\boldsymbol{\theta}$, $N$ critic parameters $\boldsymbol{w}_i$, target parameters
  $\overline{\boldsymbol{w}}_i = \boldsymbol{w}_i$, replay buffer $\mathcal{D} = \emptyset$, discount factor $\gamma$, EMA rate $\rho$, step size $\eta_w$, $\eta_\pi$.
repeat
    Take action $\boldsymbol{a} \sim \pi_{\boldsymbol{\theta}}(\cdot|\boldsymbol{s})$
    $(\boldsymbol{s}', r) = \text{step}(\boldsymbol{a}, \boldsymbol{s})$
    $\mathcal{D} := \mathcal{D} \cup \{(\boldsymbol{s}, \boldsymbol{a}, r, \boldsymbol{s}')\}$
    $\boldsymbol{s} \leftarrow \boldsymbol{s}'$
    for $G$ updates do
        Sample a minibatch $\mathcal{B} = \{(\boldsymbol{s}_j, \boldsymbol{a}_j, r_j, \boldsymbol{s}'_j)\}$ from $\mathcal{D}$
        $\boldsymbol{w} = \text{update-critics}(\boldsymbol{\theta}, \boldsymbol{w}, \mathcal{B})$
    Sample a minibatch $\mathcal{B} = \{(\boldsymbol{s}_j, \boldsymbol{a}_j, r_j, \boldsymbol{s}'_j)\}$ from $\mathcal{D}$
    $\boldsymbol{\theta} = \text{update-policy}(\boldsymbol{\theta}, \boldsymbol{w}, \mathcal{B})$
until converged;
.
def update-critics($\boldsymbol{\theta}, \boldsymbol{w}, \mathcal{B}$):
Let $(\boldsymbol{s}_j, \boldsymbol{a}_j, r_j, \boldsymbol{s}'_j)_{j=1}^{B} = \mathcal{B}$
$y_j = y(r_j, \boldsymbol{s}'_j; \overline{\boldsymbol{w}}_{1:N}, \boldsymbol{\theta})$ for $j = 1 : B$
for $i = 1 : N$ do
    $\mathcal{L}(\boldsymbol{w}_i) = \frac{1}{|\mathcal{B}|} \sum_{(\boldsymbol{s},\boldsymbol{a},r,\boldsymbol{s}')_j \in \mathcal{B}} (Q_{\boldsymbol{w}_i}(\boldsymbol{s}_j, \boldsymbol{a}_j) - \text{sg}(y_j))^2$
    $\boldsymbol{w}_i \leftarrow \boldsymbol{w}_i - \eta_{\boldsymbol{w}} \nabla \mathcal{L}(\boldsymbol{w}_i)$ // Descent
    $\overline{\boldsymbol{w}}_i := \rho \overline{\boldsymbol{w}}_i + (1 - \rho) \boldsymbol{w}_i$ //Update target networks
Return $\boldsymbol{w}_{1:N}, \overline{\boldsymbol{w}}_{1:N}$
.
def update-actor($\boldsymbol{\theta}, \boldsymbol{w}, \mathcal{B}$):
$\hat{Q}(s, a) \triangleq \frac{1}{N} \sum_{i=1}^{N} Q_{\boldsymbol{w}_i}(s, a)$ // Average critic
$J(\boldsymbol{\theta}) = \frac{1}{|\mathcal{B}|} \sum_{\boldsymbol{s} \in \mathcal{B}} \left( \hat{Q}(\boldsymbol{s}, \tilde{\boldsymbol{a}}_{\boldsymbol{\theta}}(\boldsymbol{s})) - \alpha \log \pi_{\boldsymbol{\theta}}(\tilde{\boldsymbol{a}}(\boldsymbol{s})|\boldsymbol{s}) \right)$ , $\tilde{\boldsymbol{a}}_{\boldsymbol{\theta}}(\boldsymbol{s}) \sim \pi_{\boldsymbol{\theta}}(\cdot|\boldsymbol{s})$
$\boldsymbol{\theta} \leftarrow \boldsymbol{\theta} + \eta_{\boldsymbol{\theta}} \nabla J(\boldsymbol{\theta})$ // Ascent
Return $\boldsymbol{\theta}$
```

The **deterministic policy gradient theorem** [Sil+14] tells us that the gradient of this expression is given by

$$\nabla_{\boldsymbol{\theta}} J(\mu_{\boldsymbol{\theta}}) = \mathbb{E}_{\rho_{\mu_{\boldsymbol{\theta}}}(s)} \left[\nabla_{\boldsymbol{\theta}} Q_{\mu_{\boldsymbol{\theta}}}(s, \mu_{\boldsymbol{\theta}}(s))\right] \tag{3.131}$$

$$= \mathbb{E}_{\rho_{\mu_{\boldsymbol{\theta}}}(s)} \left[\nabla_{\boldsymbol{\theta}} \mu_{\boldsymbol{\theta}}(s) \nabla_a Q_{\mu_{\boldsymbol{\theta}}}(s, a)|_{a=\mu_{\boldsymbol{\theta}}(s)}\right] \tag{3.132}$$

where $\nabla_{\boldsymbol{\theta}} \mu_{\boldsymbol{\theta}}(s)$ is the $M \times N$ Jacobian matrix, and $M$ and $N$ are the dimensions of $\mathcal{A}$ and $\boldsymbol{\theta}$, respectively. For stochastic policies of the form $\pi_{\boldsymbol{\theta}}(a|s) = \mu_{\boldsymbol{\theta}}(s) + \text{noise}$, the standard policy gradient theorem reduces to the above form as the noise level goes to zero.

Note that the gradient estimate in Equation (3.132) integrates over the states but not over the actions, which helps reduce the variance in gradient estimation from sampled trajectories. However, since the deterministic policy does not do any exploration, we need to use an off-policy method for training. This collects data from a stochastic behavior policy $\pi_b$, whose stationary state distribution is $p^{\gamma}_{\pi_b}$. The original objective, $J(\mu_{\boldsymbol{\theta}})$, is approximated by the following:

$$J_b(\mu_{\boldsymbol{\theta}}) \triangleq \mathbb{E}_{p^{\gamma}_{\pi_b}(s)} \left[V_{\mu_{\boldsymbol{\theta}}}(s)\right] = \mathbb{E}_{p^{\gamma}_{\pi_b}(s)} \left[Q_{\mu_{\boldsymbol{\theta}}}(s, \mu_{\boldsymbol{\theta}}(s))\right] \tag{3.133}$$

with the off-policy deterministic policy gradient from [DWS12] is approximated by

$$\nabla_{\boldsymbol{\theta}} J_b(\mu_{\boldsymbol{\theta}}) \approx \mathbb{E}_{p^{\gamma}_{\pi_b}(s)} \left[\nabla_{\boldsymbol{\theta}} \left[Q_{\mu_{\boldsymbol{\theta}}}(s, \mu_{\boldsymbol{\theta}}(s))\right]\right] = \mathbb{E}_{p^{\gamma}_{\pi_b}(s)} \left[\nabla_{\boldsymbol{\theta}} \mu_{\boldsymbol{\theta}}(s) \nabla_a Q_{\mu_{\boldsymbol{\theta}}}(s, a)|_{a=\mu_{\boldsymbol{\theta}}(s)}\right] \tag{3.134}$$

where we have a dropped a term that depends on $\nabla_{\boldsymbol{\theta}} Q_{\mu_{\boldsymbol{\theta}}}(s, a)$ and is hard to estimate [Sil+14].

To apply Equation (3.134), we may learn $Q_{\boldsymbol{w}} \approx Q_{\mu_{\boldsymbol{\theta}}}$ with TD, giving rise to the following updates:

$$\delta = r_t + \gamma Q_{\boldsymbol{w}}(s_{t+1}, \mu_{\boldsymbol{\theta}}(s_{t+1})) - Q_{\boldsymbol{w}}(s_t, a_t) \tag{3.135}$$

$$\boldsymbol{w}_{t+1} \leftarrow \boldsymbol{w}_t + \eta_{\boldsymbol{w}} \delta \nabla_{\boldsymbol{w}} Q_{\boldsymbol{w}}(s_t, a_t) \tag{3.136}$$

$$\boldsymbol{\theta}_{t+1} \leftarrow \boldsymbol{\theta}_t + \eta_{\boldsymbol{\theta}} \nabla_{\boldsymbol{\theta}} \mu_{\boldsymbol{\theta}}(s_t) \nabla_a Q_{\boldsymbol{w}}(s_t, a)|_{a=\mu_{\boldsymbol{\theta}}(s_t)} \tag{3.137}$$

So we learn both a state-action critic $Q_{\boldsymbol{w}}$ and an actor $\boldsymbol{\mu}_{\boldsymbol{\theta}}$. This method avoids importance sampling in the actor update because of the deterministic policy gradient, and we avoids it in the critic update because of the use of Q-learning.

If $Q_{\boldsymbol{w}}$ is linear in $\boldsymbol{w}$, and uses features of the form $\boldsymbol{\phi}(s, a) = \boldsymbol{a}^{\mathsf{T}} \nabla_{\boldsymbol{\theta}} \mu_{\boldsymbol{\theta}}(s)$, then we say the function approximator for the critic is **compatible** with the actor; in this case, one can show that the above approximation does not bias the overall gradient.

The basic off-policy DPG method has been extended in various ways, some of which we describe below.

### 3.7.1 DDPG

The **DDPG** algorithm of [Lil+16], which stands for "deep deterministic policy gradient", uses the DQN method (Section 2.5.2.2) to update $Q$ that is represented by deep neural networks. In more detail, the actor tries to minimize the output of the critic by optimize

$$\mathcal{L}_{\boldsymbol{\theta}}(s) = Q_{\boldsymbol{w}}(s, \mu_{\boldsymbol{\theta}}(s)) \tag{3.138}$$

averaged over states $s$ drawn from the replay buffer. The critic tries to minimize the 1-step TD loss

$$\mathcal{L}_{\boldsymbol{w}}(s, a, r, s') = \left[Q_{\boldsymbol{w}}(s, a) - (r + \gamma Q_{\overline{\boldsymbol{w}}}(s', \mu_{\boldsymbol{\theta}}(s')))\right]^2 \tag{3.139}$$

where $Q_{\overline{\boldsymbol{w}}}$ is the target critic network, and the samples $(s, a, r, a')$ are drawn from a replay buffer. (See Section 2.5.2.5 for a discussion of target networks.)

The **D4PG** algorithm [BM+18], which stands for "distributed distributional DDPG", extends DDPG to handle distributed training, and to handle distributional RL (see Section 7.2).

### 3.7.2 Twin Delayed DDPG (TD3)

The **TD3** ("twin delayed deep deterministic") method of [FHM18] extends DDPG in 3 main ways. First, it uses **target policy smoothing**, in which noise is added to the action, to encourage generalization:

$$\tilde{\boldsymbol{a}} = \boldsymbol{\mu}_{\boldsymbol{\theta}}(\boldsymbol{s}) + \text{noise} = \pi_{\boldsymbol{\theta}}(\boldsymbol{s}) \tag{3.140}$$

Second it uses **clipped double Q learning**, which is an extension of the double Q-learning discussed in Section 2.5.3.1 to avoid over-estimation bias. In particular, the target values for TD learning are defined using

$$y(r, \boldsymbol{s}'; \overline{\boldsymbol{w}}_{1:2}, \overline{\boldsymbol{\theta}}) = r + \gamma \min_{i=1,2} Q_{\overline{\boldsymbol{w}}_i}(\boldsymbol{s}', \pi_{\overline{\boldsymbol{\theta}}}(\boldsymbol{s}')) \tag{3.141}$$

Third, it uses **delayed policy updates**, in which it only updates the policy after the value function has stabilized. (See also Section 3.3.3.) See Algorithm 9 for the pseudocode.

**Algorithm 9:** TD3

```
Initialize environment state $\boldsymbol{s}$, policy parameters $\boldsymbol{\theta}$, target policy parameters $\overline{\boldsymbol{\theta}}$, critic parameters $\boldsymbol{w}_i$,
  target critic parameters $\overline{\boldsymbol{w}}_i = \boldsymbol{w}_i$, replay buffer $\mathcal{D} = \emptyset$, discount factor $\gamma$, EMA rate $\rho$, step size $\eta_{\boldsymbol{w}}$,
  $\eta_{\boldsymbol{\theta}}$.
repeat
    $\boldsymbol{a} = \mu_{\boldsymbol{\theta}}(\boldsymbol{s}) + \text{noise}$
    $(\boldsymbol{s}', r) = \text{step}(\boldsymbol{a}, \boldsymbol{s})$
    $\mathcal{D} := \mathcal{D} \cup \{(\boldsymbol{s}, \boldsymbol{a}, r, \boldsymbol{s}')\}$
    $\boldsymbol{s} \leftarrow \boldsymbol{s}'$
    for $G$ updates do
        Sample a minibatch $\mathcal{B} = \{(\boldsymbol{s}_j, \boldsymbol{a}_j, r_j, \boldsymbol{s}'_j)\}$ from $\mathcal{D}$
        $\boldsymbol{w} = \text{update-critics}(\boldsymbol{\theta}, \boldsymbol{w}, \mathcal{B})$
    Sample a minibatch $\mathcal{B} = \{(\boldsymbol{s}_j, \boldsymbol{a}_j, r_j, \boldsymbol{s}'_j)\}$ from $\mathcal{D}$
    $\boldsymbol{\theta} = \text{update-policy}(\boldsymbol{\theta}, \boldsymbol{w}, \mathcal{B})$
until converged;
.
def update-critics$(\boldsymbol{\theta}, \boldsymbol{w}, \mathcal{B})$:
Let $(\boldsymbol{s}_j, \boldsymbol{a}_j, r_j, \boldsymbol{s}'_j)_{j=1}^{B} = \mathcal{B}$
for $j = 1 : B$ do
    $\tilde{\boldsymbol{a}}_j = \mu_{\overline{\boldsymbol{\theta}}}(\boldsymbol{s}'_j) + \text{clip}(\text{noise}, -c, c)$
    $y_j = r_j + \gamma \min_{i=1,2} Q_{\overline{\boldsymbol{w}}_i}(\boldsymbol{s}'_j, \tilde{\boldsymbol{a}}_j)$
for $i = 1 : 2$ do
    $\mathcal{L}(\boldsymbol{w}_i) = \frac{1}{|\mathcal{B}|} \sum_{(\boldsymbol{s},\boldsymbol{a},r,\boldsymbol{s}')_j \in \mathcal{B}} (Q_{\boldsymbol{w}_i}(\boldsymbol{s}_j, \boldsymbol{a}_j) - \text{sg}(y_j))^2$
    $\boldsymbol{w}_i \leftarrow \boldsymbol{w}_i - \eta_{\boldsymbol{w}} \nabla \mathcal{L}(\boldsymbol{w}_i)$ // Descent
    $\overline{\boldsymbol{w}}_i := \rho \overline{\boldsymbol{w}}_i + (1 - \rho) \boldsymbol{w}_i$ //Update target networks with EMA
Return $\boldsymbol{w}_{1:N}, \overline{\boldsymbol{w}}_{1:N}$
.
def update-actor$(\boldsymbol{\theta}, \boldsymbol{w}, \mathcal{B})$:
$J(\boldsymbol{\theta}) = \frac{1}{|\mathcal{B}|} \sum_{\boldsymbol{s} \in \mathcal{B}} \left(Q_{\boldsymbol{w}_1}(\boldsymbol{s}, \mu_{\boldsymbol{\theta}}(\boldsymbol{s}))\right)^2$
$\boldsymbol{\theta} \leftarrow \boldsymbol{\theta} + \eta_{\boldsymbol{\theta}} \nabla J(\boldsymbol{\theta})$ // Ascent
$\overline{\boldsymbol{\theta}} := \rho \overline{\boldsymbol{\theta}} + (1 - \rho) \boldsymbol{\theta}$ //Update target policy network with EMA
Return $\boldsymbol{\theta}, \overline{\boldsymbol{\theta}}$
```

## 3.8 Gradient-free policy optimization

The policy gradient estimator computes a “zeroth order” gradient, which essentially evaluates the function with randomly sampled trajectories. Sometimes it can be more efficient to use a derivative-free optimizer that does not even attempt to estimate the gradient. For example, [MGR18] obtain good results by training linear policies with random search, and [Sal+17] show how to use evolutionary strategies to optimize the policy of a robotic controller.

# Chapter 4

# Model-based RL

## 4.1 Introduction

Model-free approaches to RL typically need a lot of interactions with the environment to achieve good performance. For example, state of the art methods for the Atari benchmark, such as rainbow (Section 2.5.2.2), use millions of frames, equivalent to many days of playing at the standard frame rate. By contrast, humans can achieve the same performance in minutes [Tsi+17]. Similarly, OpenAI's robot hand controller [And+20] needs 100 years of simulated data to learn to manipulate a rubiks cube.

One promising approach to greater sample efficiency is **model-based RL** (**MBRL**). In the simplest approach to MBRL, we first learn the state transition or dynamics model $p_S(s'|s,a)$ — also called a **world model** — and the reward function $R(s,a)$, using some offline trajectory data, and then we use these models to compute a policy (e.g., using dynamic programming, as discussed in Section 2.2, or using some model-free policy learning method on simulated data, as discussed in Chapter 3). It can be shown that the sample complexity of learning the dynamics is less than the sample complexity of learning the policy [ZHR24].

However, the above two-stage approach — where we first learn the model, and then plan with it — can suffer from the usual problems encountered in offline RL (Section 7.6), i.e., the policy may query the model at a state for which no data has been collected, so predictions can be unreliable, causing the policy to learn the wrong thing. To get better results, we have to interleave the model learning and policy learning, so that one helps the other (since the policy determines what data is collected).

There are two main ways to perform MBRL. In the first approach, known as **decision-time planning** or **model predictive control**, we use the model to choose the next action by searching over possible future trajectories. We then score each trajectory, pick the action corresponding to the best one, take a step in the environment, and repeat. (We can also optionally update the model based on the rollouts.) This is discussed in Section 4.2.

The second approach is to use the current model and policy to rollout imaginary trajectories, and to use this data (optionally in addition to empirical data) to improve the policy using model-free RL; this is called **background planning**, and is discussed in Section 4.3.

The advantage of decision-time planning is that it allows us to train a world model on reward-free data, and then use that model to optimize any reward function. This can be particularly useful if the reward contains changing constraints, or if it is an intrinsic reward (Section 7.3) that frequently changes based on the knowledge state of the agent. The downside of decision-time planning is that it is much slower. However, it is possible to combine the two methods, as we discuss below. For an empirical comparison of background planning and decision-time planning, see [AP24].

Some generic pseudo-code for an MBRL agent is given in Algorithm 10. (The `rollout` function is defined in Algorithm 11; some simple code for model learning is shown in Algorithm 12, although we discuss other loss functions in Section 4.4; finally, the code for the policy learning is given in other parts of this manuscript.) For more details on general MBRL, see e.g., [Wan+19; Moe+23; PKP21; Luo+22].

**Algorithm 10:** MBRL agent

```
def MBRL-agent($M_{\text{env}}; T, H, N$):
Initialize state $s \sim M_{\text{env}}$
Initialize data buffer $\mathcal{D} = \emptyset$, model $\hat{M}$
Initialize value function $V$, policy proposal $\pi$
repeat
    // Collect data from environment
    $\tau_{\text{env}} = \text{rollout}(s, \pi, T, M_{\text{env}})$, ;
    $s = \tau_{\text{env}}[-1]$, ;
    $\mathcal{D} = \mathcal{D} \cup \tau_{\text{env}}$
    // Update model
    if Update model online then
        $\hat{M} = \text{update-model}(\hat{M}, \tau_{\text{env}})$
    if Update model using replay then
        $\tau^n_{\text{replay}} = \text{sample-trajectory}(\mathcal{D}), n = 1 : N$
        $\hat{M} = \text{update-model}(\hat{M}, \tau^{1:N}_{\text{replay}})$
    // Update policy
    if Update on-policy with real then
        $(\pi, V) = \text{update-on-policy}(\pi, V, \tau_{\text{env}})$
    if Update on-policy with imagination then
        $\tau^n_{\text{imag}} = \text{rollout}(\text{sample-init-state}(\mathcal{D}), \pi, T, \hat{M}), n = 1 : N$
        $(\pi, V) = \text{update-on-policy}(\pi, V, \tau^{1:N}_{\text{imag}})$
    if Update off-policy with real then
        $\tau^n_{\text{replay}} = \text{sample-trajectory}(\mathcal{D}), n = 1 : N$
        $(\pi, V) = \text{update-off-policy}(\pi, V, \tau^{1:N}_{\text{replay}})$
    if Update off-policy with imagination then
        $\tau^n_{\text{imag}} = \text{rollout}(\text{sample-state}(\mathcal{D}), \pi, T, \hat{M}), n = 1 : N$
        $(\pi, V) = \text{update-off-policy}(\pi, V, \tau^{1:N}_{\text{imag}})$
until until converged;
```

**Algorithm 11:** Rollout

```
def rollout($s_1, \pi, T, M$)
$\tau = [s_1]$
for $t = 1 : T$ do
    $a_t = \pi(s_t)$
    $(s_{t+1}, r_{t+1}) \sim M(s_t, a_t)$
    $\tau += [a_t, r_{t+1}, s_{t+1}]$
Return $\tau$
```

**Algorithm 12:** Model learning

```
def update-model($M, \tau^{1:N}$) :
$\ell(M) = -\frac{1}{NT} \sum_{n=1}^{N} \sum_{(s_t, a_t, r_{t+1}, s_{t+1}) \in \tau^n} \log M(s_{t+1}, r_{t+1} | s_t, a_t)$ // NLL
$M = M - \eta_M \nabla_M \ell(M)$
Return $M$
```

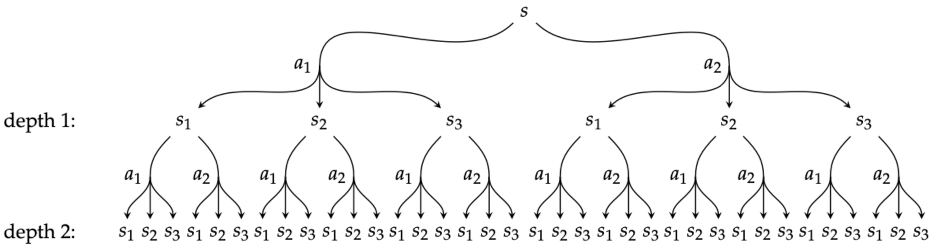


*Figure 4.1: Illustration of forward search applied to a problem with 3 discrete states and 2 discrete actions. From Figure 9.1 of [KWW22]. Used with kind permission of Mykel Kochenderfer.*

## 4.2 Decision-time (online) planning

In this section, we discuss how to choose the best action at each step based on planning forward from the current state using a known (or learned) world model. This is called **decision time planning** or "**planning in the now**" [KLP11], and is in contrast to methods that try to learn a policy which can be applied to all possible situations. In this section, we summarize some approaches to this problem. Our presentation is based in part on [KWW22, Ch. 9].

### 4.2.1 Receeding horizon control

In **receeding horizon control** or **RHC**, we plan from the current state $s_t$ to a maximum fixed depth (horizon into the future) of $d$. We then take the first action $a_t$ based on this future planning, observe the new state $s_{t+1}$, and then replan. This approach can be quite slow, since it needs to perform a search or optimization procedure at each step. However, it can give good results, since it can choose an action that is tailored to the current state (and likely future), rather than relying on the generalization properties of a policy that was learned offline. In the sections below, we discuss various ways to implement this procedure.

#### 4.2.1.1 Forward search

In **forward search**, we examine all possible transitions up to depth $d$ by starting from the current state, and then considering all possible actions, and then considering all possible next states, etc. An example of the resulting **search tree** is given in Figure 4.1. We can compute the reward associated with each edge in the tree. At the leaves of the tree, we compute the remaining reward-to-go based on a utility or value function, $V(s)$, which can be learned offline using value-based methods. We then find the path with the highest score, and return the first action on this path. This process takes $O((|\mathcal{S}| \times |\mathcal{A}|)^d)$ time.

#### 4.2.1.2 Branch and bound

In **branch and bound**, we try to avoid the exponential complexity of forward search by pruning paths that we determine are suboptimal. To do this, we need to know a lower bound on the value function, $\underline{V}(s)$, and an upper bound on the action value function, $\overline{Q}(s, a)$. At each state node $s$, we examine the actions in decreasing order of their upper bound. If we find an action $a$ where $\overline{Q}(s, a)$ is less than the current best lower bound, we prune this branch of the tree, otherwise we expand it, and explore below. We continue this process until we hit a leaf node $s$ (at the maximum depth), in which case we return the lower bound $\underline{V}(s)$. Depending on the tightness of the bounds, this approach can be significantly faster than forward search.

#### 4.2.1.3 Sparse sampling

A simple way to speed up forward search (and branch and boundd) is to sample a subset of $m$ possible next states for each action. This is called **sparse sampling** [KMN99]. The resulting complexity is $O((m \times |\mathcal{A}|)^d)$, which is independent of $|\mathcal{S}|$.

#### 4.2.1.4 Heuristic search

In **heuristic search**, we start with a heuristic function $\overline{V}(s)$, which we use to initialize the value function $V(s)$. We then perform $m$ Monte Carlo rollouts starting from the root node $s$. At each state node, we pick the greedy action wrt the current $V$, i.e., we choose $\text{argmax}_a R(s,a) + \gamma \sum_{s'} p(s'|s,a)V(s')$. We then update $V(s) = \max_a R(s,a) + \gamma \sum_{s'} p(s'|s,a)V(s')$, and sample a next state $s' \sim p(s|s,a)$. We repeat this process until we hit the max depth. Finally we return the greedy action wrt $V$ applied to the root node.

If the heuristic function is an upper bound on the optimal value function, then it is called an **admissible heuristic**. In this case, heuristic search is guaranteed to converge to the optimal value. The efficiency depends on the tighteness of the upper bound, but in the worst case it is $O(m \times d \times |\mathcal{S}| \times |\mathcal{A}|)$.

### 4.2.2 Monte Carlo tree search (MCTS)

**Monte Carlo tree search** or **MCTS** is a receeding horizon control procedure that works as follows (see e.g., [Mun14] for more details). Given the root node $s_t$, we perform $m$ Monte Carlo rollouts to estimate $Q(s_t, a)$, and then we return the best action $\text{argmax}_a Q(s_t, a)$ or the action distribution $\text{softmax}(Q(s_t, a))$. During the rollouts, we keep track of how many times we have tried each action $a$ in each state $s$ using the counter $N(s, a)$. To perform a rollout from a state $s$, we proceed as follows. If we have not visited $s$ before, we initialize the node by setting $N(s, a) = 0$ and $Q(s, a) = 0$ and returning $U(s)$ as the value, where $U$ is some estimated value function. Otherwise we pick the next action to explore from state $s$. To explore actions, we first try each action once, and we then use the UCB heuristic (see Section 7.1.2) to select subsequent actions, i.e. we use

$$a = \underset{a}{\text{argmax}}\, Q(s, a) + c\sqrt{\frac{\log N(s, a)}{N(s, a)}} \tag{4.1}$$

where $N(s) = \sum_a N(s, a)$ is the total visit count to $s$, and $c$ is an exploration bonus scaling term. After choosing action $a$, we sample the next state $s' \sim p(s'|s, a)$, and then recursively estimate $u = U(s')$ using MCTS from that node. We then update the Q function using the TD update

$$Q(s, a) \leftarrow Q(s, a) + \frac{1}{N(s, a)}(u - Q(s, a)) \tag{4.2}$$

where the learning rate is given by $\frac{1}{N(s,a)}$. We also increment $N(s, a)$ by 1. When we return from the recursive call, we are effectively backpropagating the value $u$ from the leaves up the tree, as illustrated in Figure 4.2(b). A sketch of a non-recursive version of the algorithm (Algorithm 25 of [ACS24]) is shown in Algorithm 13.

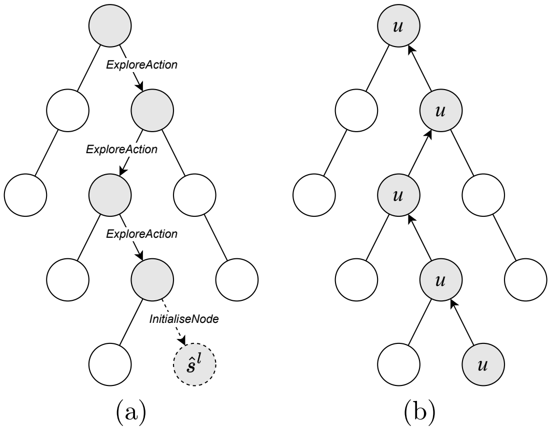


*Figure 4.2: Illustration of MCTS. (a) Expanding nodes until we hit a new (previously unexplored) leaf node. (b) Propagating leaf value u back up the tree. From Figure 9.25 of [ACS24].*

**Algorithm 13:** Monte Carlo Tree Search (MCTS)

```
for $t = 0, 1, 2, 3, \ldots$ do
    Observe current state $s_t$;
    for $k$ simulations do
        $\tau \leftarrow t$;
        $\hat{s}_\tau \leftarrow s_t$
        while $\hat{s}_\tau$ is non-terminal and node $\hat{s}_\tau$ exists in tree do
            $\hat{a}_\tau \leftarrow$ ExploreAction($\hat{s}_\tau$);
            $\hat{s}_{\tau+1} \sim \mathcal{T}(\cdot \mid \hat{s}_\tau, \hat{a}_\tau)$;
            $\hat{r}_\tau \leftarrow \mathcal{R}(\hat{s}_\tau, \hat{a}_\tau, \hat{s}_{\tau+1})$;
            $\tau \leftarrow \tau + 1$;
        if node $\hat{s}_\tau$ does not exist in tree then
            InitializeNode($\hat{s}_\tau$)
        while $\tau > t$ do
            // Backpropagate
            $\tau \leftarrow \tau - 1$;
            Update($Q, \hat{s}_\tau, \hat{a}_\tau$);
    // Select action for state $s_t$
    $\pi_t \leftarrow$ BestAction($s_t$);
    $a_t \sim \pi_t$;
```

#### 4.2.2.1 MCTS for two-player games: AlphaGo, AlphaGoZero, and AlphaZero

MCTS can be applied to any kind of MDP, but some of its most famous applications are to games. We discuss general stochastic games in Chapter 5, but here focus on the special case of two-player, zero-sum symmetric games. In this case, the agent can model the opponent using its own policy, but with the roles reversed (this is known as **self-play**). If $i$ represents the "main" player and $j$ represents its opponent, then the state transition function, as seen by $i$, has the form

$$p^\pi(s'|s, a^i) = \sum_{a^j} \pi(a^j|\psi(s))p(s'|s, a^i, a^j) \tag{4.3}$$

where $p(s'|s, a^i, a^j)$ is the world model, $\pi$ is $i$'s policy, and $\psi(s)$ performs the role reversal.[1] We see that $i$ just treats $j$ as part of the environment, thus creating the above (policy-dependent) transition function. This can be used inside of MCTS to pick actions at each step.

In addition to choosing the next best action $a_t$ (as in RHC), MCTS can be used to return a distribution over good actions for the current state $s$; we denote this by $\boldsymbol{\pi}_s^{\text{MCTS}}(a) = [N(s,a)/(\sum_b N(s,b))]^{1/\tau}$, where $\tau$ is a temperature. This can be used as a target for policy improvement.

This method was used in the **AlphaGo** system of [Sil+16], which was the first AI system to beat a human grandmaster at the board game Go. AlphaGo was followed up by **AlphaGoZero** [Sil+17a], which had a much simpler design, and did not train on any human data, i.e., it was trained entirely using RL and self play. It significantly outperformed the original AlphaGo. This was generalized to **AlphaZero** [Sil+18], which can play expert-level Go, chess, and shogi (Japanese chess), without using any domain knowledge (except in the design of the neural network used to guide MCTS).

In more detail, AlphaZero used MCTS (with self-play), combined with a neural network which computes $(v^s, \boldsymbol{\pi}^s) = f(s; \boldsymbol{\theta})$, where $v_s$ is the expected outcome of the game from state $s$ (either +1 for a win, -1 for a loss, or 0 for a draw), and $\boldsymbol{\pi}_s$ is the policy (distribution over actions) for state $s$. The policy is used internally by MCTS whenever a new node is initialized to give an additional exploration bonus to the most promising / likely actions. This controls the breadth of the search tree. In addition, the learned value function $v_s = f(s; \boldsymbol{\theta})_v$ is used to provide the value for leaf nodes in cases where we cannot afford to rollout to termination. This controls the depth of the search tree.

The policy/value network $f$ is trained by optimizing the loss

$$\mathcal{L}(\boldsymbol{\theta}) = \mathbb{E}_{(s, \boldsymbol{\pi}_s^{\text{MCTS}}, V^{\text{MCTS}}(s)) \sim \mathcal{D}} \left[ (V^{\text{MCTS}}(s) - V_{\boldsymbol{\theta}}(s))^2 - \sum_a \boldsymbol{\pi}_s^{\text{MCTS}}(a) \log \boldsymbol{\pi}_{\boldsymbol{\theta}}(a|s) \right] \tag{4.4}$$

where $\mathcal{D} = \{(s, \boldsymbol{\pi}_s^{\text{MCTS}}, V_s^{\text{MCTS}})\}$ is a dataset collected from MCTS rollouts starting at state $s$. These rollouts generate a distribution over actions at the root node $s$ using $\boldsymbol{\pi}_s^{\text{MCTS}}(a) = [N(s,a)/(\sum_b N(s,b))]^{1/\tau}$, where $\tau$ is a temperature. The rollouts also provide an MC estimate of the reward-to-go using the n-step bootstrap estimate starting at root node $s_t$ and then computing $V_{s_t}^{\text{MCTS}} = \sum_{i=0}^{n-1} \gamma^i r_{t+i} + \gamma^k v_{t+i}$ summing over each path (of length $n$) in the search tree.

The above self-play approach trains an agent against the current version of itself, which can result in overfitting. To combat this, we can store multiple past versions of the policy, and then select any of these policies as a proxy for the opponent's policy. This increases robustness of the main agent.

#### 4.2.2.2 MCTS with learned world model: MuZero and EfficientZero

AlphaZero and related methods assume the world model is known. The **MuZero** method of [Sch+20] learns a world model, by training a latent representation (embedding function) of the observations, $\boldsymbol{z}_t = e_{\boldsymbol{\phi}}(\boldsymbol{o}_t)$, and a corresponding latent dynamics (and reward) model $(\boldsymbol{z}_t, r_t) = M_{\boldsymbol{w}}(\boldsymbol{z}_t, a_t)$. The world model is trained to predict the immediate reward, the future reward (i..e, the value), and the optimal policy, where the optimal policy is computed using MCTS.

In more details, we use MCTS to select action $a_t$, take a step, and add $(\boldsymbol{o}_t, a_t, r_t, \boldsymbol{o}_{t+1}, \boldsymbol{\pi}_t^{\text{MCTS}}, V_t^{\text{MCTS}})$ to the replay buffer. To train the model, we augment the loss in Equation (4.4) by adding a term that measures how well the learned model predicts the observed rewards. Also, we now optimize this wrt the policy/value parameters $\boldsymbol{\theta}$ as well as the model parameters $\boldsymbol{w}$ and embedding parameters $\boldsymbol{\phi}$:

$$\mathcal{L}(\boldsymbol{\theta}, \boldsymbol{w}, \boldsymbol{\phi}) = \mathbb{E}_{(\boldsymbol{o}, a_t, r, \boldsymbol{o}', \boldsymbol{\pi}_z^{\text{MCTS}}, V_z^{\text{MCTS}}) \sim \mathcal{D}} \Big\{ (V^{\text{MCTS}}(z) - V_{\boldsymbol{\theta}}(e_{\boldsymbol{\phi}}(\boldsymbol{o}))^2 - \sum_a \boldsymbol{\pi}_z^{\text{MCTS}}(a) \log \boldsymbol{\pi}_{\boldsymbol{\theta}}(a|e_{\boldsymbol{\phi}}(\boldsymbol{o})) \tag{4.5}$$

$$+ (r - M_{\boldsymbol{w}}^r(e_{\boldsymbol{\phi}}(\boldsymbol{o}), a_t))^2 \Big\} \tag{4.6}$$

[1] For example, consider the game of chess, where the state is represented by $s = (x, y)$, where $x$ is a vector containing the location of player 1's pieces (or -1 if they are removed), and $y$ is a vector containing the opponent's pieces. Thus the policy for player 1, $\pi_1$, just needs to access the $x$ part of the state. For player 2, we can transform the state vector into $s' = \psi(s) = (y, x)$ and then apply $\pi_1$ to choose actions, so $\pi_2(s) = \pi_1(\psi(s))$.

MuZero was applied to 3 perfect information board games (Go, Chess, and Shogi), as well as to Atari. The **Stochastic MuZero** method of [Ant+22] extends MuZero to allow for stochastic environments. The **Sampled MuZero** method of [Hub+21] extends MuZero to allow for large and/or continuous action spaces.

The **Efficient Zero** paper [Ye+21] extends MuZero by adding an additional self-prediction loss of the form $(\boldsymbol{z}_{t+1} - M^z_{\boldsymbol{w}}(\boldsymbol{z}_t, a_t))^2$ to Equation (4.6) to help train the world model. (See Section 4.4.2.4 for further discussion of such losses.) It also makes several other changes. In particular, it replaces the empirical sum of instantaneous rewards, $\sum_{i=0}^{n-1} \gamma^i r_{t+i}$, used in computing $V_t^{\text{MCTS}}$, with an LSTM model that predicts the sum of rewards for a trajectory starting at $\boldsymbol{z}_t$; they call this the value prefix. In addition, it replaces the stored value at the leaf nodes of trajectories in the replay buffer with new values, by rerunning MCTS using the current model applied to the leaves. They show that all three changes help, but the biggest gain is from the self-prediction loss. The recent **Efficient Zero V2** [Wan+24b] extends this to also work with continuous actions, by replacing tree search with sampling-based Gumbel search, amongst other changes.

### 4.2.3 Sequential Monte Carlo (SMC) for online planning

Although MCTS is powerful, it is inherently serial, and can be complicated to apply to continuous action spaces. In this section, we discuss a more general method known as **SPO**, which stands for Sequential Monte Carlo Policy Optimisation [Mac+24].

SPO is based on the "RL as inference" framework, and is discussed in more detail in Section 3.6.6. In brief, the goal is to sample trajectories (sequences of states and actions) that are likely to be high scoring. That is, we want to sample from the following distribution

$$q(\tau) \propto d_q(s_0) \prod_{t \geq 0} \mathcal{T}(s_{t+1}|s_t, a_t) \pi(a_t|s_t, \boldsymbol{\theta}_i) \exp\left(\frac{A(s_t, a_t)}{\eta}\right) \tag{4.7}$$

where $s_0$ is the current state, $A$ is the advantage function

$$A(s_t, a_t) = Q(s_t, a_t) - V(s_t) \approx r_t + V(s_{t+1}) - V(s_t) \tag{4.8}$$

and $\eta$ is a temperature parameter obtained by maximizing Equation (3.115). (The state-value function $V$ can be learned via TD(0.)

Let the resulting empirical distribution over trajectories be denoted by

$$\hat{q}_i(\tau) = \sum_{n=1}^{N} \overline{w}^n \delta(\tau - \tau^n) \tag{4.9}$$

where $\tau^n$ is the $n$'th sample, and $\overline{w}^n$ is its (normalized) weight. We can derive the distribution over next best action as follows:

$$\hat{q}(a|s_0) = \sum_n \overline{w}^n \delta(a - a_0^n) \tag{4.10}$$

One way to sample trajectories from such a distribution is to use **SMC** (Sequential Monte Carlo), which is a generalization of **particle filtering**. This is an approach to approximate inference in state space models based on sequential importance sampling with resampling (see e.g., [NLS19]). At each step, we use a proposal distribution $\beta(\tau_t|\tau_{1:t-1})$, which extends the previous sampled trajectory with a new value of $x_t = (s_t, a_t)$. We then compute the weight of this proposed extension by comparing it to the target $q_i(\tau_t|\tau_{1:t})$ to get

$$w(\tau_{1:t}) \propto w(\tau_{1:t-1}) \frac{q_i(\tau_{1:t})}{\beta(\tau_{1:t})} \tag{4.11}$$

Suppose we use the following proposal

$$\beta_i(\tau_t|\tau_{1:t-1}) \propto \hat{\mathcal{T}}(s_{t+1}|s_t, a_t) \pi(a_t|s_t, \boldsymbol{\theta}_i) \tag{4.12}$$

Then the weight is given by

$$w(\tau_{1:t}) \propto w(\tau_{1:t-1}) \frac{\mathcal{T}(s_t|s_{t-1}, a_{t-1})}{\hat{\mathcal{T}}(s_t|s_{t-1}, a_{t-1})} \cdot \frac{\exp(A_i(s_t, a_t)/\eta_i^*)\pi(a_t|s_t, \boldsymbol{\theta}_i)}{\pi(a_t|s_t, \boldsymbol{\theta}_i)} \tag{4.13}$$

If we assume the learned model $\hat{\mathcal{T}}$ is accurate, this simplifies to

$$w(\tau_{1:t}) \propto w(\tau_{1:t-1}) \cdot \exp(A(s_t, a_t)/\eta) \tag{4.14}$$

In SMC, at each step we propose a new particle according to $\beta$, and then weight it according to the above equation. We can then optionally resample the particles every few steps, or when the effective sample size becomes too small; after a resampling step, we reset the weights to 1, since we now have a weighted sample. At the end, we return an empirical distribution over actions that correspond to high scoring trajectories, from which we can estimate the next best action (e.g., by taking the mean or mode of this distribution). See Algorithm 14 for details. (See also [Pic+19; Lio+22] for related methods.)

**Algorithm 14:** SMC-RHC (Sequential Monte Carlo for Receeding Horizon Control)

```
def SMC-RHC($s_t$, $\pi_i$, $V_i$):
Initialize particles: $\{\boldsymbol{s}_t^n = \boldsymbol{s}_t\}_{n=1}^N$
Initialize weights: $\{w_t^n = 1\}_{n=1}^N$
for $j = t+1 : t+d$ do
    $\{a_j^n \sim \pi_i(\cdot|s_j^n)\}_{n=1}^N$
    $\{s_{j+1}^n \sim \hat{\mathcal{T}}(s_j^n, a_j^n)\}_{n=1}^N$
    $\{r_j^n \sim \hat{\mathcal{R}}(s_j^n, a_j^n)\}_{n=1}^N$
    $\{x_j^n = (s_j^n, a_j^n, r_j^n)\}_{n=1}^N$
    $\{A_j^n = r_j^n + V_i(s_{t+1}^n) - V_i(s_j^n)\}_{n=1}^N$
    $\{w_j^n = w_{j-1}^n \exp(A_i^n/\eta_i^*)\}_{n=1}^N$
    if Resample then
        $\{\boldsymbol{x}_{t:j}^n\} \sim \text{Multinom}(n; w_i^1, \ldots, w_i^N)\}$
        $\{w_j^n = 1\}_{n=1}^N$
    $\{\overline{w}^n = \frac{w^n}{\sum_{n'} w^{n'}}\}_{n=1}^N$
    Let $\{a_t^n\}_{n=1}^N$ be the set of sampled actions at the start of $\{x_{t:t+d}^n\}_{n=1}^N$
    Return $\hat{q}(a|s_t) = \sum_n \overline{w}^n \delta(a - a_t^n)$
```

### 4.2.4 Model predictive control (MPC), aka open loop planning

In this section, we describe a method known as **model predictive control** (**MPC**), which is an **open loop** version of receeding horizon control [MM90; CA13; RMD22]. In particular, at each step, it solves for the sequence of subsequent actions that is most likely to achieve high expected reward:

$$\boldsymbol{a}_{t:t+d-1}^* = \underset{\boldsymbol{a}_{t:t+d-1}}{\text{argmax}} \, \mathbb{E}_{s_{t+1:t+d} \sim \mathcal{T}(\cdot|s_t, a_{t:t+d-1})} \left[ \sum_{h=0}^{d-1} R(s_{t+h}, a_{t+h}) + \hat{V}(s_{t+d}) \right] \tag{4.15}$$

where $\mathcal{T}$ is the dynamics model. It then returns $a_t^*$ as the best action, takes a step, and replans.

Crucially, the future actions are chosen without knowing what the future states are; this is what is meant by "open loop". This can be much faster than interleaving the search for actions and future states. However, it can also lead to suboptimal decisions, as we discuss below. Nevertheless, the fact that we replan at each step can reduce the harms of this approximation, making the method quite popular for some problems, especially ones where the dynamics are deterministic, and the actions are continuous (so that Equation (4.15) becomes a standard optimization problem over the real valued sequence of vectors $\boldsymbol{a}_{t:t+d-1}$).

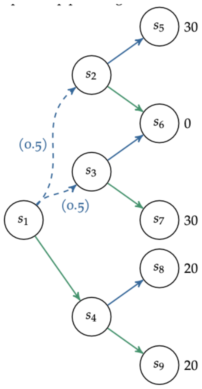


*Figure 4.3: Illustration of the suboptimality of open-loop planning. From Figure 9.9 of [KWW22]. Used with kind permission of Mykel Kochenderfer.*

#### 4.2.4.1 Suboptimality of open-loop planning for stochastic environments

Consider the example in Figure 4.3, where there are 9 states, 2 actions (going up or down), and the planning horizon is $d = 2$. All transitions are deterministic, except that going ip from $s_1$ can either end up in $s_2$ wp 0.5 or in $s_3$ wp 0.5.

There are 4 open-loop plans, with the following expected utilities:

- U(up,up) $= 0.5 \times 30 + 0.5 \times 0 = 15$
- U(up,down) $= 0.5 \times 0 + 0.5 \times 30 = 15$
- U(down,up) $= 20$
- U(down,down) $= 20$

Thus the best open-loop action is to choose down, with an expected reward of 20. However, closed-loop planning can reason that, after taking the first action, the agent can sense the resulting state. If it initially chooses to go up from $s_1$, then it can decide to next go up or down, depending on whether it is in $s_2$ or $s_3$, thereby guaranteeing a reward of 30.

#### 4.2.4.2 Trajectory optimization

If the dynamics is deterministic, the problem becomes one of solving

$$\max_{a_{1:d}, s_{2:d}} \sum_{t=1}^{d} \gamma^t R(s_t, a_t) \tag{4.16}$$

$$\text{s.t.} \quad s_{t+1} = \mathcal{T}(s_t, a_t) \tag{4.17}$$

where $\mathcal{T}$ is the transition function. This is called a **trajectory optimization** problem. We discuss various ways to solve this below.

#### 4.2.4.3 LQR

If the system dynamics are linear and the reward function is quadratic, then the optimal action sequence can be computed exactly using a method similar to Kalman filtering. This is known as the **linear quadratic regulator** (**LQR**). For details, see e.g., [AM89; HR17; Pet08].

If the model is nonlinear, we can use **differential dynamic programming** (**DDP**) [JM70; TL05] to approximately solve the problem. In each iteration, DDP starts with a reference trajectory, and linearizes the system dynamics around states on the trajectory to form a locally quadratic approximation of the reward function. This system can be solved using LQG, whose optimal solution results in a new trajectory. The algorithm then moves to the next iteration, with the new trajectory as the reference trajectory.

#### 4.2.4.4 Random shooting

For general nonlinear models (such as neural networks), a simple approach is to pick a sequence of random actions to try (from some proposal policy), evaluate the reward for each trajectory, and pick the best. This is called **random shooting** [Die+07; Rao10].

#### 4.2.4.5 CEM

As an improvement upon random shooting, it is common to use black-box (gradient-free) optimization methods like the **cross-entropy method** or **CEM** in order to find the best action sequence. The CEM method is a simple derivative-free optimization method for continuous black-box functions $f : \mathbb{R}^D \to \mathbb{R}$. We start with a multivariate Gaussian, $\mathcal{N}(\boldsymbol{\mu}_0, \boldsymbol{\Sigma}_0)$, representing a distribution over possible action $\boldsymbol{a}$. We sample from this, evaluate all the proposals, pick the top $K$, then refit the Gaussian to these top $K$, and repeat, until we find a sample with sufficiently good score (or we perform moment matching on the top $K$ scores). For details, see [Rub97; RK04; Boe+05]. In Section 4.2.4.6, we discuss the MPPI method, which is a common instantiation of CEM method. In [BXS20] they discuss how to combine CEM with gradient-based planning.

#### 4.2.4.6 MPPI

The **model predictive path integral** or **MPPI** approach [WAT17] is a version of CEM. Originally MPPI was limited to models with linear dynamics, but it was extended to general nonlinear models in [Wil+17]. The basic idea is that the initial mean of the Gaussian at step $t$, namely $\boldsymbol{\mu}_t = \boldsymbol{a}_{t:t+H}$, is computed based on shifting $\hat{\boldsymbol{\mu}}_{t-1}$ forward by one step. (Here $\boldsymbol{\mu}_t$ is known as a reference trajectory.)

In [Wag+19], they apply this method for robot control. They consider a state vector of the form $\boldsymbol{s}_t = (\boldsymbol{q}_t, \dot{\boldsymbol{q}}_t)$, where $\boldsymbol{q}_t$ is the configuration of the robot. The deterministic dynamics has the form

$$\boldsymbol{s}_{t+1} = F(\boldsymbol{s}_t, \boldsymbol{a}_t) = \begin{pmatrix} \boldsymbol{q}_t + \dot{\boldsymbol{q}}_t \Delta t \\ \dot{\boldsymbol{q}}_t + f(\boldsymbol{s}_t, \boldsymbol{a}_t)\Delta t \end{pmatrix} \tag{4.18}$$

where $f$ is a 2 layer MLP. This is trained using the **Dagger** method of [RGB11], which alternates between fitting the model (using supervised learning) on the current replay buffer (initialized with expert data), and then deploying the model inside the MPPI framework to collect new data.

A similar method was used in the **TD-MPC** paper [HSW22; HSW24], which learns a non-generative world model in latent space, and then uses MPPI to implement MPC (see Section 4.4.2.8 for details). They initialize the population of $K$ sampled action trajectories by applying the policy prior to generate $J < K$ samples, and then generate the remaining $K - J$ samples using the diagonal Gaussian prior from the previous time step.

#### 4.2.4.7 GP-MPC

[KD18] proposed **GP-MPC**, which combines a Gaussian process dynamics model with model predictive control. They compute a Gaussian approximation to the future state trajectory given a candidate action trajectory, $p(\boldsymbol{s}_{t+1:t+H}|\boldsymbol{a}_{t:t+H-1}, \boldsymbol{s}_t)$, by moment matching, and use this to deterministically compute the expected reward and its gradient wrt $\boldsymbol{a}_{t:t+H-1}$. Using this, they can solve Equation (4.15) to find $\boldsymbol{a}^*_{t:t+H-1}$; finally, they execute the first step of this plan, $a^*_t$, and repeat the whole process.

The key observation is that moment matching is a deterministic operator that maps $p(\boldsymbol{s}_t|\boldsymbol{a}_{1:t-1})$ to $p(\boldsymbol{s}_{t+1}|\boldsymbol{a}_{1:t})$, so the problem becomes one of deterministic optimal control, for which many solution methods exist. Indeed the whole approach can be seen as a generalization of the **LQG** method from classical control, which assumes a (locally) linear dynamics model, a quadratic cost function, and a Gaussian distribution over states [Rec19]. In GP-MPC, the moment matching plays the role of local linearization.

The advantage of GP-MPC over the earlier method known as **PILCO** ("probabilistic inference for learning control"), which learns a policy by maximizing the expected reward from rollouts (see [DR11; DFR15] for details), is that GP-MPC can handle constraints more easily, and it can be more data efficient, since it continually updates the GP model after every step (instead of at the end of an trajectory).

## 4.3 Background (offline) planning

In Section 4.2, we discussed how to use models to perform decision time planning. However, this can be slow. Fortunately, we can amortize the planning process into a reactive policy. To do this, we can use the model to generate synthetic trajectories "in the background" (while executing the current policy), and use this imaginary data to train the policy; this is called "**background planning**". We discuss a game theoretic formulation of this setup in Section 4.3.1. Then in Section 4.3.2, we discuss ways to combine model-based and model-free learning. Finally, in Section 4.3.3, we discuss ways to deal with model errors, that might lead the policy astray.

### 4.3.1 A game-theoretic perspective on MBRL

In this section, we discuss a game-theoretic framework for MBRL, as proposed in [RMK20]. This provides a theoretical foundation for many of the more heuristic methods in the literature.

We denote the true world model by $M_{\text{env}}$. To simplify the notation, we assume an MDP setup with a known reward function, so all that needs to be learned is the world model, $\hat{M}$, representing $p(s'|s,a)$. (It is trivial to also learn the reward function.) We define the value of a policy $\pi$ when rolled out in some model $M'$ as the (discounted) sum of expected rewards:

$$J(\pi, M') = \mathbb{E}_{M',\pi}\left[\sum_{t=0}^{\infty} \gamma^t R(s_t)\right]$$

We define the loss of a model $\hat{M}$ given a distribution $\mu(s,a)$ over states and actions as

$$\ell(\hat{M}, \mu) = \mathbb{E}_{(s,a)\sim\mu}\left[D_{\mathbb{KL}}\left(M_{\text{env}}(\cdot|s,a) \parallel \hat{M}(\cdot|s,a)\right)\right]$$

We now define MBRL as a two-player general-sum game:

$$\overbrace{\max_{\pi} J(\pi, \hat{M})}^{\text{policy player}}, \overbrace{\min_{\hat{M}} \ell(\hat{M}, \mu^{\pi}_{M_{\text{env}}})}^{\text{model player}}$$

where $\mu^{\pi}_{M_{\text{env}}} = \frac{1}{T}\sum_{t=0}^{T} M_{\text{env}}(s_t = s, a_t = a)$ is the induced state visitation distribution when policy $\pi$ is applied in the real world $M_{\text{env}}$, so that minimizing $\ell(\hat{M}, \mu^{\pi}_{M_{\text{env}}})$ gives the **maximum likelihood estimate** for $\hat{M}$.

Now consider a **Nash equilibrium** of this game, that is a pair $(\pi, \hat{M})$ that satisfies $\ell(\hat{M}, \mu^{\pi}_{M_{\text{env}}}) \leq \epsilon_{M_{\text{env}}}$ and $J(\pi, \hat{M}) \geq J(\pi', \hat{M}) - \epsilon_\pi$ for all $\pi'$. (That is, the model is accurate when predicting the rollouts from $\pi$, and $\pi$ cannot be improved when evaluated in $\hat{M}$). In [RMK20] they prove that the Nash equilibirum policy $\pi$ is near optimal wrt the real world, in the sense that $J(\pi^*, M_{\text{env}}) - J(\pi, M_{\text{env}})$ is bounded by a constant, where $\pi^*$ is an optimal policy for the real world $M_{\text{env}}$. (The constant depends on the $\epsilon$ parameters, and the TV distance between $\mu^{\pi^*}_{M_{\text{env}}}$ and $\mu^{\pi*}_{\hat{M}}$.)

A natural approach to trying to find such a Nash equilibrium is to use **gradient descent ascent** or **GDA**, in which each player updates its parameters simultaneously, using

$$\pi_{k+1} = \pi_k + \eta_\pi \nabla_\pi J(\pi_k, \hat{M}_k)$$
$$\hat{M}_{k+1} = \hat{M}_k - \eta_M \nabla_{\hat{M}} \ell(\hat{M}_k, \mu^{\pi_k}_{M_{\text{env}}})$$

Unfortunately, GDA is often an unstable algorithm, and often needs very small learning rates $\eta$. In addition, to increase sample efficiency in the real world, it is better to make multiple policy improvement steps using synthetic data from the model $\hat{M}_k$ at each step.

Rather than taking small steps in parallel, the **best response** strategy fully optimizes each player given the previous value of the other player, in parallel:

$$\pi_{k+1} = \underset{\pi}{\operatorname{argmax}}\, J(\pi, \hat{M}_k)$$
$$\hat{M}_{k+1} = \underset{\hat{M}}{\operatorname{argmin}}\, \ell(\hat{M}, \mu_{M_{\text{env}}}^{\pi_k})$$

Unfortunately, making such large updates in parallel can often result in a very unstable algorithm.

To avoid the above problems, [RMK20] propose to replace the min-max game with a **Stackelberg game**, which is a generalization of min-max games where we impose a specific player ordering. In particular, let the players be $A$ and $B$, let their parameters be $\theta_A$ and $\theta_B$, and let their losses be $\mathcal{L}_A(\theta_A, \theta_B)$ and $\mathcal{L}_B(\theta_A, \theta_B)$. If player $A$ is the leader, the Stackelberg game corresponds to the following nested optimization problem, also called a bilevel optimization problem:

$$\min_{\theta_A} \mathcal{L}_A(\theta_A, \theta_B^*(\theta_A)) s \theta_B^*(\theta_A) = \underset{\theta}{\operatorname{argmin}}\, \mathcal{L}_B(\theta_A, \theta)$$

Since the follower $B$ chooses the best response to the leader $A$, the follower's parameters are a function of the leader's. The leader is aware of this, and can utilize this when updating its own parameters.

The main advantage of the Stackelberg approach is that one can derive gradient-based algorithms that will provably converge to a local optimum [CMS07; ZS22]. In particular, suppose we choose the **policy as leader** (**PAL**). We then just have to solve the following optimization problem:

$$\hat{M}_{k+1} = \underset{\hat{M}}{\operatorname{argmin}}\, \ell(\hat{M}, \mu_{M_{\text{env}}}^{\pi_k})$$
$$\pi_{k+1} = \pi_k + \eta_\pi \nabla_\pi J(\pi_k, \hat{M}_{k+1})$$

We can solve the first step by executing $\pi_k$ in the environment to collect data $\mathcal{D}_k$ and then fitting a local (policy-specific) dynamics model by solving $\hat{M}_{k+1} = \operatorname{argmin} \ell(\hat{M}, \mathcal{D}_k)$. (For example, this could be a locally linear model, such as those used in trajectory optimization methods discussed in Section 4.2.4.6.) We then (slightly) improve the policy to get $\pi_{k+1}$ using a conservative update algorithm, such as natural actor-critic (Section 3.3.4) or TRPO (Section 3.4.2), on "imaginary" model rollouts from $\hat{M}_{k+1}$.

Alternatively, suppose we choose the **model as leader** (**MAL**). We now have to solve

$$\pi_{k+1} = \underset{\pi}{\operatorname{argmax}}\, J(\pi, \hat{M}_k)$$
$$\hat{M}_{k+1} = \hat{M}_k - \eta_M \nabla_{\hat{M}} \ell(\hat{M}, \mu_{M_{\text{env}}}^{\pi_{k+1}})$$

We can solve the first step by using any RL algorithm on "imaginary" model rollouts from $\hat{M}_k$ to get $\pi_{k+1}$. We then apply this in the real world to get data $\mathcal{D}_{k+1}$, which we use to slightly improve the model to get $\hat{M}_{k+1}$ by using a conservative model update applied to $\mathcal{D}_{k+1}$. (In practice we can implement a conservative model update by mixing $\mathcal{D}_{k+1}$ with data generated from earlier models, an approach known as **data aggregation** [RB12].) Compared to PAL, the resulting model will be a more global model, since it is trained on data from a mixture of policies (including very suboptimal ones at the beginning of learning).

### 4.3.2 Dyna

The **Dyna** paper [Sut90] proposed an approach to MBRL that is related to the approach discussed in Section 4.3.1, in the sense that it trains a policy and world model in parallel, but it differs in one crucial way: the policy is also trained on real data, not just imaginary data. That is, we define $\pi_{k+1} = \pi_k + \eta_\pi \nabla_\pi J(\pi_k, \hat{D}_k \cup \mathcal{D}_k)$, where $\mathcal{D}_k$ is data from the real environment and $\hat{D}_k = \text{rollout}(\pi_k, \hat{M}_k)$ is imaginary data from the model. This makes Dyna a hybrid model-free and model-based RL method, rather than a "pure" MBRL method.

In more detail, at each step of Dyna, the agent collects new data from the environment and adds it to a real replay buffer. This is then used to do an off-policy update. It also updates its world model given the real data. Then it simulates imaginary data, starting from a previously visited state (see `sample-init-state` function in Algorithm 10), and rolling out the current policy in the learned model. The imaginary data is then added to the imaginary replay buffer and used by an on-policy learning algorithm. This process continue until the agent runs out of time and must take the next step in the environment.

#### 4.3.2.1 Tabular Dyna

**Algorithm 15:** Tabular Dyna-Q

```
def dyna-Q-agent($s, M_{\text{env}}; \epsilon, \eta, \gamma$):
Initialize data buffer $\mathcal{D} = \emptyset$, $Q(s,a) = 0$ and $\hat{M}(s,a) = 0$
repeat
    // Collect real data from environment
    $a = \text{eps-greedy}(Q, \epsilon)$
    $(s', r) = \text{env.step}(s, a)$
    $\mathcal{D} = \mathcal{D} \cup \{(s, a, r, s')\}$
    // Update policy on real data
    $Q(s,a) := Q(s,a) + \eta[r + \gamma \max_{a'} Q(s', a') - Q(s,a)]$
    // Update model on real data
    $\hat{M}(s,a) = (s', r)$
    $s := s'$
    // Update policy on imaginary data
    for $n$=1:$N$ do
        Select $(s,a)$ from $\mathcal{D}$
        $(s', r) = \hat{M}(s,a)$
        $Q(s,a) := Q(s,a) + \eta[r + \gamma \max_{a'} Q(s', a') - Q(s,a)]$
until until converged;
```

The original Dyna paper was developed under the assumption that the world model $s' = M(s,a)$ is deterministic and tabular, and the $Q$ function is also tabular. See Algorithm 15 for the simplified pseudocode for this case. Since we assume a deterministic world model of the form $s' = M(s,a)$, then sampling a single step from this starting at a previously visited state is equivalent to experience replay (Section 2.5.2.3). Thus we can think of ER as a kind of non-parametric world model [HHA19].

#### 4.3.2.2 Dyna with function approximation

It is easy to extend Dyna to work with function approximation and policy gradient methods. The code is identical to the MBRL code in Algorithm 10, where now we train the policy on real as well as imaginary data. ([Lai+21] argues that we should gradually increase the fraction of real data that is used to train the policy, to avoid suboptimal performance due to model limitations.) If we use real data from the replay buffer, we have to use an off-policy learner, since the replay buffer contains trajectories that may have been generated from old policies. (The most recent real trajectory, and all imaginary trajectories, are always from the current policy.)

We now mention some examples of this "generalized Dyna" framework. In [Sut+08] they extended Dyna to the case where the $Q$ function is linear, and in [HTB18] they extended it to the DQN case. In [Jan+19a], they present the **MBPO** (model based policy optimization) algorithm, which uses Dyna with the off-policy SAC method. Their world model is an **ensemble of DNNs**, which generates diverse predictions (an approach which was originally proposed in the **PETS** (probabilistic ensembles with trajectory sampling) paper of [Chu+18]).[2] In [Kur+19], they combine Dyna with TRPO (Section 3.4.2) and ensemble world models, and in [Wu+23] they combine Dyna with PPO and GP world models. (Technically speaking, these on-policy approaches are not valid with Dyna, but they can work if the replay buffer used for policy training is not too stale.)

### 4.3.3 Dealing with model errors and uncertainty

The theory in Section 4.3.1 tells us that the model-as-leader approach, which trains a new policy in imagination at each inner iteration while gradually improving the model in the outer loop, will converge to the optimal policy, provided the model converges to the true model (or one that is value equivalent to it, see Section 4.4.2.3). This can be assured provided the model is sufficiently powerful, and the policy explores sufficiently widely to collect enough diverse but task-relevant data. Nevertheless, models will inevitably have errors, and it can be useful for the policy learning to be aware of this. We discuss some approaches to this below.

#### 4.3.3.1 Avoiding compounding errors in rollouts

In MBRL, we have to rollout imaginary trajectories to use for training the policy. It makes intuitive sense to start from a previously visited real-world state, since the model will likely be reliable there. We should start rollouts from different points along each real trajectory, to ensure good state coverage, rather than just expanding around the initial state [Raj+17]. However, if we roll out too far from a previously seen state, the trajectories are likely to become less realistic, due to **compounding errors** from the model [LPC22].

In [Jan+19a], they present the MBPO method, which uses short rollouts (inside Dyna) to prevent compounding error (an approach which is justified in [Jia+15]). [Fra+24] is a recent extension of MBPO which dynamically decides how much to roll out, based on model uncertainty.

Another approach to mitigating compounding errors is to learn a trajectory-level dynamics model, instead of a single-step model, see e.g., [Zho+24b] which uses diffusion to train $p(s_{t+1:t+H}|s_t, a_{t:t+H-1})$, and uses this inside an MPC loop.

If the model is able to predict a reliable distribution over future states, then we can leverage this uncertainty estimate to compute an estimate of the expected reward. For example, PILCO [DR11; DFR15] uses Gaussian processes as the world model, and uses this to analytically derive the expected reward over trajectories as a function of policy parameters, which are then optimized using a deterministic second-order gradient-based solver. In [Man+19], they combine the MPO algorithm (Section 3.6.5) for continuous control with **uncertainty sets** on the dynamics to learn a policy that optimizes for a worst case expected return objective.

#### 4.3.3.2 End-to-end differentiable learning of model and planner

One solution to the mismatch problem between model fitting and policy learning is to use **differentiable planning**, in which we learn the model so as to minimize the planning loss. This bilevel optimization problem was first proposed in the **Value Iteration Network** paper of [Tam+16] and extended in the **TreeQN** paper of [Far+18]. In [AY20] they proposed a version of this for continuous actions based on the differentiable cross entropy method. In [Nik+22; Ban+23] they propose to use implicit differentation to avoid explicitly unrolling the inner optimization.

#### 4.3.3.3 Unified model and planning variational lower bound

In [Eys+22], they propose a method called **Mismatched No More** (MNM) to solve the objective mismatch problem. They define an optimality variable (see Section 3.6) based on the entire trajectory, $p(O = 1|\tau) =$

[2] In [Zhe+22b] they argue that the main benefit of an ensemble is that it limits the Lipschitz constant of the value function. They show that more direct methods for regularizing this can work just as well, and are much faster.

$R(\tau) = \sum_{t=1}^{\infty} \gamma^t R(s_t, a_t)$. This gives rise to the following variational lower bound on the log probability of optimality:

$$\log p(O=1) = \log \int_\tau P(O=1,\tau) = \log \mathbb{E}_{P(\tau)}\left[P(O=1|\tau)\right] \geq \mathbb{E}_{Q(\tau)}\left[\log R(\tau) + \log P(\tau) - \log Q(\tau)\right]$$

where $P(\tau)$ is the distribution over trajectories induced by policy applied to the true world model, $P(\tau) = \mu(s_0)\prod_{t=0}^{\infty} M(s_{t+1}|s_t,a_t)\pi(a_t|s_t)$, and $Q(\tau)$ is the distribution over trajectories using the estimated world model, $Q(\tau) = \mu(s_0)\prod_{t=0}^{\infty} \hat{M}(s_{t+1}|s_t,a_t)\pi(a_t|s_t)$. They then maximize this bound wrt $\pi$ and $\hat{M}$.

In [Ghu+22] they extend MNM to work with images (and other high dimensional states) by learning a latent encoder $\hat{E}(\boldsymbol{z}_t|\boldsymbol{o}_t)$ as well as latent dynamics $\hat{M}(\boldsymbol{z}_{t+1}|\boldsymbol{z}_t,a_t)$, similar to other self-predictive methods (Section 4.4.2.4). They call their method **Aligned Latent Models**.

#### 4.3.3.4 Dynamically switching between MFRL and MBRL

One problem with the above methods is that, if the model is of limited capacity, or if it learns to model "irrelevant" aspects of the environment, then any MBRL method may be dominated by a MFRL method that directly optimizes the true expected reward. A safer approach is to use a model-based policy only when the agent is confident it is better, but otherwise to fall back to a model-free policy. This is the strategy proposed in the **Unified RL** method of [Fre+24].

## 4.4 World models

| | **Background planning** | **Online planning** | **Exploration** |
|---|---|---|---|
| **Observation prediction** | Dyna, DreamerV3, IRIS, Delta-IRIS, Diamond | CEM: PlaNet<br>Rnd shooting: TDM | SPR |
| **Value + self prediction** | DreamingV2, AIS | MCTS: MuZero, EfficientZero<br>CEM: TD-MPC | BYOL-Explore |

*Table 4.1: Comparison of different world model-based methods.*

In this section, we discuss various kinds of world models that have been proposed in the literature. These models can be trained to predict future observations (generative WMs) or just future rewards/values and/or future latent embeddings (non-generative / non-reconsructive WMs). Once trained, the models can be used for decision-time planning, background planning, or just as an auxiliary signal to aid in things like intrinsic curiosity. See Table 4.1 for a summary.

### 4.4.1 World models which are trained to predict observation targets

In this section, we discuss different kinds of world model $\mathcal{T}(\boldsymbol{s}'|\boldsymbol{s},a)$. We can use this to generate imaginary trajectories by sampling from the following joint distribution:

$$p(\boldsymbol{s}_{t+1:T}, \boldsymbol{r}_{t+1:T}, \boldsymbol{a}_{t:T-1}|\boldsymbol{s}_t) = \prod_{i=t}^{T-1} \pi(\boldsymbol{a}_i|\boldsymbol{s}_i)\mathcal{T}(\boldsymbol{s}_{i+1}|\boldsymbol{s}_i,\boldsymbol{a}_i)R(r_{i+1}|\boldsymbol{s}_i,\boldsymbol{a}_i) \tag{4.19}$$

The model may be augmented with latent variables, as we discuss in Section 4.4.1.2.

In this section, we assume the model is always trained to predict the entire observation vector, even if we use latent variables. (This is what we mean by "generative world model".) One big disadvantage of this approach is that the observations may contain irrelevant or distractor variables; this is particularly likely to occur in the case of image data. In addition, there may be a distribution shift in th observation process between train and test time. Both of these factors can adversely affect the performance of generative WMs (see e.g., [Tom+23]). We discuss some non-generative approaches to WMs in Section 4.4.2.

#### 4.4.1.1 Generative world models without latent variables

The simplest approach is to define $\mathcal{T}(\boldsymbol{s}'|\boldsymbol{s}, a)$ as a conditional generative model over states. If the observed states are low-dimensional vectors, such as proprioceptive states, we can use transformers (see e.g., the **Transformer Dynamics Model** of [Sch+23a]).

In some cases, the dimensions of the state vector $\boldsymbol{s}$ represent distinct variables, and the joint Markov transition matrix $p(\boldsymbol{s}'|\boldsymbol{s}, a)$ has conditional independence properties which can be represented as a sparse graphical model, This is called a **factored MDP** [BDG00].

If the state space is high dimensional (e.g., images), then we denote the observable data by $\boldsymbol{o}$. We can then learn $\mathcal{T}(\boldsymbol{o}'|\boldsymbol{o}, a)$ using standard techniques for conditional image generation such as diffusion (see e.g., the **Diamond** method of [Alo+24], the **Genie2** method of [al24], the GAIA-1 model of [Hu+23], etc).

#### 4.4.1.2 Generative world models with latent variables

In this section, we describe some methods that use latent variables as part of their world model. This can improve the speed of generating imaginary futures, and can provide a compact latent space as input to a policy.

We let $\boldsymbol{z}_t$ denote the latent (or hidden) state at time $t$; this can be a discrete or continuous variable (or vector of variables). The generative model has the form of a controlled HMM:

$$p(\boldsymbol{o}_{t+1:T}, \boldsymbol{z}_{t+1:T}, \boldsymbol{r}_{t+1:T}, \boldsymbol{a}_{t:T-1}|\boldsymbol{z}_t) = \prod_{i=t}^{T-1} \pi(\boldsymbol{a}_i|\boldsymbol{z}_i)\mathcal{M}(\boldsymbol{z}_{i+1}|\boldsymbol{z}_i, \boldsymbol{a}_i)R(r_i|\boldsymbol{z}_{i+1}, \boldsymbol{a}_i)D(\boldsymbol{o}_i|\boldsymbol{z}_i) \tag{4.20}$$

where $p(\boldsymbol{o}_t|\boldsymbol{z}_t) = D(\boldsymbol{o}_t|\boldsymbol{z}_t)$ is the decoder or likelihood function, $\mathcal{M}(\boldsymbol{z}'|\boldsymbol{z}, \boldsymbol{a})$ is the dunamics in latent space. $\pi(\boldsymbol{a}_t|\boldsymbol{z}_t)$ is the policy in latent space.

The world model is usually trained by maximizing the marginal likelihood of the observed outputs given an action sequence. (We discuss non-likelihood based loss functions in Section 4.4.2.) Computing the marginal likelihood requires marginalizing over the hidden variables $\boldsymbol{z}_{t+1:T}$. To make this computationally tractable, it is common to use amortized variational inference, in which we train an encoder network, $p(\boldsymbol{z}_t|\boldsymbol{o}_t) = E(\boldsymbol{z}_t|\boldsymbol{o}_t)$, to approximate the posterior over the latents. Many papers have followed this basic approach, such as the **"world models"** paper [HS18], and the methods we discuss below.

#### 4.4.1.3 Example: Dreamer

In this section, we summarize the approach used in **Dreamer** paper [Haf+20] and its recent extensions, such as DreamerV2 [Haf+21] and DreamerV3 [Haf+23]. These are all based on the background planning approach, in which the policy is trained on imaginary trajectories generated by a latent variable world model. (Note that Dreamer is based on an earlier approach called **PlaNet** [Haf+19], which used MPC instead of background planning.)

In Dreamer, the stochastic dynamic latent variables in Equation (4.20) are replaced by deterministic dynamic latent variables $\boldsymbol{h}_t$, since this makes the model easier to train. (We will see that $\boldsymbol{h}_t$ acts like the posterior over the hidden state at time $t-1$; this is also the prior predictive belief state before we see $\boldsymbol{o}_t$.) A "static" stochastic variable $\boldsymbol{z}_t$ is now generated for each time step, and acts like a "random effect" in order to help generate the observations, without relying on $\boldsymbol{h}_t$ to store all of the necessary information. (This simplifies the recurrent latent state.) In more detail, Dreamer defines the following functions:[3]

- A hidden dynamics (sequence) model: $\boldsymbol{h}_{t+1} = \mathcal{U}(\boldsymbol{h}_t, \boldsymbol{a}_t, \boldsymbol{z}_t)$

[3] We can map from our notation to the notation in the paper as follows: $\boldsymbol{o}_t \to x_t$, $U \to f_\phi$ (sequence model), $P_0 \to p_\phi(\hat{z}_t|h_t)$ (dynamics predictor), $D \to p_\phi(\hat{x}_t|h_t, \hat{z}_t)$ (decoder), $E \to q_\phi(\boldsymbol{z}_t|h_t, x_t)$ (encoder).

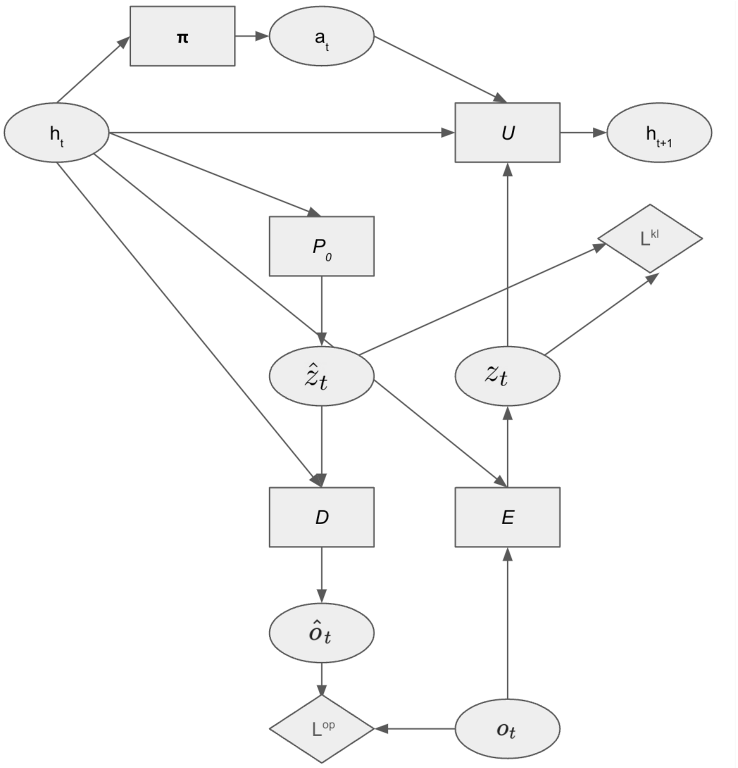


*Figure 4.4: Illustration of Dreamer world model as a factor graph (squares are learnable functions, circles are variables, diamonds are fixed cost functions). We have unrolled the forwards prediction for only 1 step. Also, we have omitted the reward prediction loss.*

- A latent state conditional prior: $\hat{\boldsymbol{z}}_t \sim P(\hat{\boldsymbol{z}}_t|\boldsymbol{h}_t)$
- A latent state decoder (observation predictor): $\hat{\boldsymbol{o}}_t \sim D(\hat{\boldsymbol{o}}_t|\boldsymbol{h}_t, \hat{\boldsymbol{z}}_t)$.
- A reward predictor: $\hat{r}_t \sim R(\hat{r}_t|\boldsymbol{h}_t, \hat{\boldsymbol{z}}_t)$
- A latent state encoder: $\boldsymbol{z}_t \sim E(\boldsymbol{z}_t|\boldsymbol{h}_t, \boldsymbol{o}_t)$.
- A policy function: $\boldsymbol{a}_t \sim \pi(\boldsymbol{a}_t|\boldsymbol{h}_t)$

See Figure 4.4 for an illustration of the system.

We now give a simplified explanation of how the world model is trained. The loss has the form

$$\mathcal{L}^{\text{WM}} = \mathbb{E}_{q(\boldsymbol{z}_{1:T})}\left[\sum_{t=1}^{T} \beta_o \mathcal{L}^o(\boldsymbol{o}_t, \hat{\boldsymbol{o}}_t) + \beta_z \mathcal{L}^z(\boldsymbol{z}_t, \hat{\boldsymbol{z}}_t)\right] \tag{4.21}$$

where the $\beta$ terms are different weights for each loss, and $q$ is the posterior over the latents, given by

$$q(\boldsymbol{z}_{1:T}|\boldsymbol{h}_0, \boldsymbol{o}_{1:T}, \boldsymbol{a}_{1:T}) = \prod_{t=1}^{T} E(\boldsymbol{z}_t|\boldsymbol{h}_t, \boldsymbol{o}_t)\delta(\boldsymbol{h}_t - \mathcal{U}(\boldsymbol{h}_{t-1}, \boldsymbol{a}_{t-1}, \boldsymbol{z}_{t-1})) \tag{4.22}$$

The loss terms are defined as follows:

$$\mathcal{L}^o = -\ln D(\boldsymbol{o}_t|\boldsymbol{z}_t, \boldsymbol{h}_t) \tag{4.23}$$

$$\mathcal{L}^z = D_{\mathbb{KL}}\left(E(\boldsymbol{z}_t|\boldsymbol{h}_t, \boldsymbol{o}_t)\right) \parallel P(\boldsymbol{z}_t|\boldsymbol{h}_t))) \tag{4.24}$$

where we abuse notation somewhat, since $\mathcal{L}^z$ is a function of two distributions, not of the variables $\boldsymbol{z}_t$ and $\hat{\boldsymbol{z}}_t$.

In addition to the world model loss, we have the following actor-critic losses

$$\mathcal{L}^{\text{critic}} = \sum_{t=1}^{T} (V(\boldsymbol{h}_t) - \text{sg}(G_t^\lambda))^2 \tag{4.25}$$

$$\mathcal{L}^{\text{actor}} = -\sum_{t=1}^{T} \text{sg}((G_t^\lambda - V(\boldsymbol{h}_t))) \log \pi(\boldsymbol{a}_t|\boldsymbol{h}_t) \tag{4.26}$$

where $G_t^\lambda$ is the GAE estimate of the reward to go:

$$G_t^\lambda = r_t + \gamma\left((1-\lambda)V(\boldsymbol{h}_t) + \lambda G_{t+1}^\lambda\right) \tag{4.27}$$

There have been several extensions to the original Dreamer paper. DreamerV2 [Haf+21] adds categorical (discrete) latents and KL balancing between prior and posterior estimates. This was the first imagination-based agent to outperform humans in Atari games. DayDreamer [Wu+22] applies DreamerV2 to real robots. DreamerV3 [Haf+23] builds upon DreamerV2 using various tricks — such as symlog encodings[4] for the reward, critic, and decoder — to enable more stable optimization and domain independent choice of hyper-parameters. It was the first method to create diamonds in the Minecraft game without requiring human demonstration data. (However, reaching this goal took 17 days of training.) [Lin+24a] extends DreamerV3 to also model language observations.

Many variants of Dreamer have been explored. For example, TransDreamer [Che+21a] and STORM [Zha+23b] replace the RNN world model with transformers, and the S4WM method of [DPA23] uses S4 (Structured State Space Sequence) models. The DreamingV2 paper of [OT22] replaces the generative loss with a non-generative self-prediction loss (see Section 4.4.2.4), and [RHH23; Sgf] use the VicReg non-generative representation learning method (see Section 4.4.2.7).

[4] The symlog function is defined as $\text{symlog}(x) = \text{sign}(x)\ln(|x|+1)$, and its inverse is $\text{symexp}(x) = \text{sign}(x)(\exp(|x|) - 1)$. The symlog function squashes large positive and negative values, while preserving small values.

#### 4.4.1.4 Example: IRIS

The **IRIS** method ("Imagination with auto-Regression over an Inner Speech") of [MAF22] follows the MBRL paradigm, in which it alternates beween (1) learning a world model using real data $D_r$ and then generate imaginary rollouts $D_i$ using the WM, and (2) learning the policy given $D_i$ and collecting new data $D'_r$ for learning. In the model learning stage, Iris learns a discrete latent encoding using the VQ-VAE method, and then fits a transformer dynamics model to the latent codes. In the policy learning stage, it uses actor critic methods. The **Delta-IRIS** method of [MAF24] extends this by training the model to only predict the delta between neighboring frames. Note that, in both cases, the policy has the form $a_t = \pi(\boldsymbol{o}_t)$, where $\boldsymbol{o}_t$ is an image, so the the rollouts need to ground to pixel space, and cannot only be done in latent space.

#### 4.4.1.5 Code world models (WIP)

Recently it has become popular to represent the world model $p(s'|s, a)$ using code, such as Python. This is called a **code world model**. It is possible to learn such models from trajectory data using LLMs (large language models). See Section 6.2.3 for details.

#### 4.4.1.6 Partial observation prediction

Predicting all the pixels in image may waste capacity and may distract the agent from the important bits. A natural alternative is to predict some of the observations, or at least some function of them. This is known as a **partial world model** (see e.g., [AP23]). One way to implement this is to impose an information bottleneck between the latent state and the observed variables, to prevent the agent focusing on irrelevant observational details. See e.g., the **denoised MDP** method of [Wan+22].

### 4.4.2 World models that are trained to predict other targets

In this section, we discuss training world models that are not necessarily able to predict all the future observations. These are often still (conditional) generative models (in that they return a distribution over potentially high dimensional outputs), but they are *lossy* models, because they do not capture all the details of the data.

#### 4.4.2.1 The objective mismatch problem

In Section 4.3.1, we argued that, if we can learn a sufficiently accurate world model, then solving for the optimal policy in simulation will give a policy that is close to optimal in the real world. However, a simple agent may not be able to capture the full complexity of the true environment; this is called the "**small agent, big world**" problem [DVRZ22; Lu+23; Aru+24a; Kum+24].

Consider what happens when the agent's model is misspecified (i.e., it cannot represent the true world model), which is nearly always the case. The agent will train its model to reduce state (or observation) prediction error, by minimizing $\ell(\hat{M}, \mu^{\pi}_{M})$. However, not all features of the state are useful for planning. For example, if the states are images, a dynamics model with limited representational capacity may choose to focus on predicting the background pixels rather than more control-relevant features, like small moving objects, since predicting the background reliably reduces the MSE more. This is due to "**objective mismatch**" [Lam+20; Wei+24], which refers to the discrepancy between the way a model is usually trained (to predict the observations) vs the way its representation is used for control. To tackle this problem, in this section we discuss methods for learning representations and models that don't rely on predicting all the observations. Our presentation is based in part on [Ni+24] (which in turn builds on [Sub+22]). See Table 4.2 for a summary of some of the methods we will discuss.

| Loss | Policy | Usage | Examples |
|---|---|---|---|
| OP | Observables | Dyna | Diamond [Alo+24], Delta-Iris [MAF24] |
| OP | Observables | MCTS | TDM [Sch+23a] |
| OP | Latents | Dyna | Dreamer [Haf+23] |
| RP, VP, PP | Latents | MCTS | MuZero [Sch+20] |
| RP, VP, PP, ZP | Latents | MCTS | EfficientZero [Ye+21] |
| RP, VP, ZP | Latents | MPC-CEM | TD-MPC [HSW22; HSW24] |
| VP, ZP | Latents | Aux. | Minimalist [Ni+24] |
| VP, ZP | Latents | Dyna | DreamingV2 [OT22] |
| VP, ZP, OP | Latents | Dyna | AIS [Sub+22] |
| POP | Latents | Dyna | Denoised MDP [Wan+22] |

*Table 4.2: Summary of some world-modeling methods. The "loss" column refers to the loss used to train the latent encoder (if present) and the dynamics model (OP = observation prediction, ZP = latent state prediction, RP = reward prediction, VP = value prediction, PP = policy prediction, POP = partial observation prediction). The "policy" column refers to the input that is passed to the policy. (For MCTS methods, the policy is just used as a proposal over action sequences to initialize the search/ optimization process.) The "usage" column refers to how to the world model is used: for background planning (which we call "Dyna"), or for decision-time planning (which we call "MCTS"), or just as an auxiliary loss on top of standard policy/value learning (which we call "Aux"). Thus Aux methods are single-stage ("end-to-end"), whereas the other methods alternate are two-phase, and alternate between improving the world model and then using it for improving the policy (or searching for the optimal action).*

#### 4.4.2.2 Observation prediction

We consider a modeling paradigm where we learn an encoder, $\boldsymbol{z} = \phi(\boldsymbol{o})$[5]; a dynamics model in latent space, $\boldsymbol{z}' = \mathcal{M}(\boldsymbol{z}, \boldsymbol{a})$, for future prediction; and an update model in latent space, $\boldsymbol{z}' = \mathcal{U}(\boldsymbol{z}, a, \boldsymbol{o})$, for belief state tracking.

A natural target to use for learning the encoder and dynamics is the next observation, using a one-step version of Equation (4.19). Indeed, [Ni+24] say that a representation $\phi$ satisifies the **OP** (observation prediction) criterion if it satisfies the following condition:

$$\exists D \quad \text{s.t.} \quad p^*(\boldsymbol{o}'|\boldsymbol{h}, a) = D(\boldsymbol{o}'|\phi(\boldsymbol{h}), a) \;\; \forall \boldsymbol{h}, a \tag{4.28}$$

where $D$ is the decoder. In order to repeatedly apply this, we need to be able to update the encoding $\boldsymbol{z} = \phi(\boldsymbol{h})$ in a recursive or online way. Thus we must also satisfify the following recurrent encoder condition, which [Ni+24] call **Rec**:

$$\exists U \quad \text{s.t.} \quad \phi(\boldsymbol{h}') = \mathcal{U}(\phi(\boldsymbol{h}), a, \boldsymbol{o}') \;\; \forall \boldsymbol{h}, a, \boldsymbol{o}' \tag{4.29}$$

where $\mathcal{U}$ is the update operator. Note that belief state updates (as in a POMDP) satisfy this property. Furthermore, belief states are a sufficient statistic to satisfy the OP condition. See Section 4.4.1.2 for a discussion of generative models of this form.

The drawback of this approach is that in general it is very hard to predict future observations, at least in high dimensional settings like images. Fortunately, such prediction is not necessary for optimal behavior. Thus we now turn our attention to other training objectives.

[5] Note that in general, the encoder may depend on the entire history of previous observations, denoted $\boldsymbol{z} = \phi(\mathcal{D})$.

#### 4.4.2.3 Value prediction

Let $\boldsymbol{h}_t = (\boldsymbol{h}_{t-1}, \boldsymbol{a}_{t-1}, r_{t-1}, \boldsymbol{o}_t)$ be all the visible data (history) at time $t$, and let $\boldsymbol{z}_t = \phi(\boldsymbol{h}_t)$ be a latent representation (compressed encoding) of this history, where $\phi$ is called an encoder or a **state abstraction** function. We will train the policy $\boldsymbol{a}_t = \pi(\boldsymbol{z}_t)$ in the usual way, so our focus will be on how to learn good latent representations.

An optimal representation $\boldsymbol{z}_t = \phi(\boldsymbol{h}_t)$ is a sufficient statistic for the optimal action-value function $Q^*$. Thus it satifies the **value equivalence** principle [LWL06; Cas11; Gri+20b; GBS22; AP23; ARKP24], which says that two states $s_1$ and $s_2$ are value equivalent (given a policy) if $V^\pi(s_1) = V^\pi(s_2)$. In particular, if the representation is optimal, it will satisfy value equivalence wrt the optimal policy, i.e., if $\phi(\boldsymbol{h}_i) = \phi(\boldsymbol{h}_j)$ then $Q^*(\boldsymbol{h}_i, a) = Q^*(\boldsymbol{h}_j, a)$. We can train such a representation function by using its output $\boldsymbol{z} = \phi(\boldsymbol{h})$ as input to the Q function or to the policy. (We call such a loss **VP**, for value prediction.) This will cause the model to focus its representational power on the relevant parts of the observation history.

Note that there is a stronger property than value equivalence called **bisimulation** [GDG03]. This says that two states $s_1$ and $s_2$ are bisimiliar if $P(s'|s_1, a) \approx P(s'|s_2, a)$ and $R(s_1, a) = R(s_2, a)$. From this, we can derive a continuous measure called the **bisimulation metric** [FPP04]. This has the advantage (compared to value equivalence) of being policy independent, but the disadvantage that it can be harder to compute [Cas20; Zha+21], although there has been recent progress on computaitonally efficient methods such as MICo [Cas+21] and KSMe [Cas+23].

#### 4.4.2.4 Self prediction (self distillation)

Unfortunately, in problems with sparse reward, predicting the value may not provide enough of a feedback signal to learn quickly. Consequently it is common to augment the training with a **self-prediction** loss where we train $\phi$ to ensure the following condition hold:

$$\exists M \quad \text{s.t.} \quad \mathbb{E}_{M^*}\left[\boldsymbol{z}'|\boldsymbol{h}, a\right] = \mathbb{E}_M\left[\boldsymbol{z}'|\phi(\boldsymbol{h}), a)\right] \quad \forall \boldsymbol{h}, a \tag{4.30}$$

where the LHS is the predicted mean of the next latent state under the true model, and the RHS is the predicted mean under the learned dynamics model. We call this the **EZP**, which stands for expected $\boldsymbol{z}$ prediction.[6]

A trivial way to minimize the (E)ZP loss is for the embedding to map everything to a constant vector, say $E(\boldsymbol{h}) = \boldsymbol{0}$, in which case $\boldsymbol{z}_{t+1}$ will be trivial for the dynamics model $M$ to predict. However this is not a useful representation. This problem is **representational collapse** [Jin+22]. Fortunately, we can provably prevent collapse (at least for linear encoders) by using a frozen target network [TCG21; Tan+23; Ni+24]. That is, we use the following auxiliary loss

$$\mathcal{L}_{\text{EZP}}(\boldsymbol{\phi}, \boldsymbol{\theta}; \boldsymbol{h}, a, \boldsymbol{h}') = ||M_{\boldsymbol{\theta}}(E_{\boldsymbol{\phi}}(\boldsymbol{h}, a)) - E_{\overline{\boldsymbol{\phi}}}(\boldsymbol{h}')||_2^2 \tag{4.31}$$

where

$$\overline{\boldsymbol{\phi}} = \rho\overline{\boldsymbol{\phi}} + (1-\rho)\text{sg}(\boldsymbol{\phi}) \tag{4.32}$$

is the (stop-gradient version of) the EMA of the encoder weights. (If we set $\rho = 0$, this is called a detached network.)

Methods that optimize ZP and VP loss have been used in many papers, such as **Predictron** [Sil+17b], **Value Prediction Networks** [OSL17], **Self Predictive Representations** (SPR) [Sch+21], **Efficient Zero** (Section 4.2.2.2), **BYOL-Explore** (Section 4.4.2.9), etc.

#### 4.4.2.5 Reward prediction

We can also train the latent encoder to predict the reward. Formally, we want to ensure we can satisfy the following condition, which we call **RP** for "reward prediction":

$$\exists R \quad \text{s.t.} \quad \mathbb{E}_{R^*}\left[r|\boldsymbol{h}, a\right] = \mathbb{E}_R\left[r|\phi(\boldsymbol{h}), a)\right] \quad \forall \boldsymbol{h}, a \tag{4.33}$$

[6] In [Ni+24], they also describe the ZP loss, which requires predicting the full distribution over $\boldsymbol{z}'$ using a stochastic transition model. This is strictly more powerful, but somewhat more complicated, so we omit it for simplicity.

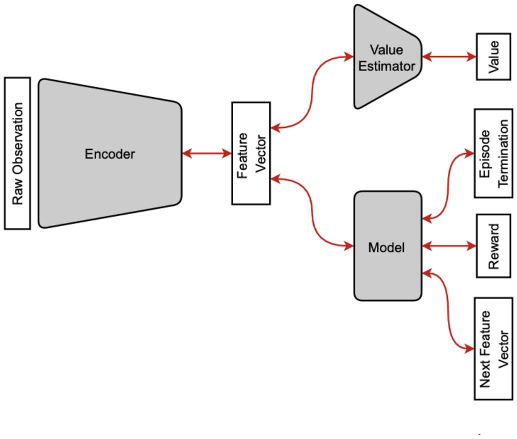


*Figure 4.5: Illustration of an encoder $z_t = E(o_t)$, which is passed to a value estimator $v_t = V(z_t)$, and a world model, which predicts the next latent state $\hat{z}_{t+1} = \mathcal{M}(z_t, a_t)$, the reward $r_t = R(z_t, a_t)$, and the termination (done) flag, $d_t = done(z_t)$. From Figure C.2 of [AP23]. Used with kind permission of Doina Precup.*

See Figure 4.5 for an illustration. In [Ni+24], they prove that a representation that satisfies ZP and RP is enough to satisfy value equivalence (sufficiency for $Q^*$).

#### 4.4.2.6 Policy prediction

The value function and reward losses may be too sparse to learn efficiently. Although self-prediction loss can help somewhat, it does not use any extra information from the environment as feedback. Consequently it is natural to consider other kinds of prediction targets for learning the latent encoder (and dynamics). When using MCTS, it is possible compute what the policy should be for a given state, and this can be used as a prediction target for the reactive policy $a_t = \pi(z_t)$, which in turn can be used as a feedback signal for the latent state. This method is used by MuZero (Section 4.2.2.2) and EfficientZero (Section 4.2.2.2).

#### 4.4.2.7 JEPA

In this section, we discuss the **JEPA** (Joint embedding Prediction Architecture) approach to world modeling, first proposed in [LeC22]. The basic idea is to jointly embed the current and following observations, to compute $\boldsymbol{z}_t = E(\boldsymbol{o}_t)$ and $\boldsymbol{z}_{t+1} = E(\boldsymbol{o}_{t+1})$, and then to compare the actual latent embedding $\boldsymbol{z}_{t+1}$ to its prediction $\boldsymbol{z}'_{t+1} = \mathcal{M}(\boldsymbol{z}_t, a_t; \epsilon_t)$, where $\epsilon_t$ is a random noise source, and $M$ is the deterministic world model. We then train the encoder to minimize the difference between $\boldsymbol{z}_t$ and $\boldsymbol{z}'_t$.

To prevent the encoder collapsing to a trivial function, such as $E(\boldsymbol{o}) = \mathbf{0}$, two different classes of methods have been considered. The first is based on self-prediction or self-distillation, discussed in Section 4.4.2.4; here we ensure that the encoder used to compute the target $\boldsymbol{z}_{t+1}$ is a frozen EMA version of the encoder used to compute the source $\boldsymbol{z}_t$ (see Figure 4.6(a)). This approach is used in **BYOL** [Gri+20a] (BYOL stands for "bootstrap your own latent"), **SimSiam** [CH20], **DinoV2** [Oqu+24], **I-JEPA** [Ass+23], **V-JEPA** [Bar+24], **Image World Models** [Gar+24], etc. Unfortunately, the self-prediction method has only been proven to be theoretical sound for the case of linear encoders.

An alternative way to avoid the latent collapse problem is to add regularization terms that try to maximize the information content in $\boldsymbol{z}_t$ and $\boldsymbol{z}_{t+1}$ (see Figure 4.6(b)), while also minimizing the prediction error. That is, the objective becomes

$$\begin{aligned} J(\boldsymbol{\phi}) &= E_{\boldsymbol{o}_t, \boldsymbol{a}_t, \boldsymbol{o}_{t+1}, \boldsymbol{\epsilon}_t} \left( ||\boldsymbol{z}_{t+1} - \hat{\boldsymbol{z}}_{t+1}||_2^2 - \lambda I(\boldsymbol{z}_t) - \lambda I(\boldsymbol{z}_{t+1}) \right) \\ &\quad \text{where } \boldsymbol{z}_t = E(\boldsymbol{o}_t; \boldsymbol{\phi}), \boldsymbol{z}_{t+1} = E(\boldsymbol{o}_{t+1}; \boldsymbol{\phi}), \hat{\boldsymbol{z}}_{t+1} = \mathcal{M}(\boldsymbol{z}_t, \boldsymbol{a}_t, \boldsymbol{\epsilon}_t; \boldsymbol{\theta}) \end{aligned} \tag{4.34}$$

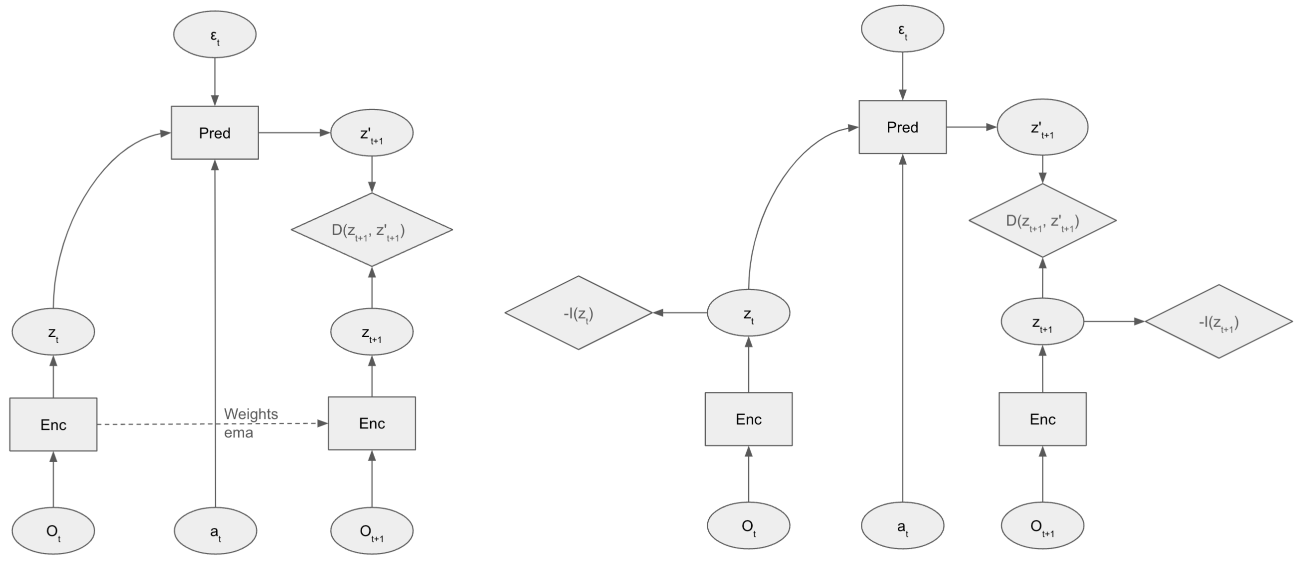


*Figure 4.6: Illustration of the JEPA (Joint embedding Prediction Architecture) world model approach using two different approaches to avoid latent collapse: (a) self-distillation; (b) information theoretic regularizers. Diamonds represent fixed cost functions, squares represent learnable functions, circles are variables.*

Various methods have been proposed to approximate the information content $I(\boldsymbol{z}_t)$, mostly based on some function of the outer product matrix $\sum_t \boldsymbol{z}_t \boldsymbol{z}_t^\mathsf{T}$ (since this captures second order moments, it is an implicit assumption of Gaussanity of the embedding distribution). Examples of such methods include **Barlow Twins** [Zbo+21], **VICReg** [BPL22a], **VICRegL** [BPL22b], **MCR2** (Maximal Coding Rate Reduction) [Yu+20b], **MMCR** (Maximum Manifold Capacity Representation) [Yer+23], etc. Unfortunately, the methods in these papers do not provide a lower bound on $I(\boldsymbol{z}_t)$ and $I(\boldsymbol{z}_{t+1})$, which is needed to optimize Equation (4.34).

#### 4.4.2.8 Example: TD-MPC

In this section, we describe **TD-MPC2** [HSW24], which is an extension of **TD-MPC** of [HSW22]. This learns the following functions:

- Encoder: $\boldsymbol{e}_t = E(\boldsymbol{o}_t)$
- Latent dynamics (for rollouts): $\boldsymbol{z}'_t = \mathcal{M}(\boldsymbol{z}_{t-1}, \boldsymbol{a}_t)$
- Latent update (after each observation): $\boldsymbol{z}_t = \mathcal{U}(\boldsymbol{z}_{t-1}, \boldsymbol{e}_t, \boldsymbol{a}_t) = \boldsymbol{e}_t$
- Reward: $\hat{r}_t = R(\boldsymbol{z}_t, \boldsymbol{a}_t)$
- Value: $\hat{q}_t = Q(\boldsymbol{z}_t, \boldsymbol{a}_t)$
- Policy prior: $\hat{\boldsymbol{a}}_t = \pi_{\text{prior}}(\boldsymbol{z}_{t-1})$

The model is trained using the following VP+ZP loss applied to trajectories sampled from the replay buffer:

$$\mathcal{L}(\boldsymbol{\theta}) = \mathbb{E}_{(\boldsymbol{o},\boldsymbol{a},r,\boldsymbol{o}')_{0:H}\sim\mathcal{B}}\left[\sum_{t=0}^{H} \lambda^t \left(||\boldsymbol{z}'_t - \text{sg}(E(\boldsymbol{o}'_t))||_2^2 + \text{CE}(\hat{r}_t, r_t) + \text{CE}(\hat{q}_t, q_t)\right)\right] \tag{4.35}$$

We use cross-entropy loss on a discretized representation of the reward and Q value in a log-transformed space, in order to be robust to different value scales across time and problem settings (see Section 7.2.2). The

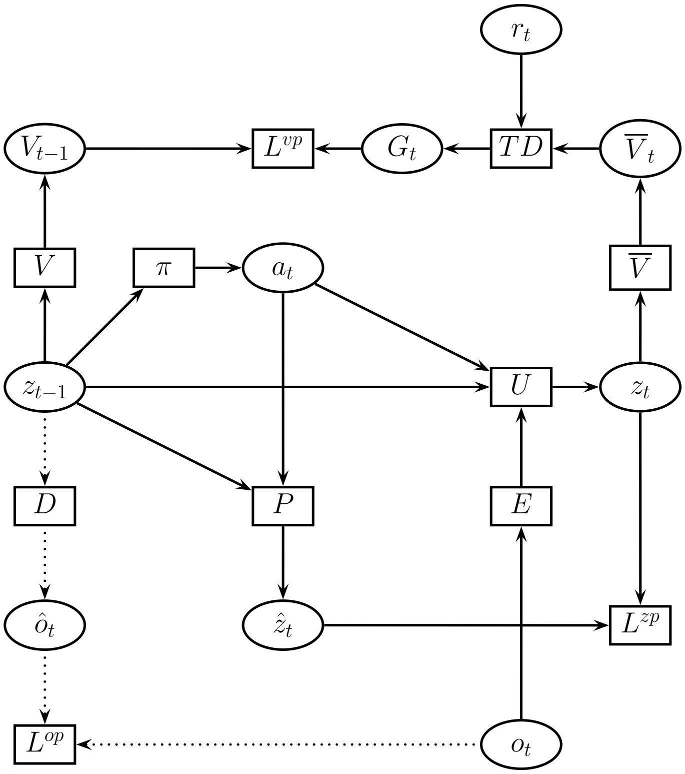


*Figure 4.7: Illustration of (a simplified version of) the BYOL-Explore architecture, represented as a factor graph (so squares are functions, circles are variables). The dotted lines represent an optional observation prediction loss. The map from notation in this figure to the paper is as follows: $U \rightarrow h^c$ (closed-loop RNN update), $P \rightarrow h^o$ (open-loop RNN update), $D \rightarrow g$ (decoder), $E \rightarrow f$ (encoder). We have unrolled the forwards prediction for only 1 step. Also, we have omitted the reward prediction loss. The $\overline{V}$ node is the EMA version of the value function. The TD node is the TD operator.*

target value for the Q function update is defined by

$$q_t = r_t + \gamma \overline{Q}(\boldsymbol{z}'_t, \pi_{\text{prior}}(\boldsymbol{z}'_t)) \tag{4.36}$$

where $\overline{Q}$ is the EMA for the Q function.

The policy is trained using the SAC objective (see Section 3.6.8) on imaginary rollouts in latent space using observations and actions from the replay buffer:

$$\mathcal{L}_\pi(\boldsymbol{\theta}) = \mathbb{E}_{(\boldsymbol{o},\boldsymbol{a})_{0:H}\sim\mathcal{B}}\left[\sum_{t=0}^{H} \lambda^t \left[\alpha Q(\boldsymbol{z}_t, \pi_{\text{prior}}(\boldsymbol{z}_t)) - \beta\,\mathbb{H}(\pi_{\text{prior}}(\cdot|\boldsymbol{z}_t))\right]\right], \boldsymbol{z}_{t+1} = \mathcal{M}(\boldsymbol{z}_t, \boldsymbol{a}_t), \boldsymbol{z}_0 = E(\boldsymbol{o}_0) \tag{4.37}$$

This policy is used as a proposal (prior), in conjunction with the MPPI trajectory planning method (Section 4.2.4.6) to select actions at run time.

#### 4.4.2.9 Example: BYOL-Explore

As an example of a non-generative WM, consider the **BYOL-Explore** paper [Guo+22], which uses the ZP and VP loss. See Figure 4.7 for the computation graph, which we see is slightly simpler than the Dreamer computation graph in Figure 4.4 due to the lack of stochastic latents. In addition to using self-prediction loss to help train the latent representation, the error in this loss can be used to define an intrinsic reward, to encourage the agent to explore states where the model is uncertain. See Section 7.3 for further discussion of this topic.

#### 4.4.2.10 Example: imagination-augmented agents

In [Web+17], they train a model to predict future states and rewards, and then use the hidden states of this model as additional context for a policy-based learning method. This can help overcome partial observability. They call their method **imagination-augmented agents**.

#### 4.4.2.11 Using pre-trained visual representations

In the case where the observations are high-dimensional, such as images, it it natural to use a pre-trained representation, $\boldsymbol{z}_t = \phi(\boldsymbol{o}_t)$, as input to the world model (or policy). The representation function $\phi$ can be pretrained on a large dataset using a non-reconstructive loss, such as the DINOv2 method [Oqu+24]. Although this can sometimes give gains (as in the **DinoWM** paper [Zho+24a]), in other cases, better results are obtained by training the representaton from scratch [Han+23; Sch+24]; the performance is, not surprisingly, highly dependent on the similarity or differences between between the pretraining distribution and the agent's distribution, the form of the representation function, and its training objective.

### 4.4.3 Exploration for learning world models

In Section 1.3.5, we discussed the exploration-exploitation tradeoff, which contrasts the need to (1) collect diverse experiences (by trying many new actions in many new states) so as to learn a better policy to help long-run performance with (2) the need to stay in familiar parts of the state space where the optimal policy has already been learned, so as to ensure short-term rewards. When using MBRL, the need for diverse data becomes even more important, to ensure we learn the correct underlying world model (which is then used to train the policy, or for online planning).

One popular approach to this is to use posterior sampling RL, which applies Thompson sampling to the MDP parameters (i.e., the world model), as explained in Section 7.1.3.2. This was applied to MBRL in [WCM24].

If we are in the reward-free setting, we can view the problem of learning a world model as similar to the scientist's job of trying to create a **causal model** of the world, which can explain the effects of actions (interventions). This requires designing and carrying out experiments in order to collect informative trajectories for model fitting. Recently it has become popular to use LLMs to tackle this problem, using methods known as **AI scientists** (see e.g., [Gan+25b]). It is also possible to combine LLMs as hypothesis generators with Bayesian inference and information theoretic reasoning principles for a more principled approach to the problem (see e.g., **Piriyakulkij2024**).

## 4.5 Beyond one-step models: predictive representations

The "world models" we described in Section 4.4 are **one-step models** of the form $p(s'|s,a)$, or $p(z'|z,a)$ for $z = \phi(s)$, where $\phi$ is a state-abstraction function. However, such models are problematic when it comes to predicting many kinds of future events, such as "will a car pull in front of me?" or "when will it start raining?", since it is hard to predict exactly when these events will occur, and these events may correspond to many different "ground states". In principle we can roll out many possible long term futures, and apply some abstraction function to the resulting generated trajectories to extract features of interest, and thus derive a predictive model of the form $p(t', \phi(s_{t+1:t'})|s_t, \pi)$, where $t'$ is the random duration of the sampled trajectory, and $\phi$ maps from state trajectories to features. However, it would be more efficient if we could directly predict this distribution without having to know the value of $t'$, and without having to predict all the details of all the intermediate future states, many of which will be irrelevant after we pass them into the abstraction function $\phi$. This motivates the study of multi-step world models, that predict multiple steps into the future, either at the state level, or at the feature level. These are called **predictive representations**, and are a compromise between standard model-based RL and model-free RL, as we will see. Our presentation on this topic is based on [Car+24]. (See also Section 7.4, where we discuss the related topic of temporal abstraction from a model-free perspective.)

### 4.5.1 General value functions

The value function is based on predicting the sum of expected discounted future rewards. But the reward is just one possible signal of interest we can extract from the environment. We can generalize this by considering a **cumulant** $C_t \in \mathbb{R}$, which is some scalar of interest derived from the state or observation (e.g., did a loud bang just occur? is there a tree visible in the image?). We then define the **general value function** or **GVF** as follows [Sut95; Sut+11; Rin21; Xu+22]:

$$V^{\pi,C,\gamma}(s) = \mathbb{E}\left[\sum_{t=0}^{\infty} \gamma^t C(s_{t+1}) | s_0 = s, a_{0:\infty} \sim \pi\right] \tag{4.38}$$

If $C(s_{t+1}) = R_{t+1}$, this reduces to the value function.[7] If we define the cumulatant to be the observation vector, then the GVF will learn to predict future observations at multiple time scales; this is called **nexting** [MS14; MWS14]. Predicting the GVFs for multiple cumulants can be useful as an auxiliary task to learn a useful non-generative representation for the solving the main task, as shown in [Jad+17].

[Vee+19] present an approach (based on meta-gradients) to learn which cumulants are worth predicting, In the inner loop, the model $f$ predicts the policy $\pi_t$ and value function $V_t$, as usual, and also predicts the GVFs $\boldsymbol{y}_t$ for the specified cumulants; the function $f$ is called the answer network, and is denoted by $(\pi_t, V_t, \boldsymbol{y}_t) = f_{\boldsymbol{\theta}}(\boldsymbol{o}_{t-i-1:t})$. In the outerloop, the model $g$ learns to extract the cumulants and their discounts given future observations; this called the question network and is denoted by $(\boldsymbol{c}_t, \boldsymbol{\gamma}_t) = g_{\boldsymbol{\eta}}(\boldsymbol{o}_{t+1:t+j})$. The outer update to $\boldsymbol{\eta}$ is based on the gradient of the RL loss after performing $K$ inner updates to $\boldsymbol{\theta}$ using the RL loss and auxiliary loss.

### 4.5.2 Successor representations

In this section we consider a variant of GVF where the cumulant corresponds to a state occupancy vector $C_{\tilde{s}}(s_{t+1}) = \mathbb{I}(s_{t+1} = \tilde{s})$, which provides a dense feedback signal. Computing this for each possible state $\tilde{s}$ gives us the **successor representation** or **SR** [Day93]:

$$M^\pi(s, \tilde{s}) = \mathbb{E}\left[\sum_{t=0}^{\infty} \gamma^t \mathbb{I}\left(s_{t+1} = \tilde{s}\right) | S_0 = s\right] \tag{4.39}$$

If we define the policy-dependent state-transition matrix by

$$T^\pi(s, s') = \sum_a \pi(a|s) T(s'|s, a) \tag{4.40}$$

then the SR matrix can be rewritten as

$$\mathbf{M}^\pi = \sum_{t=0}^{\infty} \gamma^t [\mathbf{T}^\pi]^{t+1} = \mathbf{T}^\pi(\mathbf{I} - \gamma \mathbf{T}^\pi)^{-1} \tag{4.41}$$

Thus we see that the SR replaces information about individual transitions with their cumulants, just as the value function replaces individual rewards with the reward-to-go.

Like the value function, the SR obeys a Bellman equation

$$M^\pi(s, \tilde{s}) = \sum_a \pi(a|s) \sum_{s'} T(s'|s, a) \left(\mathbb{I}\left(s' = \tilde{s}\right) + \gamma M^\pi(s', \tilde{s})\right) \tag{4.42}$$

$$= \mathbb{E}\left[\mathbb{I}\left(s' = \tilde{s}\right) + \gamma M^\pi(s', \tilde{s})\right] \tag{4.43}$$

[7] This follows the convention of [SB18], where we write $(s_t, a_t, r_{t+1}, s_{t+1})$ — as opposed to $(s_t, a_t, r_t, s_{t+1})$ — to represent the transitions, since $r_{t+1}$ and $s_{t+1}$ are both generated by applying $a_t$ in state $s_t$.

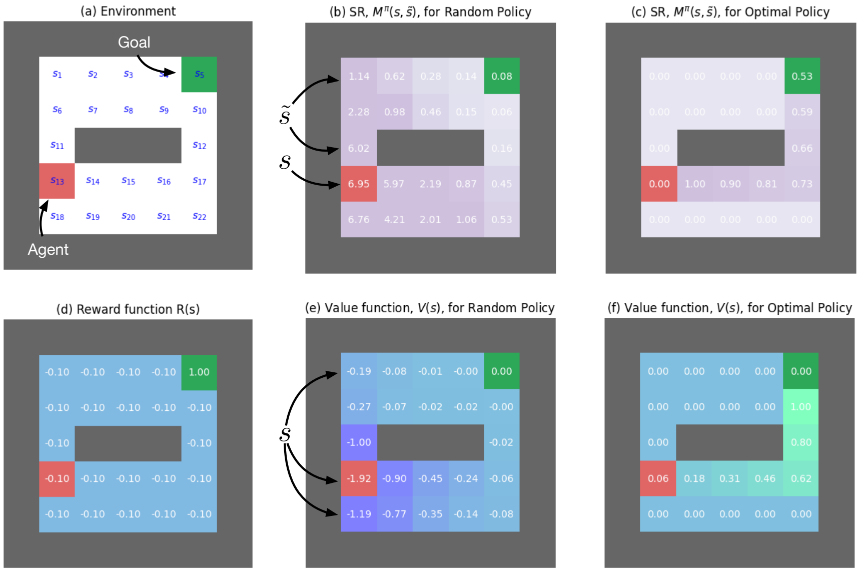


*Figure 4.8: Illustration of successor representation for the 2d maze environment shown in (a) with reward shown in (d), which assigns all states a reward of -0.1 except for the goal state which has a reward of 1.0. In (b-c) we show the SRs for a random policy and the optimal policy. In (e-f) we show the corresponding value functons. In (b), we see that the SR under the random policy assigns high state occupancy values to states which are close (in Manhattan distance) to the current state $s_{13}$ (e.g., $M^\pi(s_{13}, s_{14}) = 5.97$) and low values to states that are further away (e.g., $M^\pi(s_{13}, s_{12}) = 0.16$). In (c), we see that the SR under the optimal policy assigns high state occupancy values to states which are close to the optimal path to the goal (e.g., $M^\pi(s_{13}, s_{14}) = 1.0$) and which fade with distance from the current state along that path (e.g., $M^\pi(s_{13}, s_{12}) = 0.66$). From Figure 3 of [Car+24]. Used with kind permission of Wilka Carvalho. Generated by https://github.com/wcarvalho/jaxneurorl/blob/main/successor_representation.ipynb.*

Hence we can learn an SR using a TD update of the form

$$M^\pi(s, \tilde{s}) \leftarrow M^\pi(s, \tilde{s}) + \eta \underbrace{\left(\mathbb{I}\left(s' = \tilde{s}\right) + \gamma M^\pi(s', \tilde{s}) - M^\pi(s, \tilde{s})\right)}_{\delta} \tag{4.44}$$

where $s'$ is the next state sampled from $T(s'|s, a)$. Compare this to the value-function TD update in Equation (2.16):

$$V^\pi(s) \leftarrow V^\pi(s) + \eta \underbrace{\left(R(s') + \gamma V^\pi(s') - V^\pi(s)\right)}_{\delta} \tag{4.45}$$

However, with an SR, we can easily compute the value function for any reward function (given a fixed policy) as follows:

$$V^{R,\pi} = \sum_{\tilde{s}} M^\pi(s, \tilde{s}) R(\tilde{s}) \tag{4.46}$$

See Figure 4.8 for an example.

We can also make a version of SR that depends on the action as well as the state to get

$$M^\pi(s, a, \tilde{s}) = \mathbb{E}\left[\sum_{t=0}^{\infty} \gamma^t \mathbb{I}\left(s_{t+1} = \tilde{s}\right) | s_0 = s, a_0 = a, a_{1:\infty} \sim \pi\right] \tag{4.47}$$

$$= \mathbb{E}\left[\mathbb{I}\left(s' = \tilde{s}\right) + \gamma M^\pi(s', a, \tilde{s}) | s_0 = s, a_0 = a, a_{1:\infty} \sim \pi\right] \tag{4.48}$$

This gives rise to a TD update of the form

$$M^\pi(s, a, \tilde{s}) \leftarrow M^\pi(s, a, \tilde{s}) + \eta \underbrace{\left(\mathbb{I}\left(s' = \tilde{s}\right) + \gamma M^\pi(s', a', \tilde{s}) - M^\pi(s, a, \tilde{s})\right)}_{\delta} \tag{4.49}$$

where $s'$ is the next state sampled from $T(s'|s,a)$ and $a'$ is the next action sampled from $\pi(s')$. Compare this to the (on-policy) SARSA update from Equation (2.28):

$$Q^\pi(s,a) \leftarrow Q^\pi(s,a) + \eta \underbrace{(R(s') + \gamma Q^\pi(s',a') - Q^\pi(s,a))}_{\delta} \tag{4.50}$$

However, from an SR, we can compute the state-action value function for any reward function:

$$Q^{R,\pi}(s,a) = \sum_{\tilde{s}} M^\pi(s,a,\tilde{s}) R(\tilde{s}) \tag{4.51}$$

This can be used to improve the policy as we discuss in Section 4.5.4.1.

We see that the SR representation has the computational advantages of model-free RL (no need to do explicit planning or rollouts in order to compute the optimal action), but also the flexibility of model-based RL (we can easily change the reward function without having to learn a new value function). This latter property makes SR particularly well suited to problems that use intrinsic reward (see Section 7.3), which often changes depending on the information state of the agent.

Unfortunately, the SR is limited in two key ways: (1) it assumes a finite, discrete state space; (2) it depends on a given policy. We discuss ways to overcome limitation 1 in Section 4.5.3, and limitation 2 in Section 4.5.4.1.

### 4.5.3 Successor models

In this section, we discuss the **successor model** (also called a $\gamma$-model), which is a probabilistic extension of SR [JML20; Eys+21]. This allows us to generalize SR to work with continuous states and actions, and to simulate future state trajectories. The approach is to define the cumulant as the $k$-step conditional distribution $C(s_{k+1}) = P(s_{k+1} = \tilde{s}|s_0 = s, \pi)$, which is the probability of being in state $\tilde{s}$ after following $\pi$ for $k$ steps starting from state $s$. (Compare this to the SR cumulant, which is $C(s_{k+1}) = \mathbb{I}(s_{k+1} = \tilde{s})$.) The SM is then defined as

$$\boldsymbol{\mu}^\pi(\tilde{s}|s) = (1-\gamma) \sum_{t=0}^{\infty} \gamma^t P(s_{t+1} = \tilde{s}|s_0 = s) \tag{4.52}$$

where the $1-\gamma$ term ensures that $\boldsymbol{\mu}^\pi$ integrates to 1. (Recall that $\sum_{t=0}^{\infty} \gamma^t = \frac{1}{1-\gamma}$ for $\gamma < 1$.) In the tabular setting, the SM is just the normalized SR, since

$$\begin{aligned}
\boldsymbol{\mu}^\pi(\tilde{s}|s) &= (1-\gamma) M^\pi(s,\tilde{s}) && (4.53)\\
&= (1-\gamma)\mathbb{E}\left[\sum_{t=0}^{\infty} \gamma^t \mathbb{I}(s_{t+1} = \tilde{s}) \,|s_0 = s, a_{0:\infty} \sim \pi\right] && (4.54)\\
&= (1-\gamma) \sum_{t=0}^{\infty} \gamma^t P(s_{t+1} = \tilde{s}|s_0 = s, \pi) && (4.55)
\end{aligned}$$

Thus $\boldsymbol{\mu}^\pi(\tilde{s}|s)$ tells us the probability that $\tilde{s}$ can be reached from $s$ within a horizon determined by $\gamma$ when following $\pi$, even though we don't know exactly when we will reach $\tilde{s}$.

SMs obey a Bellman-like recursion

$$\boldsymbol{\mu}^\pi(\tilde{s}|s) = \mathbb{E}\left[(1-\gamma)T(\tilde{s}|s,a) + \gamma \boldsymbol{\mu}^\pi(\tilde{s}|s')\right] \tag{4.56}$$

We can use this to perform policy evaluation by computing

$$V^\pi(s) = \frac{1}{1-\gamma} \mathbb{E}_{\boldsymbol{\mu}^\pi(\tilde{s}|s)}\left[R(\tilde{s})\right] \tag{4.57}$$

We can also define an action-conditioned SM

$$\boldsymbol{\mu}^\pi(\tilde{s}|s,a) = (1-\gamma)\sum_{t=0}^{\infty}\gamma^t P(s_{t+1}=\tilde{s}|s_0=s, a_0=a) \tag{4.58}$$

$$= (1-\gamma)T(\tilde{s}|s,a) + \gamma\mathbb{E}\left[\boldsymbol{\mu}^\pi(\tilde{s}|s',a',\pi)\right] \tag{4.59}$$

Hence we can learn an SM using a TD update of the form

$$\boldsymbol{\mu}^\pi(\tilde{s}|s,a) \leftarrow \boldsymbol{\mu}^\pi(\tilde{s}|s,a) + \eta\underbrace{\left((1-\gamma)T(s'|s,a) + \gamma\boldsymbol{\mu}^\pi(\tilde{s}|s',a') - \boldsymbol{\mu}^\pi(\tilde{s}|s,a)\right)}_{\delta} \tag{4.60}$$

where $s'$ is the next state sampled from $T(s'|s,a)$ and $a'$ is the next action sampled from $\pi(s')$. With an SM, we can compute the state-action value for any reward:

$$Q^{R,\pi}(s,a) = \frac{1}{1-\gamma}\mathbb{E}_{\boldsymbol{\mu}^\pi(\tilde{s}|s,a)}\left[R(\tilde{s})\right] \tag{4.61}$$

This can be used to improve the policy as we discuss in Section 4.5.4.1.

#### 4.5.3.1 Learning SMs

Although we can learn SMs using the TD update in Equation (4.60), this requires evaluating $T(s'|s,a)$ to compute the target update $\delta$, and this one-step transition model is typically unknown. Instead, since $\boldsymbol{\mu}^\pi$ is a conditional density model, we will optimize the cross-entropy TD loss [JML20], defined as follows

$$\mathcal{L}_\mu = \mathbb{E}_{(s,a)\sim p(s,a),\tilde{s}\sim(T^\pi\boldsymbol{\mu}^\pi)(\cdot|s,a)}\left[\log\boldsymbol{\mu}_{\boldsymbol{\theta}}(\tilde{s}|s,a)\right] \tag{4.62}$$

where $(T^\pi\boldsymbol{\mu}^\pi)(\cdot|s,a)$ is the Bellman operator applied to $\boldsymbol{\mu}^\pi$ and then evaluated at $(s,a)$, i.e.,

$$(T^\pi\boldsymbol{\mu}^\pi)(\tilde{s}|s,a) = (1-\gamma)T(s'|s,a) + \gamma\sum_{s'}T(\tilde{s}|s,a)\sum_{a'}\pi(a'|s')\boldsymbol{\mu}^\pi(\tilde{s}|s',a') \tag{4.63}$$

We can sample from this as follows: first sample $s' \sim T(s'|s,a)$ from the environment (or an offline replay buffer), and then with probability $1-\gamma$ set $\tilde{s} = s'$ and terminate. Otherwise sample $a' \sim \pi(a'|s')$ and then create a bootstrap sample from the SM using $\tilde{s} \sim \boldsymbol{\mu}^\pi(\tilde{s}|s',a')$.

There are many possible density models we can use for $\boldsymbol{\mu}^\pi$. In [Tha+22], they use a VAE. In [Tom+24], they use an autoregressive transformer applied to a set of discrete latent tokens, which are learned using VQ-VAE or a non-reconstructive self-supervised loss. They call their method **Video Occcupancy Models**.

An alternative approach to learning SMs, that avoids fitting a normalized density model over states, is to use contrastive learning to estimate how likely $\tilde{s}$ is to occur after some number of steps, given $(s,a)$, compared to some randomly sampled negative state [ESL21; ZSE24]. Although we can't sample from the resulting learned model (we can only use it for evaluation), we can use it to improve a policy that achieves a target state (an approach known as goal-conditioned policy learning, discussed in Section 7.4.1).

#### 4.5.3.2 Jumpy models using geometric policy composition

In [Tha+22], they propose **geometric policy composition** or GPC as a way to learn a new policy by sequencing together a set of $N$ policies, as opposed to taking $N$ primitive actions in a row. This can be thought of as a **jumpy model**, since it predicts multiple steps into the future, instead of one step at a time (c.f., [Zha+23a]).

In more detail, in GPC, the agent picks a sequence of $n$ policies $\pi_i$ for $i = 1:n$, and then samples states according to their corresponding SMs: starting with $(s_0, a_0)$, we sample $s_1 \sim \boldsymbol{\mu}_\gamma^{\pi_1}(\cdot|s_0,a_0)$, then $a_1 \sim \pi_1(\cdot|s_1)$, then $s_2 \sim \boldsymbol{\mu}_\gamma^{\pi_2}(\cdot|s_1,a_1)$, etc. This continues for $n-1$ steps. Finally we sample $s_n \sim \boldsymbol{\mu}_{\gamma'}^{\pi_n}(\cdot|s_{n-1},a_{n-1})$, where $\gamma' > \gamma$ represents a longer horizon SM. The reward estimates computed along this sampled path can then be combined to compute the value of each candidate policy sequence.

### 4.5.4 Successor features

Both SRs and SMs require defining expectations or distributions over the entire future state vector, which can be problematic in high dimensional spaces. In [Bar+17] they introduced **successor features**, that generalize SRs by working with features $\boldsymbol{\phi}(s)$ instead of primitive states. In particular, if we define the cumulant to be $C(s_{t+1}) = \boldsymbol{\phi}(s_{t+1})$, we get the following definition of SF:

$$\boldsymbol{\psi}^{\pi,\boldsymbol{\phi}}(s) = \mathbb{E}\left[\sum_{t=0}^{\infty} \gamma^t \boldsymbol{\phi}(s_{t+1}) | s_0 = s, a_{0:\infty} \sim \pi\right] \tag{4.64}$$

We will henceforth drop the $\boldsymbol{\phi}$ superscript from the notation, for brevity. SFs obey a Bellman equation

$$\boldsymbol{\psi}(s) = \mathbb{E}\left[\boldsymbol{\phi}(s') + \gamma \boldsymbol{\psi}(s')\right] \tag{4.65}$$

If we assume the reward function can be written as

$$R(s, \boldsymbol{w}) = \boldsymbol{\phi}(s)^{\mathsf{T}} \boldsymbol{w} \tag{4.66}$$

then we can derive the value function for any reward as follows:

$$\begin{aligned} V^{\pi,\boldsymbol{w}}(s) &= \mathbb{E}\left[R(s_1) + \gamma R(s_2) + \cdots | s_0 = s\right] &(4.67)\\ &= \mathbb{E}\left[\boldsymbol{\phi}(s_1)^{\mathsf{T}} \boldsymbol{w} + \gamma \boldsymbol{\phi}(s_2)^{\mathsf{T}} \boldsymbol{w} + \cdots | s_0 = s\right] &(4.68)\\ &= \mathbb{E}\left[\sum_{t=0}^{\infty} \gamma^t \boldsymbol{\phi}(s_{t+1}) | s_0 = s\right]^{\mathsf{T}} \boldsymbol{w} = \boldsymbol{\psi}^{\pi}(s)^{\mathsf{T}} \boldsymbol{w} &(4.69) \end{aligned}$$

Similarly we can define an action-conditioned version of SF as

$$\begin{aligned} \boldsymbol{\psi}^{\pi,\boldsymbol{\phi}}(s,a) &= \mathbb{E}\left[\sum_{t=0}^{\infty} \gamma^t \boldsymbol{\phi}(s_{t+1}) | s_0 = s, a_0 = a, a_{1:\infty} \sim \pi\right] &(4.70)\\ &= \mathbb{E}\left[\boldsymbol{\phi}(s') + \gamma \boldsymbol{\psi}(s', a')\right] &(4.71) \end{aligned}$$

We can learn this using a TD rule

$$\boldsymbol{\psi}^{\pi}(s,a) \leftarrow \boldsymbol{\psi}^{\pi}(s,a) + \eta \underbrace{\left(\boldsymbol{\phi}(s') + \gamma \boldsymbol{\psi}^{\pi}(s',a') - \boldsymbol{\psi}^{\pi}(s,a)\right)}_{\delta} \tag{4.72}$$

And we can use it to derive a state-action value function:

$$Q^{\pi,\boldsymbol{w}}(s) = \boldsymbol{\psi}^{\pi}(s,a)^{\mathsf{T}} \boldsymbol{w} \tag{4.73}$$

This allows us to define multiple $Q$ functions (and hence policies) just by changing the weight vector $\boldsymbol{w}$, as we discuss in Section 4.5.4.1.

#### 4.5.4.1 Generalized policy improvement

So far, we have discussed how to compute the value function for a new reward function but using the SFs from an existing known policy. In this section we discuss how to create a new policy that is better than an existing set of policies, by using **Generalized Policy Improvement** or **GPI** [Bar+17; Bar+20].

Suppose we have learned a set of $N$ (potentially optimal) policies $\pi_i$ and their corresponding SFs $\boldsymbol{\psi}^{\pi_i}$ for maximizing rewards defined by $\boldsymbol{w}_i$. When presented with a new task $\boldsymbol{w}_{\text{new}}$, we can compute a new policy using GPI as follows:

$$a^*(s; \boldsymbol{w}_{\text{new}}) = \underset{a}{\operatorname{argmax}} \max_i Q^{\pi_i}(s, a, \boldsymbol{w}_{\text{new}}) = \underset{a}{\operatorname{argmax}} \max_i \boldsymbol{\psi}^{\pi_i}(s,a)^{\mathsf{T}} \boldsymbol{w}_{\text{new}} \tag{4.74}$$

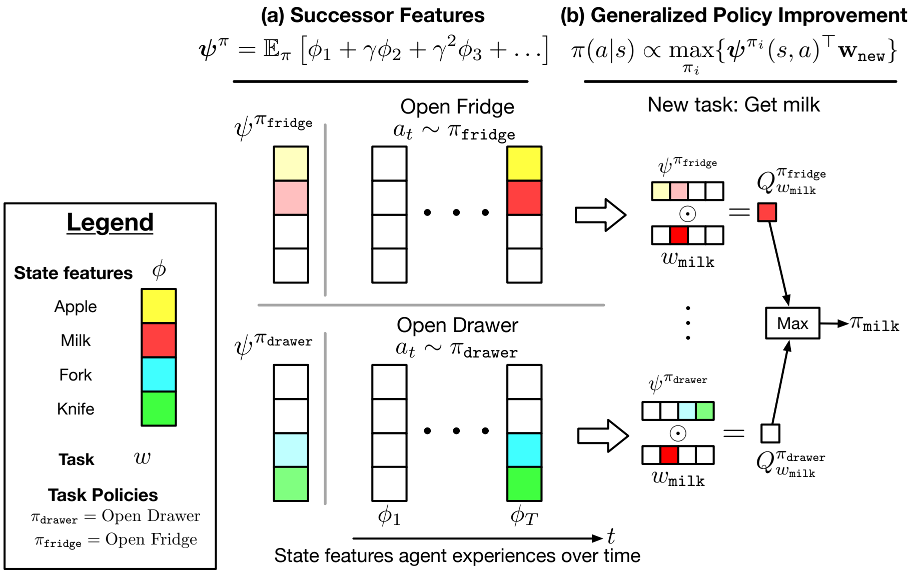

(a) Successor Features
$\boldsymbol{\psi}^{\pi} = \mathbb{E}_{\pi}\left[\phi_1 + \gamma\phi_2 + \gamma^2\phi_3 + \dots\right]$
(b) Generalized Policy Improvement
$\pi(a|s) \propto \max_{\pi_i}\{\boldsymbol{\psi}^{\pi_i}(s,a)^{\top}\mathbf{w}_{\texttt{new}}\}$
New task: Get milk
$\psi^{\pi_{\texttt{fridge}}}$
Open Fridge
$a_t \sim \pi_{\texttt{fridge}}$
$\psi^{\pi_{\texttt{fridge}}}$
$\odot$
$w_{\texttt{milk}}$
$=$
$Q^{\pi_{\texttt{fridge}}}_{w_{\texttt{milk}}}$
Max
$\pi_{\texttt{milk}}$
Legend
State features $\phi$
Apple
Milk
Fork
Knife
Task $w$
Task Policies
$\pi_{\texttt{drawer}}$ = Open Drawer
$\pi_{\texttt{fridge}}$ = Open Fridge
$\psi^{\pi_{\texttt{drawer}}}$
Open Drawer
$a_t \sim \pi_{\texttt{drawer}}$
$\psi^{\pi_{\texttt{drawer}}}$
$\odot$
$w_{\texttt{milk}}$
$=$
$Q^{\pi_{\texttt{drawer}}}_{w_{\texttt{milk}}}$
$\phi_1$
$\phi_T$
$t$
State features agent experiences over time

*Figure 4.9: Illustration of successor features representation. (a) Here $\boldsymbol{\phi}_t = \boldsymbol{\phi}(s_t)$ is the vector of features for the state at time t, and $\boldsymbol{\psi}^{\pi}$ is the corresponding SF representation, which depends on the policy $\pi$. (b) Given a set of existing policies and their SFs, we can create a new one by specifying a desired weight vector $\boldsymbol{w}_{new}$ and taking a weighted combination of the existing SFs. From Figure 5 of [Car+24]. Used with kind permission of Wilka Carvalho.*

If $\boldsymbol{w}_{\text{new}}$ is in the span of the training tasks (i.e., there exist weights $\alpha_i$ such that $\boldsymbol{w}_{\text{new}} = \sum_i \alpha_i \boldsymbol{w}_i$), then the GPI theorem states that $\pi(a|s) = \mathbb{I}\left(a = a^*(s, \boldsymbol{w}_{\text{new}})\right)$ will perform at least as well as any of the existing policies, i.e., $Q^{\pi}(s,a) \geq \max_i Q^{\pi_i}(s,a)$ (c.f., policy improvement in Section 3.4). See Figure 4.9 for an illustration.

Note that GPI is a model-free approach to computing a new policy, based on an existing library of policies. In [Ale+23], they propose an extension that can also leverage a (possibly approximate) world model to learn better policies that can outperform the library of existing policies by performing more decision-time search.

### 4.5.4.2 Option keyboard

One limitation of GPI is that it requires that the reward function, and the resulting policy, be defined in terms of a fixed weight vector $\boldsymbol{w}_{\text{new}}$, where the preference over features is constant over time. However, for some tasks we might want to initially avoid a feature or state and then later move towards it. To solve this, [Bar+19; Bar+20] introduced the **option keyboard**, in which the weight vector for a task can be computed dynamically in a state-dependent way, using $\boldsymbol{w}_s = g(s, \boldsymbol{w}_{\text{new}})$. (Options are discussed in Section 7.4.2.) Actions can then be chosen as follows:

$$a^*(s; \boldsymbol{w}_{\text{new}}) = \underset{a}{\text{argmax}} \max_i \boldsymbol{\psi}^{\pi_i}(s,a)^{\mathsf{T}} \boldsymbol{w}_s \tag{4.75}$$

Thus $\boldsymbol{w}_s$ induces a set of policies that are active for a period of time, similar to playing a chord on a piano.

### 4.5.4.3 Learning SFs

A key question when using SFs is how to learn the cumulants or state-features $\boldsymbol{\phi}(s)$. Various approaches have been suggested, including leveraging meta-gradients [Vee+19], image reconstruction [Mac+18b], and maximizing the mutual information between task encodings and the cumulants that an agent experiences when pursuing that task [Han+19]. The cumulants are encouraged to satisfy the linear reward constraint by minimizing

$$\mathcal{L}_r = ||r - \boldsymbol{\phi}_{\boldsymbol{\theta}}(s)^{\mathsf{T}} \boldsymbol{w}||_2^2 \tag{4.76}$$

Once the cumulant function is known, we have to learn the corresponding SF. The standard approach learns a different SF for every policy, which is limiting. In [Bor+19] they introduced **Universal Successor Feature Approximators** which takes an input a policy encoding $\boldsymbol{z}_{\boldsymbol{w}}$, representing a policy $\pi_{\boldsymbol{w}}$ (typically we set $\boldsymbol{z}_{\boldsymbol{w}} = \boldsymbol{w}$). We then define

$$\boldsymbol{\psi}^{\pi_{\boldsymbol{w}}}(s,a) = \boldsymbol{\psi}_{\boldsymbol{\theta}}(s,a,\boldsymbol{z}_{\boldsymbol{w}}) \tag{4.77}$$

The GPI update then becomes

$$a^*(s;\boldsymbol{w}_{\text{new}}) = \operatorname*{argmax}_a \max_{\boldsymbol{z}_{\boldsymbol{w}}} \boldsymbol{\psi}_{\boldsymbol{\theta}}(s,a,\boldsymbol{z}_{\boldsymbol{w}})^\mathsf{T}\boldsymbol{w}_{\text{new}} \tag{4.78}$$

so we replace the discrete over a finite number of policies, $\max_i$, with a continuous optimization problem $\max_{z_w}$, to be solved per state.

If we want to learn the policies and SFs at the same time, we can optimize the following losses in parallel:

$$\mathcal{L}_Q = ||\boldsymbol{\psi}_{\boldsymbol{\theta}}(s,a,\boldsymbol{z}_w)^\mathsf{T}\boldsymbol{w} - \boldsymbol{y}_Q||, \ \boldsymbol{y}_Q = R(s';\boldsymbol{w}) + \gamma\boldsymbol{\psi}_{\boldsymbol{\theta}}(s',a^*,\boldsymbol{z}_w)^\mathsf{T}\boldsymbol{w} \tag{4.79}$$

$$\mathcal{L}_{\boldsymbol{\psi}} = ||\boldsymbol{\psi}_{\boldsymbol{\theta}}(s,a,\boldsymbol{z}_{\boldsymbol{w}}) - \boldsymbol{y}_{\boldsymbol{\psi}}||, \ \boldsymbol{y}_{\boldsymbol{\psi}} = \boldsymbol{\phi}(s') + \gamma\boldsymbol{\psi}_{\boldsymbol{\theta}}(s',a^*,\boldsymbol{z}_{\boldsymbol{w}}) \tag{4.80}$$

where $a^* = \operatorname{argmax}_{a'} \boldsymbol{\psi}_{\boldsymbol{\theta}}(s',a',\boldsymbol{z}_{\boldsymbol{w}})^\mathsf{T}\boldsymbol{w}$. The first equation is standard Q learning loss, and the second is the TD update rule in Equation (4.72) for the SF. In [Car+23], they present the **Successor Features Keyboard**, that can learn the policy, the SFs and the task encoding $\boldsymbol{z}_{\boldsymbol{w}}$, all simultaneously. They also suggest replacing the squared error regression loss in Equation (4.79) with a cross-entropy loss, where each dimension of the SF is now a discrete probability distribution over $M$ possible values of the corresponding feature. (c.f. Section 7.2.2).

#### 4.5.4.4 Choosing the tasks

A key advantage of SFs is that they provide a way to compute a value function and policy for any given reward, as specified by a task-specific weight vector $\boldsymbol{w}$. But how do we choose these tasks? In [Han+19] they sample $\boldsymbol{w}$ from a distribution at the start of each task, to encourage the agent to learn to explore different parts of the state space (as specified by the feature function $\boldsymbol{\phi}$). In [LA21] they extend this by adding an intrinsic reward that favors exploring parts of the state space that are surprising (i.e., which induce high entropy), c.f., Section 7.3. In [Far+23], they introduce **proto-value networks**, which is a way to define auxiliary tasks based on successor measures.

### 4.5.5 Forwards-backwards representations: TODO

[TO21; TRO23]

# Chapter 5

# Multi-agent RL

In this section, we give a brief introduction to **multi-agent RL** or **MARL**. Our presentation is based on [ACS24]. MARL is closely related to game theory (see e.g. [LBS08]) and multi-agent systems design (see e.g. [SLB08]), as we will see. For other surveys on MARL, see e.g. [YW20; Won+22; GD22].

## 5.1 Types of games

Multi-agent environments are often called **games**, even if they represent "real-world" problems such as multi-robot coordination (e.g., a fleet of autonomous vehicles) or agent-based trading. In this section, we discuss different kinds of games that have been proposed, summarized in Figure 5.1.

In the **game theory** community, the rules of the game (i.e., dynamics and reward function of the environment) are usually assumed known, and the focus is on computing **strategies** (i.e., policies) for each **player** (i.e., agent), whereas in MARL, we usually assume the environment is unknown and the agents have to learn just by interacting with it. (This is analogous to the distinction between DP methods, that assume a known MDP, and RL methods, that just assume sample-based access to the MDP.)

### 5.1.1 Normal-form games

A **normal-form game** defines a single interaction between $n \geq 2$ agents. In particular, we have a finite set of agents $\mathcal{I} = \{1, \ldots, n\}$ (we assume that $n$ is fixed). For each agent $i \in \mathcal{I}$ we have a finite set of actions $\mathcal{A}_i$ and a reward function $\mathcal{R}_i : \mathcal{A}_{1:n} \rightarrow \mathbb{R}$, where $\mathcal{A}_{1:n} = \mathcal{A}_1 \times \cdots \times \mathcal{A}_n$. A single round of the game proceeds

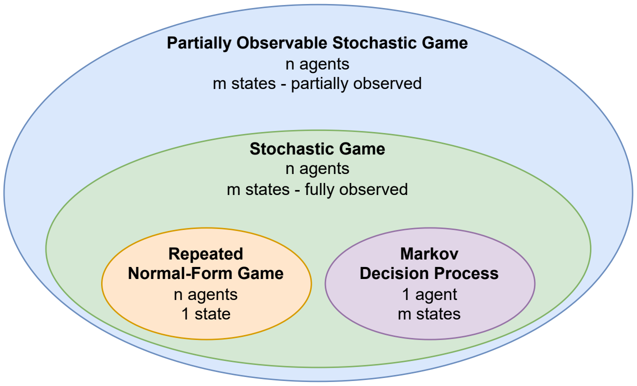


*Figure 5.1: Hierarchy of games. From Fig 3.1 of [ACS24]. Used with kind permission of Stefano Albrecht.*

as follows. Each agent samples an action $a_i \in \mathcal{A}_i$ with probability $\pi_i(a_i)$, then the resulting **joint action** $\boldsymbol{a} = (a_1, \ldots, a_n)$ is taken and the reward $\boldsymbol{r} = (r_1, \ldots, r_m)$ is given to each player, where $r_i = \mathcal{R}_i(\boldsymbol{a})$.

Games can be classified based on the type of rewards they contain. In **zero-sum games**, we have $\sum_i \mathcal{R}_i(\boldsymbol{a}) = 0$ for all $\boldsymbol{a}$. (For a two-player zero-sum game, we must have $R_1(\boldsymbol{a}) = -R_2(\boldsymbol{a})$.) In **common-reward games**, we have $\mathcal{R}_i(\boldsymbol{a}) = \mathcal{R}_j(\boldsymbol{a})$ for all $\boldsymbol{a}$. And in **general-sum games**, there are no restrictions on the rewards.

In zero-sum games, the agents must compete against each other, whereas in common-reward games, the agents generally must cooperate (although they may compete with each other over a shared resource). In general-sum games, there can be a mix of cooperation and competition. Although common-reward games can be easier to solve than general-sum games, it can be challenging to disentangle the contribution of each agent to the shared reward (this is a multi-agent version of the **credit assignment** problem), and coordinating actions across agents can also be difficult.

Normal-form games with 2 agents are called **matrix games** because they can be defined by a 2d reward matrix. We give some well-known examples in Table 5.1.

- In **rock-paper-scissors**, rock can blunt scissors, paper can cover rock, and scissors can cut paper; from these constraints, we can determine which player wins or loses. This is a zero-sum game.
- In the **coordination game**, players only achieve positive reward if they play the same action; this is a common-reward game.
- In the **Prisoner's dilemma**, which is a general-sum game, the players (who are prisoners being interogated independently in different cells) can either cooperate with each other (by both "staying mum", i.e., denying they committed the crime), or one can defect on the other (by claiming the other person committed the crime). If they both cooperate, they only have to serve 1 year in jail each, based on weak evidence. If they both defect, they each serve 3 years. But if the row player cooperates (stays silent) and the column player defects (implicates his partner), the row player gets 5 years and the column player gets out of jail free. This leads to an incentive for both players to defect, even though they would be better off if they both cooperated. We discuss this more in Section 5.2.3.

|   | R | P | S |
|---|---|---|---|
| R | 0,0 | -1,1 | 1,-1 |
| P | 1,-1 | 0,0 | -1,1 |
| S | -1,1 | 1,-1 | 0,0 |

*(a) Rock-Paper-Scissors*

|   | A | B |
|---|---|---|
| A | 10 | 0 |
| B | 0 | 10 |

*(b) Coordination Game*

|   | C | D |
|---|---|---|
| C | -1,-1 | -5,0 |
| D | 0,5 | -3,-3 |

*(c) Prisoner's Dilemma*

*Table 5.1: Three different matrix games.*

Suppose we consider matrix games with just 2 actions each. In this case, we can represent the game as follows:

$$\begin{pmatrix} a_{11}, b_{11} & a_{12}, b_{12} \\ a_{21}, b_{21} & a_{22}, b_{22} \end{pmatrix} \tag{5.1}$$

where $a_{ij}$ is the reward to player 1 (row player) and $b_{ij}$ is the reward to player 2 (column player) if player 1 picks action $i$ and player 2 picks action $j$. Suppose we further restrict attention to strictly ordinal games, meaning that each agent ranks the 4 possible outcomes from 1 (least preferred) to 4 (most preferred)). In this case, there are 78 structurally distinct games [RG66]. These can be grouped into two main kinds. In **no-conflict games**, both players have the same set of most preferred outcomes, whereas in **conflict games**, the players disagree about what is best. If we consider general ordinal $2 \times 2$ games (where one or both players may have equal preference for two or more outcomes), we find that there are 726 of them [KF88].

A **repeated matrix game** is the multi-agent analog of a multi-armed bandit problem, discussed in Section 1.2.4. In this case, the policy has the form $\pi_i(a_t^i|\boldsymbol{h}_t)$, where $\boldsymbol{h}_t = (\boldsymbol{a}_0, \ldots, \boldsymbol{a}_{t-1})$ is the history of joint-actions. In some cases, the agent may choose to ignore the history, or only look at the last $n$ joint actions. For example, in the **tit-for-tat** strategy in the prisoner's dilemma, the policy for agent $i$ at step $t$ is to do the same action that agent $-i$ did at step $t-1$ (where $-i$ means the agent other than $i$), so the policy is conditioned on $\boldsymbol{a}_{t-1}$. (Note that this strategy will punish players who defect, and can lead to the evolution of cooperative behavior, even in selfish agents [AH81; Axe84].)

### 5.1.2 Stochastic games

A **stochastic game** is a multi-agent version of an MDP. It is defined by a finite set of agents $\mathcal{I} = \{1, \ldots, n\}$; a finite set of states $\mathcal{S}$, of which a subset $\overline{S} \subset \mathcal{S}$ are terminal; a finite action set $\mathcal{A}_i$ for each agent $i \in \mathcal{I}$; a reward function $\mathcal{R}_i(s, a, s')$ for each agent $i \in \mathcal{I}$[1]; a state transition distribution $\mathcal{T}(s_{t+1}|s_{1:t}, \boldsymbol{a}_t) \in [0,1]$; and an initial state distribution $\mu(s_0) \in [0,1]$. Typically the transition distribution is Markovian (i.e., $\mathcal{T}(s_{t+1}|s_{1:t}, \boldsymbol{a}_t) = \mathcal{T}(s_{t+1}|s_t, \boldsymbol{a}_t)$, in which case this is called a **Markov game**.) See Figure 5.2 for an example.

The policy for each agent in such a game has the form $\pi_i(a_t^i|\boldsymbol{h}_t)$ where $\boldsymbol{h}_t = (s_0, \boldsymbol{a}_1, \ldots, s_t)$ is the state-action history. (We omit rewards from the definition of history for notational simplicity.) The overal **joint policy** is denoted by $\boldsymbol{\pi} = (\pi_1, \ldots, \pi_n)$; if the agents make their decisions independently (which we assume), then this has the form

$$\boldsymbol{\pi}(\boldsymbol{a}_t|\boldsymbol{h}_t) = \prod_i \pi_i(a_t^i|\boldsymbol{h}_t) \tag{5.2}$$

Often we assume the policies are Markovian, in which case they can be written as $\pi_i(a_t^i|s_t)$.

Note that, from the perspective of each agent $i$, the environment transition function has the form

$$\mathcal{T}_i(s_{t+1}|s_t, a_t^i) = \sum_{\boldsymbol{a}_t^{-i}} \mathcal{T}(s_{t+1}|s_t, (a_t^i, \boldsymbol{a}_t^{-i})) \prod_{j \neq i} \pi_j(a_t^j|s_t) \tag{5.3}$$

Thus $\mathcal{T}_i$ depends on the policies of the other players, which are often changing, which makes these local/agent-centric transition matrices non-stationary, even if the underlying environment is stationary. Typically agent $i$ does not know the policies of the other agents $j$, so it has to learn them (as we discuss in Section 5.4.2), or it can just treat the other agents as part of the environment (i.e., as another source of unmodeled "noise") and then use single agent RL methods (see Section 5.3.2).

### 5.1.3 Partially observed stochastic games (POSG)

A **Partially Observed Stochastic Game** or **POSG** is a multi-agent version of a POMDP. We augment the stochastic game with the observation distributions $\mathcal{O}_i(o_{t+1}^i|s_{t+1}, \boldsymbol{a}_t) \in [0,1]$ for each agent $i$. (Alternatively, the $i$'th observation distribution may just depend on $i$'s actions.) Let $\boldsymbol{o}_t = (o_t^1, \ldots, o_t^n)$ be the **joint observation** generated by the product distribution $\mathcal{O}_{1:n}(\boldsymbol{o}_t|s_t, \boldsymbol{a}_{t-1})$. The policy for each agent in such a game has the form $\pi_i(a_t^i|\boldsymbol{h}_t^i)$ where $\boldsymbol{h}_t^i = (o_0^i, a_0^i, o_1^i, \ldots, o_t^i)$ is the observation history for agent $i$. (Note that the environment decides what is included in each observation; for example, it may or may not contain information about the other agent's actions.) Note that a **Decentralized POMDP** or **Dec-POMDP** is a special case of a POMDP where the reward function is the same for all agents (thus it can only capture cooperative behavior).

The data generating process for a POSG proceeds as follows. First the environment samples an initial state from $\mu(s_0)$ and generates an initial observation from $\mathcal{O}_{1:n}^0(\boldsymbol{o}_0|s_0)$. Then for $t = 0, 1, \ldots$, we repeat the folowing

[1] Here $R(s, a, s')$ is the reward we receive if we take action $a$ in state $s$ and end up in $s'$. As explained in [ACS24, Sec 2.8], we can convert from $R(s, a, s')$ to the more common $R(s, a)$ notation, representing the expected reward, by noting that $R(s, a) = \sum_{s'} \mathcal{T}(s'|s, a) R(s, a, s')$.

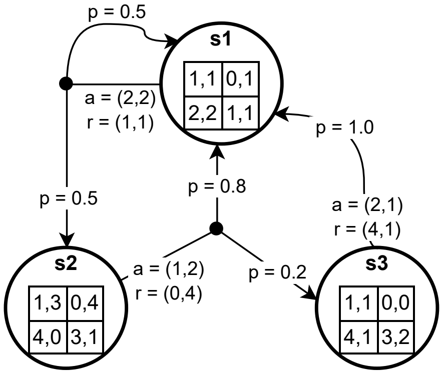


*Figure 5.2: Example of a two-player general-sum stochastic game. Circles represent the states, inside of which we show the reward function in matrix form. Only one of the 4 possible transitions out of each state are shown. The little black dots are called the* **after states***, and correspond to an intermediate point where a joint action has been decided by the players, but nature hasn't yet sampled the next transition, which occurs with the specified probabilities. From Fig 3.3(b) of [ACS24]. Used with kind permission of Stefano Albrecht.*

1. Each agent generates action from $\pi_i(a_t^i|\boldsymbol{h}_t^i)$
2. Environment generates next state from $\mathcal{T}(s_{t+1}|s_t, \boldsymbol{a}_t)$
3. Environment generates observation from $\mathcal{O}_i(o_{t+1}^i|s_{t+1}, \boldsymbol{a}_t)$ for each $i$.
4. Environment generates reward from $\mathcal{R}_i(s_t, \boldsymbol{a}_t, s_{t+1})$ for each $i$.
5. Each agent updates its history using $\boldsymbol{h}_{t+1}^i = (\boldsymbol{h}_{t-1}^i, a_t^i, o_{t+1}^i)$

From the perspective of agent $i$, it just observes a sequence of observations generated by the following non-Markovian "sensor stream distribution":

$$p_i(o_{t+1}^i|\boldsymbol{h}_t^i, a_t^i) = \sum_{s_{t+1}} \sum_{\boldsymbol{a}_t^{-i}} \hat{\mathcal{O}}_i(o_{t+1}^i|s_{t+1}, \boldsymbol{a}_t) p_i(\boldsymbol{a}_t^{-i}|\boldsymbol{h}_t^i) p_i(s_{t+1}|\boldsymbol{h}_t^i, \boldsymbol{a}_t) \tag{5.4}$$

$$p_i(\boldsymbol{a}_t^{-i}|\boldsymbol{h}_t^i) = \prod_{j \neq i} \hat{\pi}_i^j(a_t^j|\boldsymbol{h}_t^i) \tag{5.5}$$

$$p_i(s_{t+1}|\boldsymbol{h}_t^i, \boldsymbol{a}_t) = \sum_{s_t} \hat{\mathcal{T}}_i(s_{t+1}|s_t, \boldsymbol{a}_t) b_i(s_t|\boldsymbol{h}_t^i) \tag{5.6}$$

where $\hat{\pi}_i^j$ in Equation (5.5) is $i$'s estimate of $j$'s policy, $\hat{\mathcal{T}}_i$ is $i$'s estimate of $\mathcal{T}$ (based on $\boldsymbol{h}_t^i$), $\hat{\mathcal{O}}_i$ is $i$'s estimate of $\mathcal{O}_i$ (based on $\boldsymbol{h}_t^i$), and $b_i(s_t|\boldsymbol{h}_t^i)$ is $i$'s **belief state** (ie., its posterior distributiion over the underlying latent state given its local observation history).

### 5.1.4 Extensive form games (EFG)

In the game theory literature, it is common to use the **extensive form game** representation, Rather than representing a sequence of world states that evolve over time, we represent a tree of possible choices or actions take by each player (and optionally a **chance player**, if the game is stochastic, e.g., backgammon). Each node represents a unique sequence (history) of actions leading up to that point.

In the context of EFGs, some additional terminology is commonly used. If all the nodes are observed (including chance nodes), we say the game has perfect and complete information. If the moves of some players are not visible and/or the state of the game is not fully known (e.g., poker), the game has **imperfect information**. In this case, we define an **information set** as the set of nodes that an agent cannot distinguish between. If an agent does not know the other player's type or payoff function (e.g. in an auction, or playing against players with unknown skill level), then the game has **incomplete information**. In this case, the agent should maintain a Bayesian belief state about the unknown factors.

EFGs and POSGs are closely related, as explained in [Kov+22], although POSGs are arguably simpler and more general. In a POSG, the imperfect information is due to partial observability, and requires estimating a distribution over the latent states $p(s_t|\boldsymbol{h}_t)$; this is analogous to an information set. If the world model $\mathcal{T}(s'|s, \boldsymbol{a}; \boldsymbol{\theta})$ and/or reward functions $\mathcal{R}_i(s, a^i, s'; \boldsymbol{\theta}_i)$ are not known, the agent will also have incomplete information, which requires estimating a distribution over the model parameters $p(\boldsymbol{\theta}|\boldsymbol{h}_t)$, in addition to a distribution over latent states (which we could call a "doubly Bayesian" approach). This is equivalent to a multi-agent version of a Bayes Adaptive POMDP [RCdP07].

## 5.2 Types of solutions

In the multi-agent setting the definition of "optimality" is much more complex than in the single agent setting, as we will see. That is, there are multiple **solution concepts**.

### 5.2.1 Notation and definitions

First we define some notation. Let $\hat{\boldsymbol{h}}_t = \{(s_k, \boldsymbol{o}_k, \boldsymbol{a}_k)_{k=1}^{t-1}, s_t, \boldsymbol{o}_t\}$ be the **full history**, containing all the past states, joint observations, and joint actions. Let $\sigma(\hat{\boldsymbol{h}}_t) = \boldsymbol{h}_t = (\boldsymbol{o}_1, \ldots, \boldsymbol{o}_t)$ be the history of joint observations, and $\sigma_i(\hat{\boldsymbol{h}}_t) = \boldsymbol{h}_t^i = (o_1^i, \ldots, o_t^i)$ be the history of observations for agent $i$. (This typically also includes the actions chosen by agent $i$.)

We define the expected return for agent $i$ under joint policy $\boldsymbol{\pi}$ by

$$U_i(\boldsymbol{\pi}) = \sum_{\hat{\boldsymbol{h}}_t} p(\hat{\boldsymbol{h}}_t|\boldsymbol{\pi}) u_i(\hat{\boldsymbol{h}}_t) \tag{5.7}$$

where the distribution over full histories is given by

$$p(\hat{\boldsymbol{h}}_t|\boldsymbol{\pi}) = \mu(s_0)\mathcal{O}_{1:n}^0(\boldsymbol{o}_0|s_0) \prod_{k=1}^{t-1} \boldsymbol{\pi}(\boldsymbol{a}_k|\hat{\boldsymbol{h}}_k)\mathcal{T}(s_{k+1}|s_k, \boldsymbol{a}_k)\mathcal{O}_{1:n}(\boldsymbol{o}_{k+1}|s_{k+1}, \boldsymbol{a}_k) \tag{5.8}$$

and $u_i(\hat{\boldsymbol{h}}_t)$ is the discounted actual return for agent $i$ in a given full history

$$u_i(\hat{\boldsymbol{h}}_t) = \sum_{k=0}^{t-1} \gamma^k \mathcal{R}_i(s_k, \boldsymbol{a}_k, s_{k+1}) \tag{5.9}$$

We can also derive the following Bellman-like equations:

$$V_i^{\boldsymbol{\pi}}(\hat{\boldsymbol{h}}) = \sum_{\boldsymbol{a}} \boldsymbol{\pi}(\boldsymbol{a}|\sigma(\hat{\boldsymbol{h}}))Q_i^{\boldsymbol{\pi}}(\hat{\boldsymbol{h}}, \boldsymbol{a}) \tag{5.10}$$

$$Q_i^{\boldsymbol{\pi}}(\hat{\boldsymbol{h}}, \boldsymbol{a}) = \sum_{s'} \mathcal{T}(s'|s(\hat{\boldsymbol{h}}), \boldsymbol{a}) \left[\mathcal{R}_u(s(\hat{\boldsymbol{h}}), \boldsymbol{a}, s') + \gamma \sum_{\boldsymbol{o}'} \mathcal{O}_{1:n}(\boldsymbol{o}'|\boldsymbol{a}, s') V_i^{\boldsymbol{\pi}}((\hat{\boldsymbol{h}}, \boldsymbol{a}, s', \boldsymbol{o}'))\right] \tag{5.11}$$

where $s(\hat{\boldsymbol{h}})$ extracts the last state from $\hat{\boldsymbol{h}}$. With this, we can define the expected return using

$$U_i(\boldsymbol{\pi}) = \mathbb{E}_{\mu(s_0)\mathcal{O}_{1:n}^0(\boldsymbol{o}_0|s_0)}\left[V_i^{\pi}((s_0, \boldsymbol{o}_0))\right] \tag{5.12}$$

Finally, We define the **best response** policy for agent $i$ as the one that maximizes the expected return for agent $i$ against a given set of policies for all the other agents, $\boldsymbol{\pi}_{-i} = (\pi_1, \ldots, \pi_{i-1}, \pi_{i+1}, \ldots, \pi_n)$. That is,

$$\mathrm{BR}_i(\boldsymbol{\pi}_{-i}) = \operatorname*{argmax}_{\pi_i} U_i((\pi_i, \boldsymbol{\pi}_{-i})) \tag{5.13}$$

### 5.2.2 Minimax

The **minimax** solution is defined for two-agent zero-sum games. Its existence for normal-form games was first proven by John von Neumann in 1928. We say that joint policy $\boldsymbol{\pi} = (\pi_i, \pi_j)$ is a minimax solution if

$$U_i(\boldsymbol{\pi}) = \max_{\pi_i'} \min_{\pi_j'} U_i(\pi_i', \pi_j') \tag{5.14}$$

$$= \min_{\pi_j'} \max_{\pi_i'} U_i(\pi_i', \pi_j') \tag{5.15}$$

$$= -U_j(\boldsymbol{\pi}) \tag{5.16}$$

In other words, $\boldsymbol{\pi}$ is a minimax solution iff $\pi_i \in \text{BR}_i(\pi_j)$ and $\pi_j \in \text{BR}_j(\pi_i)$. We can solve for the minimax solution using linear programming.

Minimax solutions also exist for two-player zero-sum stochastic games with finite episode lengths, such as chess and Go, although it is computationally intractable to compute exact solutions to these problems.

### 5.2.3 Nash equilibrium

The **Nash equilibrium** generalized the idea of mutual best response to general-sum games with two or more agents. That is, we say that $\boldsymbol{\pi}$ is a Nash equilibrium (NE) if no agent $i$ can improve its expected returns by changing its policy $\pi_i$, assuming the other agents policies remain fixed:

$$\forall, \pi_i'. U_i(\pi_i', \boldsymbol{\pi}_{-i}) \leq U_i(\boldsymbol{\pi}) \tag{5.17}$$

John Nash proved the existence of such a solution for general-sum non-repeated normal form games in 1950.

For example, consider the games shown in Table 5.1. For the rock-paper-scissors, the only NE is the **mixed strategy** (i.e., stochastic policy) where each agent chooses actions uniformly at random, so $\pi_i = (1/3, 1/3, 1/3)$. This yields an expected return of 0. For the coordination game, there are two NEs, corresponding to the **pure strategy** (i.e., deterministic policy) of always playing A (with expected return of 10), or always playing B (with expected return of 10). Finally, for the Prisoner's Dilemma, the only NE is the pure strategy of (D,D), which yields an expected return of (-3,-3). Note that this is worse than the maximum possible expected return, which is (-1,-1) given by the strategy of (C,C). However, such a strategy is not an NE, since each player could improve its return if it unilaterally deviates from it (i.e., defects on its partner). In general, computing Nash equilibria can be computationally expensive.

It is possible to relax the definition of exact inequality by defining an $\epsilon$-Nash equilibrium as a joint policy that satisfies

$$\forall, \pi_i'. U_i(\pi_i', \boldsymbol{\pi}_{-i}) - \epsilon \leq U_i(\boldsymbol{\pi}) \tag{5.18}$$

Unfortunatelt, the expected return from a $\epsilon$-Nash equilibrium can be very different from the expected return from a true NE. For example, consider this matrix game:

$$\begin{array}{c|cc} & \text{C} & \text{D} \\ \hline \text{A} & 100{,}100 & 0{,}0 \\ \text{B} & 1{,}2 & 1{,}1 \end{array} \tag{5.19}$$

The unique NE is (A,C), but the $\epsilon$-NE with $\epsilon = 1$ is either (A,C) or (B,D), which clearly have very different rewards.

Interestingly, it can be shown that two agents that use rational (Bayesian) learning rules to update their beliefs about the opponent's strategy (based on observed outcomes of earlier games), and then compute a best response to this belief, will eventually converge to Nash equilibrium [KL93].

### 5.2.4 Correlated equilibrium

Nash equilibrium assumes the policies are independent, which can limit the expectd returns. A **correlated equilibrium** (CE) allows for correlated policies. Specifically, we assume there is a central policy $\boldsymbol{\pi}_c$ that defines a distribution over joint actions. Agents can follow this recommended policy, or can choose to deviate from it by using an action modified $\xi_i : \mathcal{A}_i \to \mathcal{A}_i$. We then say that $\boldsymbol{\pi}_c$ is a CE is for all $i$ and $\xi_i$ we have

$$\sum_{\boldsymbol{a}} \boldsymbol{\pi}_c(\boldsymbol{a})\mathcal{R}_i((\xi_i(a^i), \boldsymbol{a}^{-i})) \leq \sum_{\boldsymbol{a}} \boldsymbol{\pi}_c(\boldsymbol{a})\mathcal{R}_i(\boldsymbol{a}) \tag{5.20}$$

That is, player $i$ has no incentive to deviate from the recommendation, after receiving it. It can be shown that the set of correlated equilibria contains the set of Nash equilibria. In particular, since Nash equilibrium is a special case of correlated equilibrium in which the joint policy $\boldsymbol{\pi}_c$ is factored into independent agent policies with $\boldsymbol{\pi}_c(\boldsymbol{a}) = \prod_i \pi_i(a_i)$.

To see how a correlated equilibrium can give higher returns than a Nash equilibrium, consider the **Chicken game**. This models two agents that are driving towards each other. Each agent can either stay on course (S) or leave (L) and avoid a crash. The payoff matrix is as follows:

| | S | L |
|---|---|---|
| S | 0,0 | 7,2 |
| L | 2,7 | 6,6 |

(5.21)

This reflects the fact that if they both stay on course, then they both die and get reward 0; if they both leave, they both survive and get reward 6; but if player $i$ chooses to stay and the other one leaves, then $i$ gets a reward of 7 for being brave, and $-i$ only gets a reward of 2 for chickening out.

We can represent $\pi_i$ by the scalar $\pi_i(S)$, since $\pi_i(L)) = 1 - \pi_i(S)$. Hence $\boldsymbol{\pi}$ can be defined by the tuple $(\pi_1, \pi_2)$. There are 3 uncorrelated NEs: $\boldsymbol{\pi} = (1, 0)$ with return $(7, 2)$; $\boldsymbol{\pi} = (0, 1)$ with return $(2, 7)$; and $\boldsymbol{\pi} = (\frac{1}{3}, \frac{1}{3})$ with return $(4.66, 4.66)$. There is 1 CE, namely $\boldsymbol{\pi}_c(L, L) = \boldsymbol{\pi}_c(S, L) = \boldsymbol{\pi}_c(L, S) = \frac{1}{3}$ and $\boldsymbol{\pi}_c(S, S) = 0$. The central policy has an expected return of

$$7 \cdot \frac{1}{3} + 2 \cdot \frac{1}{3} + 6 \cdot \frac{1}{3} = 5 \tag{5.22}$$

which we see is higher than the NE of 4.66. This is because it avoids the deadly joint (S,S) action. To show that this is a CE, consider the case where $i$ (e.g., row player) receives recommendation $L$; they know that $j$ (column player) will choose either $S$ or $L$ with probability 0.5 (because the central policy is uniform). If $i$ sticks with the recommendation, its expected return is $0.5 \cdot 2 + 0.5 \cdot 6 = 4$; this is greater than deviating from the recommendation and picking $S$, which has expected return of $0.5 \cdot 0 + 0.5 \cdot 7 = 3.5$. Thus $\boldsymbol{\pi}_c$ is a CE.

The correleated equilibrium solution can be computed via linear programming.

### 5.2.5 Limitations of equilibrium solutions

Equilibrium solutions have several limitations. First, they do not always maximize expected returns. For example, in Prisoner's Dilemma, (D,D) is Nash but (C,C) yields higher returns. Second, there can be multiple (even infinitely many) equilibria, each with different expected returns, as we have seen. Third, equilibria for sequential games don't specify what to do if the history deviates from the equilibrium path, i.e., they do not define the policy for full histories where $p(\hat{\boldsymbol{h}}|\boldsymbol{\pi}) = 0$; this can be problematic when the agents are learning, or the environment is changing in some other way. Consequently it is common to define additional solution requirements, as we discuss below.

### 5.2.6 Pareto optimality

We say a joint policy $\boldsymbol{\pi}$ is **Pareto optimal** if it is not **Pareto dominated** by any other joint policy $\boldsymbol{\pi}'$. We sat that $\boldsymbol{\pi}$ is Pareto dominated by $\boldsymbol{\pi}'$ if $\boldsymbol{\pi}'$ improves the expected return for at least one agent:

$$\forall i. U_i(\boldsymbol{\pi}') \geq U_i(\boldsymbol{\pi}) \text{ and } \exists i. U_i(\boldsymbol{\pi}') L U_i(\boldsymbol{\pi}) \tag{5.23}$$

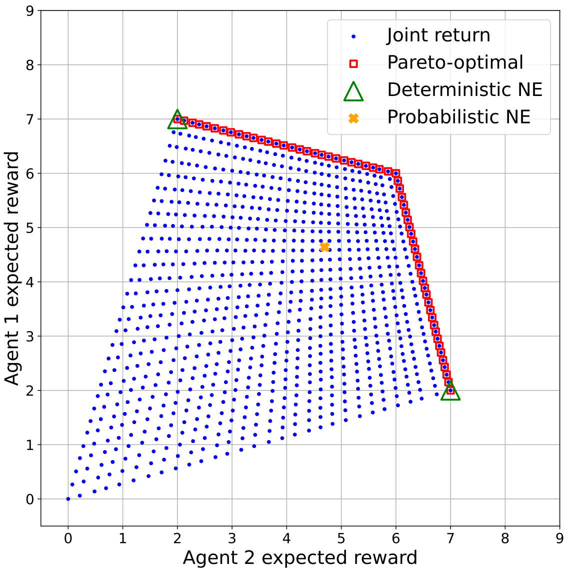


*Figure 5.3: Space of (discretized) joint policies for Chicken game. From Fig 4.4 of [ACS24]. Used with kind permission of Stefano Albrecht.*

Figure 5.3 illustrates the expected joint rewards and the Pareto frontier for all feasible policies (up to quantization error) applied to the Chicken game in Equation (5.21). We see that the two pure NEs are on the Pareto frontier (as are many other policies that are not Nash), but the mixed NE is not Pareto optimal.

### 5.2.7 Social welfare and fairness

Pareto optimality ensures there is no other solution in which at least one agent is better off, without making other agents worse off. However, it does not make any guarantees about the total rewards, or their distribution amongst agents. For example, along the Pareto frontier in Figure 5.3, the joint returns vary from (7,2) to (6,6) to (2,7).

To further constrain the space of desirable solutions, we can consider additional concepts. For example, we define **welfare optimality** as

$$W(\boldsymbol{\pi}) = \sum_i U_i(\boldsymbol{\pi}) \tag{5.24}$$

A joint policy is welfare-optimal if $\boldsymbol{\pi} \in \text{argmax}_{\boldsymbol{\pi}'} W(\boldsymbol{\pi}')$. One can show that welfare optimality implies Pareto optimality, but not (in general) vice versa.

Similarly, we define **fairness optimality** as

$$F(\boldsymbol{\pi}) = \prod_i U_i(\boldsymbol{\pi}) \tag{5.25}$$

A joint policy is fairness-optimal if $\boldsymbol{\pi} \in \text{argmax}_{\boldsymbol{\pi}'} F(\boldsymbol{\pi}')$.

In the Chicken game in Figure 5.3, there is only one solution that is both welfare-optimal and fairness-optimal, namely the joint policy with expected return of (6,6). Note, however, that this is not a Nash policy.

### 5.2.8 No regret

The quantity known as **regret** measures the difference between the rewards an agent received versus the maximum rewards it could have received if it had chosen a different action. For a non-repeated normal-form general-sum game, played over $E$ episodes, this is defined as

$$\text{Regret}_i^E = \max_{a^i} \sum_{e=1}^{E} [\mathcal{R}_i((a^i, \boldsymbol{a}_e^{-i})) - \mathcal{R}_i(\boldsymbol{a}_e)] \tag{5.26}$$

We can generalize the definition of regret to stochastic games and POSGs by defining the regret over policies instead of actions. That is,

$$\text{Regret}_i^E = \max_{\pi^i} \sum_{e=1}^{E} [U_i((\pi^i, \boldsymbol{\pi}_e^{-i})) - U_i(\boldsymbol{\pi}_e)] \tag{5.27}$$

In all these cases, an agent is said to have no-regret if

$$\forall i. \lim_{E \to \infty} \frac{1}{E} \text{Regret}_i^E \leq 0 \tag{5.28}$$

## 5.3 Reductions to single agent learning

The simplest way to solve a MARL problem is to reduce it to a single agent RL (SARL) problem. This can be done in two different ways, as we disuss below.

### 5.3.1 Central learning

In **central learning**, we learn a single joint policy over the joint action space. This requires that we can transform the joint reward $\boldsymbol{r}_t = (r_t^1, \ldots, r_t^n)$ into a scalar $r_t$. This is easy to do in common reward games, where the agents must cooperate. However, for general sum games, it may be impossible to define a single scalar reward across all agents. And even if we can define such a shared reward, the resulting method may not scale well with the number of agents, and learns a policy that requires global access to all of the observations for each agent.

### 5.3.2 Independent learning

In **independent learning**, each agent treats all other agents as part of the environment, and then uses any standard single-agent RL algorithm for training. This is done in parallel across all agents. For example, if we use Q learning for each agent, the method is known as independent Q-learning or **IQL**; see Algorithm 16 for the pseudocode.

One problem with IQL is that it trains the Q function on data from a replay buffer (at least in the deep learning context). However, since the other agents are changing their policies $\pi^j$, then $i$'s transition matrix $\mathcal{T}_i$ in Equation (5.3) will become non-stationary (as is illustrated in Figure 5.4), making old data in the buffer potentially misleading. One can get better performance using an on-policy method such as PPO, which can be easily extended to the independent multi-agent case; this is known as **IPPO** [Wit+20].

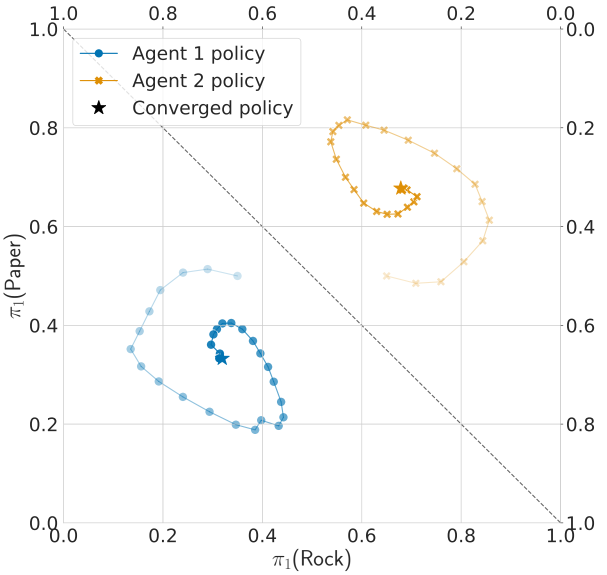


*Figure 5.4: Learning dynamics of two policies for the rock-paper-scissors game. The upper and lower triangles illustrate the policies for each agent over time as a point in the 2d simplex (noting that $\pi_e^i(S) = 1 - (\pi_e^i(P) + \pi_e^i(R))$, where $S$ is the scissors action, $P$ is paper action, and $R$ is rock action). The update rule is $\boldsymbol{\pi}_{e+1} = LR(\mathcal{D}_e, \boldsymbol{\pi}_e)$, where $LR$ is the learning rule known as WoLF-PHC (see Section 5.4.3.1). From Fig 5.5 of [ACS24]. Used with kind permission of Stefano Albrecht.*

**Algorithm 16:** Independent Q learning (DQN for multiple independent agents)

```
Initialize $n$ value networks with random parameters $\theta_1, \ldots, \theta_n$;
Initialize $n$ target networks with parameters $\bar{\theta}_1 = \theta_1, \ldots, \bar{\theta}_n = \theta_n$;
Initialize a replay buffer for each agent $D_1, D_2, \ldots, D_n$;
for time step $t = 0, 1, 2, \ldots$ do
    Collect current observations $o_t^1, \ldots, o_t^n$;
    for agent $i = 1, \ldots, n$ do
        With probability $\epsilon$: choose random action $a_t^i$;
        Otherwise: choose $a_t^i \in \operatorname{argmax}_{a_i} Q(h_t^i, a_i; \theta_i)$;
    Apply actions $(a_t^1, \ldots, a_t^n)$; collect rewards $r_t^1, \ldots, r_t^n$ and next observations $o_{t+1}^1, \ldots, o_{t+1}^n$;
    for agent $i = 1, \ldots, n$ do
        Store transition $(h_t^i, a_t^i, r_t^i, h_{t+1}^i)$ in replay buffer $D_i$;
        Sample random mini-batch of $B$ transitions $(h_k^i, a_k^i, r_k^i, h_{k+1}^i)$ from $D_i$;
        if $s_{k+1}^i$ is terminal then
            Targets $y_k^i \leftarrow r_k^i$;
        else
            Targets $y_k^i \leftarrow r_k^i + \gamma \max_{a_i' \in \mathcal{A}_i} Q(h_{k+1}^i, a_i'; \overline{\theta_i})$;
        Loss $\mathcal{L}(\theta_i) \leftarrow \frac{1}{B} \sum_{k=1}^{B} \left( y_k^i - Q(h_k^i, a_k^i; \theta_i) \right)^2$;
        Update parameters $\theta_i$ by minimizing the loss $\mathcal{L}(\theta_i)$;
        In a set interval, update target network parameters $\bar{\theta}_i$;
```

## 5.4 Model-free MARL algorithms

In this section, we discuss how to learn policies in the multi-agent setting without having to know the world model. We consider both fully and partially observed stochastic games.

### 5.4.1 Best response against game-theoretic agents

Since the optimal action depends on the other agents, we will learn a joint-action value function $Q_i(s, \boldsymbol{a})$ for each agent $i$; this is called **joint-action learning**.

In the fully observed stochastic game setting, with tabular state representation and known reward functions, we can do this as follows. For each state $s$ that we encounter, we define a normal-form game $\Gamma_s = (\mathcal{R}_1 = Q_1(s, \cdot), \cdots, R_n = Q_n(s, \cdot))$. We can solve this game to find a joint policy $\boldsymbol{\pi}_s^* = (\pi_{s,1}^*, \ldots, \pi_{s,n}^*)$ with certain properties. Once we have computed $\boldsymbol{\pi}_s^*$, the best response for agent $i$ is then given by

$$\text{BR}_i(s) = \boldsymbol{\pi}_s^*[i] \tag{5.29}$$

We can amortize this process by learning a Q function, as follows. We define the value of $\Gamma_s$ for agent $i$ as its expected reward under the joint policy $\boldsymbol{\pi}_s^*$:

$$\text{Value}_i(\Gamma_s) = \sum_{\boldsymbol{a}} Q_i(s, \boldsymbol{a}) \boldsymbol{\pi}_s^*(\boldsymbol{a}) \tag{5.30}$$

We can then update $Q_i$ at state $s_t$ as follows:

$$Q_i(s_t, \boldsymbol{a}_t) \leftarrow Q_i(s_t, \boldsymbol{a}_t) + \alpha[r_t^i + \gamma \text{Value}_i(\Gamma_{s_{t+1}}) - Q_i(s_t, \boldsymbol{a}_t)] \tag{5.31}$$

where $\alpha$ is the learning rate, $\gamma$ is the discount factor, and $s_{t+1}$ is the next sampled state. If $\boldsymbol{\pi}_s^*$ corresponds to a minimax equilibrium (for zero-sum games), then this is called **minimax Q learning**. If $\boldsymbol{\pi}_s^*$ corresponds to a Nash equilibrium (for general-sum games), this is called **Nash Q learning**.

### 5.4.2 Best response against learned agents

In Section 5.4.1, each agent $i$ assumes the other agents choose their actions according to some normative approach, such as picking a Nash equilibrium. However, it is possible to do better by learning a model of the other agents, and then picking the best response wrt this learned model.

Agent $i$ can learn to predict agent $j$'s actions by using supervised fitting a model of the form $\hat{\pi}_j^i(a_j|\boldsymbol{h}_t^i)$ to $(\boldsymbol{h}_t^i, a_t^j)$ pairs. (In the fully observed setting, we have $\boldsymbol{h}_t^i = s_t$, so we can just write $\hat{\pi}_j$, and drop the conditioning on $i$.) There are many kinds of **agent model** or **opponent model** (see e.g. [AS18] for a review); we give some examples below. Note that, for symmetric games, we can assume that each player uses the same policy, which lets us use self-play, as we discuss in Section 4.2.2.1.

#### 5.4.2.1 Fictitious play for normal-form games

For non-repeated normal-form games (which are stateless), we can estimate agent models by counting. That is,

$$\hat{\pi}^j(a^j) = \frac{C(a^j)}{\sum_{a'} C(a')} \tag{5.32}$$

where $C(a^j)$ is the number of times agent $i$ chose action $a^j$ in prior episodes. The best response is given by

$$\text{BR}_i = \underset{a^i}{\text{argmax}} \sum_{\boldsymbol{a}^{-i}} \mathcal{R}_i((a^i, \boldsymbol{a}^{-i}) \prod_{j \neq i} \hat{\pi}_j(a^j) \tag{5.33}$$

This is known as **fictitious play**. If the empirical distribution of agents' actions converge (e.g., in two-player zero-sum finite games), then this procedure will converge to a NE.

#### 5.4.2.2 Tabular agent learning

We can extend fictitious play to fully observed stochastic games by conditioning the agent models on the state:

$$\hat{\pi}_j(a^j|s) = \frac{C(s, a^j)}{\sum_{a'} C(s, a')} \tag{5.34}$$

Given the agent models, the action values are defined as

$$AV_i(s, a^i) = \sum_{\boldsymbol{a}^{-i}} Q_i(s, (a^i, \boldsymbol{a}^{-i})) \prod_{j \neq i} \hat{\pi}_j(a^j|s) \tag{5.35}$$

where the $Q$ function is learned using the following update:

$$Q_i(s_t, \boldsymbol{a}_t) \leftarrow Q_i(s_t, \boldsymbol{a}_t) + \alpha[r_t^i + \gamma \max_{a'} AV_i(s_{t+1}, a') - Q_i(s_t, \boldsymbol{a}_t)] \tag{5.36}$$

The best response is then given by

$$\text{BR}_i(s) = \operatorname*{argmax}_{a^i} AV_i(s, a^i) \tag{5.37}$$

Of course, we also need to incrementally update the agent models $\hat{\pi}^j$ given the observed $(s_t, a_t^j)$ data. This is called Joint Action Learning with Agent Modeling or **JAL-AM**.

#### 5.4.2.3 Parametric agent learning

We now extend the agent modeling paradigm to the partially observed setting, and using non-tabular representations. The basic idea is that each agent $i$ will learn a model of $j$'s policy, denoted by $\hat{\pi}_j^i(a_t^j|\boldsymbol{h}_t^i; \boldsymbol{\theta}_j^i)$, by minimizing the cross entropy loss

$$\mathcal{L}(\boldsymbol{\theta}_j^i) = \mathbb{E}_{a_t^j \sim \pi_j(\boldsymbol{h}_t^j)} \left[ -\log \hat{\pi}_j^i(a_t^j|\boldsymbol{h}_t^i; \boldsymbol{\theta}_j^i) \right] \tag{5.38}$$

where $\pi_j$ is $j$'s true policy. Given this, the agent can compute its expected action values as using

$$AV_i(\boldsymbol{h}^i, a^i) = \sum_{\boldsymbol{a}^{-i}} Q_i(\boldsymbol{h}^i, (a^i, \boldsymbol{a}^{-i})) \prod_{j \neq i} \hat{\pi}_j^i(a^j|\boldsymbol{h}^i; \boldsymbol{\theta}_j^i) \tag{5.39}$$

We can approximate the sum over $\boldsymbol{a}^{-i}$ using Monte Carlo sampling. This gives an efficient way to compute $AV_i$ and hence the best response.

### 5.4.3 Policy learning

One disadvantage of the best-response approach is that the resulting policies are deterministic, and thus cannot represent probabilistic equilibria, such as the uniform-random NE in Rock-Paper-Scissors. In this section, we discus how to learn differentiable policies directly using gradient ascent.

#### 5.4.3.1 Warmup: two-player normal-form games

To start, consider a non-repeated normal-form general-sum game with two players and two actions. Denote the reward matrices by

$$\mathcal{R}_i = \begin{pmatrix} r_{11} & r_{12} \\ r_{21} & r_{22} \end{pmatrix}, \ \mathcal{R}_j = \begin{pmatrix} c_{11} & c_{12} \\ c_{21} & c_{22} \end{pmatrix} \tag{5.40}$$

Denote the policies by

$$\pi^i = (\alpha, 1 - \alpha), \ \pi^j = (\beta, 1 - \beta) \tag{5.41}$$

We can now learn the policy using gradient ascent:

$$\alpha_{k+1} = \alpha_k + \kappa \frac{\partial U_i(\alpha_k, \beta_k)}{\partial \alpha_k}, \quad \beta_{k+1} = \beta_k + \kappa \frac{\partial U_j(\alpha_k, \beta_k)}{\partial \beta_k} \tag{5.42}$$

where $\kappa$ is the learning rate. The expected reward is given by

$$U_i(\alpha, \beta) = \alpha\beta r_{11} + \alpha(1-\beta) r_{12} + (1-\alpha)\beta r_{21} + (1-\alpha)(1-\beta) r_{22} \tag{5.43}$$

The expression $U_j(\alpha, \beta)$ is analogous, with $r_{ij}$ replaced with $c_{ij}$. (Note that computing $U_i$ requires knowledge of $\mathcal{R}_i$ but also of $\pi_j$ (and vice versa for computing $U_j$); we will relax this assumption below.)

We can analyse the dynamics of the above procedure as $\kappa \to 0$; this is known as **infinitesimal gradient ascent** or **IGA**. One can show that $(\alpha, \beta)$ does not always converge (depending on the values in $\mathcal{R}_i$ and $\mathcal{R}_j$), but if it does, the resulting converged joint policy is a NE [SKM00]. However, there is a method called **Win or Learn Fast** or **WoLF** from [BV02] which can ensure that IGA policies always converge to a NE for two-agent two-action normal-form games. The trick is to learn slow (by using smaller $\kappa$) when winning (i.e., if $U_i(\alpha_k, \beta_k) > U_i(\alpha_e, \beta_k)$ where $\alpha_e$ is a policy from some NE), and to learn fast (by using larger $\kappa$) when losing (i.e., when not winning). This approach can be extended to stochastic games, without requiring knowledge of reward functions or policies. The resulting method is called **WoLF-PHC**, which stands WoLF with Policy Hill Climbing [BV02]. See Figure 5.4 for an example. (and see [Blo+15] for a more general analysis of the dynamics of multiple interacting learning agents).

#### 5.4.3.2 Policy gradient methods

Recall from Equation (3.11) that the policy gradient theorem for a single agent in the fully observed setting is given by

$$\nabla_{\boldsymbol{\theta}} J(\boldsymbol{\theta}) \propto \mathbb{E}_{s \sim p(s|\pi), a \sim \pi(a|s)} \left[ Q^\pi(s, a) \nabla_{\boldsymbol{\theta}} \log \pi(a|s; \boldsymbol{\theta}) \right] \tag{5.44}$$

In the multi-agent partially observed case, this becomes

$$\nabla_{\boldsymbol{\theta}_i} J(\boldsymbol{\theta}_{1:n}) \propto \mathbb{E}_{\hat{\boldsymbol{h}} \sim p(\hat{\boldsymbol{h}}|\pi), a^i \sim \pi_i, \boldsymbol{a}^{-i} \sim \boldsymbol{\pi}^{-i}} \left[ Q_i^\pi(\hat{\boldsymbol{h}}, (a^i, \boldsymbol{a}^{-i}) \nabla_{\boldsymbol{\theta}_i} \log \pi(a_i | h_i = \sigma_i(\hat{\boldsymbol{h}}); \boldsymbol{\theta}_i) \right] \tag{5.45}$$

where $\sigma_i(\hat{\boldsymbol{h}}_t) = \boldsymbol{h}_t^i = (o_1^i, \ldots, o_t^i)$ is the history of observations for agent $i$. In practice, we usually subtract a baseline term from $Q$, to reduce the variance. If we use the value function for the baselne, then the first term inside the expectation becomes

$$Q_i^\pi(\hat{\boldsymbol{h}}, (a^i, \boldsymbol{a}^{-i})) - V_i^\pi(\hat{\boldsymbol{h}}) = \text{Adv}_i^\pi(\hat{\boldsymbol{h}}, \boldsymbol{a}) \tag{5.46}$$

where Adv is the advantage, as we discussed in Section 3.3.1. This can be used inside a multi-agent version of the advantage actor critic or A2C method (known as **MAA2C**) shown in Algorithm 17, or inside a multi-agent version of PPO, known as **MAPPO** [Yu+22]. (To combat the fact that we cannot use replay buffers with an on-policy method, we assume instead that we can parallelize over multiple (synchronous) environments, to ensure we have a sufficiently large minibatch to estimate the loss function at each step.)

#### 5.4.3.3 Centralized training and decentralized execution (CTDE)

We focus on the paradigm known as Centralized Training and Decentralized eEecution (**CTDE**), where the learing algorithm has access to all the information (from all agents) at training time, but at test time, agents only observe their own local observations. This is the most common scenario in the literature. The **central information** can contain the joint action taken by all agents, and/or the joint observation vector, even such joint information is not available at execution time. It is perfectly valid for the *critics* to have this kind of central information, as long as the *policies* do not rely on this, since the critics are not used during execution. This is known as **centralized critics** with **decentralized actors**. See Algorithm 17 for an example (where the central information is denoted by $z$).

**Algorithm 17:** Multi-agent Advantage Actor-Critic (MAA2C)

```
Initialize $n$ actor networks with random parameters $\boldsymbol{\theta}_1, \dots, \boldsymbol{\theta}_n$
Initialize $n$ critic networks with random parameters $\boldsymbol{w}_1, \dots, \boldsymbol{w}_n$
Initialize $K$ parallel environments
Initialize histories $h_0^{i,k}$ for each agent $i$ and environment $k$
for time step $t = 0 \dots$ do
    for environment $k = 1, \dots, K$ do
        Sample actions: $\{a_t^{i,k} \sim \pi(\cdot | h_t^{i,k}, \boldsymbol{\theta}^i)\}_{i=1}^n$
        Sample next state: $s_{t+1}^k \sim T(\cdot | s_t^k, \boldsymbol{a}_t^{1:n,k})$
        Sample observations: $\{o_{t+1}^{i,k} \sim O_i(\cdot | s_t^k, a_t^{i,k})\}_{i=1}^n$
        Sample rewards: $\{r_t^{i,k} \sim R_i(\cdot | s_t^k, \boldsymbol{a}_t^{1:n,k}, s_{t+1}^k)\}_{i=1}^n$
        Update histories: $\{h_{t+1}^{i,k} = (h_t^{i,k}, o_{t+1}^{i,k})\}_{i=1}^n$
        Collect central information $z_{t+1}^k$
    for agent $i = 1, \dots, n$ do
        if $s_{t+1}^k$ is terminal then
            $\text{Adv}(h_t^{i,k}, z_t^k, a_t^{i,k}) \leftarrow r_t^{i,k} - V(h_t^{i,k}, z_t^k; \boldsymbol{w}_i)$;
            Critic target $y_t^{i,k} \leftarrow r_t^{i,k}$;
        else
            $\text{Adv}(h_t^{i,k}, z_t^{i,k}, a_t^{i,k}) \leftarrow r_t^{i,k} + \gamma V(h_{t+1}^{i,k}, z_{t+1}^k; \boldsymbol{w}_i) - V(h_t^{i,k}, z_t^k; \boldsymbol{w}_i)$;
            Critic target $y_t^{i,k} \leftarrow r_t^{i,k} + \gamma V(h_{t+1}^{i,k}, z_{t+1}^k; \boldsymbol{w}_i)$;
        Actor loss:
            $$\mathcal{L}(\boldsymbol{\theta}_i) \leftarrow \frac{1}{K} \sum_{k=1}^{K} \text{Adv}(h_t^{i,k}, z_t^k, a_t^{i,k}) \log \pi(a_t^{i,k} \mid h_t^{i,k}; \boldsymbol{\theta}_i)$$
        Critic loss:
            $$\mathcal{L}(\boldsymbol{w}_i) \leftarrow \frac{1}{K} \sum_{k=1}^{K} \Big(y_t^{i,k} - V(h_t^{i,k}, z_t^k; \boldsymbol{w}_i)\Big)^2$$
        Update parameters $\boldsymbol{\theta}_i$ by minimizing the actor loss $\mathcal{L}(\boldsymbol{\theta}_i)$;
        Update parameters $\boldsymbol{w}_i$ by minimizing the critic loss $\mathcal{L}(\boldsymbol{w}_i)$;
```

#### 5.4.3.4 Policy learning with agent models

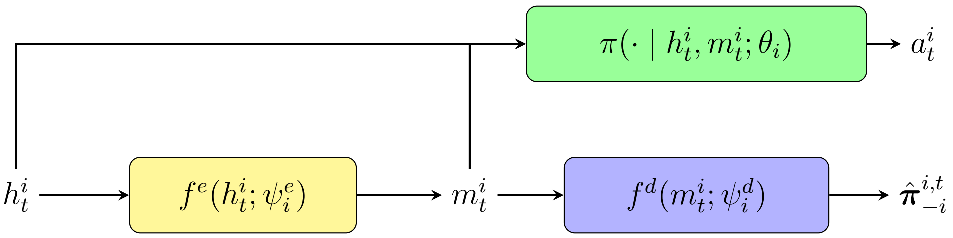

$\pi(\cdot \mid h_t^i, m_t^i; \theta_i)$
$a_t^i$
$h_t^i$
$f^e(h_t^i; \psi_i^e)$
$m_t^i$
$f^d(m_t^i; \psi_i^d)$
$\hat{\boldsymbol{\pi}}_{-i}^{i,t}$

*Figure 5.5: Encoder-decoder architecture for agent modeling. From Fig 9.21 of [ACS24]. Used with kind permission of Stefano Albrecht.*

It is possible to combine agent modeling (discussed in Section 5.4.2) with policy gradient methods, as opposed to using best response methods. For example, we can train an encoder-decoder network to predict the actions of other agents via a bottleneck, and then pass this bottleneck embedding to the policy as side information, as proposed in [PCA21]. In more detail, let $m_t^i = f^e(h_t^i; \psi_i^e)$ be the encoding of $i$'s history, which is then passed to the decoder $f^d$ to predict the other agents actions using $\hat{\boldsymbol{\pi}}_{-i}^{i,t} = f^d(m_t^i; \psi_i^d)$. In addition, we pass $m_t^i$ to $i$'s policy to compute the action using $a_t^i \sim \pi(\cdot|h_t^i, m_t^i; \theta_i)$. This is illustrated in Figure 5.5. (A similar method could be used to predict other properties of agent $j$, as long as their as observable by agent $i$.)

### 5.4.4 Value decomposition methods for common-reward games

In this section, we discuss methods for deriving a policy from a centralized state-action value function $Q(\boldsymbol{h}, z, \boldsymbol{a})$. To ensure that the per-agent policy can be implemented using only locally available information, we need to use **value decomposition** methods, which assume that the global value function can be decomposed into separate value functions, one per agent. (This is only possible if we are solving a common-reward or cooperative game.) This decomposition is valid provided the separate value functions satisfy a property known as the **individual global max** or **IGM** property, which says that

$$\forall \boldsymbol{a}.\boldsymbol{a} \in A^*(\boldsymbol{h}, z; \boldsymbol{\theta}) \Leftrightarrow \forall i.a_i \in A_i^*(h^i; \boldsymbol{\theta}_i) \tag{5.47}$$

where $A^*(\boldsymbol{h}, z; \boldsymbol{\theta}) = \operatorname{argmax}_{\boldsymbol{a}} Q(\boldsymbol{h}, z, \boldsymbol{a}; \boldsymbol{\theta})$ and $A_i^*(h^i; \boldsymbol{\theta}) = \operatorname{argmax}_{\boldsymbol{a}} Q(h^i, a^i; \boldsymbol{\theta}_i)$. This ensures that picking actions locally for each agent will also be optimal globally.

For example, consider the **value decomposition network** or **VDN** method of [Sun+17]. This assumes a linear decomposition

$$Q(\boldsymbol{h}_t, z_t, \boldsymbol{a}_t; \boldsymbol{\theta}) = \sum_i Q(h_t^i, a_t^i; \boldsymbol{\theta}_i) \tag{5.48}$$

This clearly satisfies IGM. A more general method, known as **QMIX**, is presented in [Ras+18]. This assumes

$$Q(\boldsymbol{h}_t, z_t, \boldsymbol{a}_t; \boldsymbol{\theta}) = f_{\text{mix}}(Q(h_t^1, a_t^1; \boldsymbol{\theta}_1), \ldots, Q(h_t^n, a_t^n; \boldsymbol{\theta}_n)) \tag{5.49}$$

where $f_{\text{mix}}$ is monotonically increasing in each of its arguments. This satisfies IGM since

$$\max_{\boldsymbol{a}} Q(\boldsymbol{h}_{t+1}, z_{t+1}, \boldsymbol{a}; \overline{\boldsymbol{\theta}}) = f_{\text{mix}}\left(\max_{a^1} Q(h_{t+1}^1, a^1; \overline{\theta}_1), \ldots, \max_{a^n} Q(h_{t+1}^n, a^n; \overline{\theta}_n)\right) \tag{5.50}$$

Hence we can fit this Q function by minimzing the TD loss (with target network $\overline{\boldsymbol{\theta}}$):

$$\mathcal{L}(\boldsymbol{\theta}) = \frac{1}{B} \sum_{(\boldsymbol{h}_t, z_t, \boldsymbol{a}_t, r_t, \boldsymbol{h}_{t+1}, z_{t+1}) \in \mathcal{B}} \left(r_t + \gamma \max_{\boldsymbol{a}} Q(\boldsymbol{h}_{t+1}, z_{t+1}, \boldsymbol{a}; \overline{\boldsymbol{\theta}}) - Q(\boldsymbol{h}_t, z_t, \boldsymbol{a}; \boldsymbol{\theta})\right)^2 \tag{5.51}$$

### 5.4.5 Population-based training

In Section 4.2.2.1, we discussed the concept of **self-play**, which is a way to train an agent to play a two-player game by modeling the opponent as using the same policy as the agent itself. To avoid overfitting, we typically train against multiple versions of the agent's own policy. This concept can be generalized to work with general-sum games with two or more players, by training against a population of different policies. This is called **population based training** [Jad+19].

#### 5.4.5.1 PSRO

In this section, we describe the **policy space response oracle** or **PSRO** method of [Lan+17], which is a game-theoretic instance of population based training, which can compute policies that satisfy various solution concepts for any kind of stochastic game, including partially observed, general sum games.

The idea behind PSRO is as follows. At generation $k$, each agent $i$ has a finite set of policies it can use, denoted $\Pi_i^k$. We can define a normal-form meta-game $M^k$ from this by letting each agent choose one of its policies, where the reward for the joint action $\boldsymbol{a} = \boldsymbol{\pi} = (\pi_1, \pi_n)$ is given by $\mathcal{R}_i(\boldsymbol{\pi}) = U_i(\boldsymbol{\pi})$. These returns can be estimated empirically by simulating $n$ agents interacting with each other according to these

| $k$ | $\Pi_1^k$ | $\Pi_2^k$ | $\delta_1^k$ | $\delta_2^k$ | $\pi_1'$ | $\pi_2'$ |
|---|---|---|---|---|---|---|
| 1 | $\underline{\text{R}}$ | $\underline{\text{P}}$ | 1 | 1 | S | P |
| 2 | R,$\underline{\text{S}}$ | P | $(0, 1)$ | 1 | S | R |
| 3 | R,S | $\underline{\text{R}}$,P | $(\frac{2}{3}, \frac{1}{3})$ | $(\frac{2}{3}, \frac{1}{3})$ | P | R/P |
| 4 | R,$\underline{\text{P}}$,S | R,P | $(0, \frac{2}{3}, \frac{1}{3})$ | $(\frac{1}{3}, \frac{2}{3})$ | R | S |
| 5 | R,P,S | R,P,$\underline{\text{S}}$ | $(\frac{1}{3}, \frac{1}{3}, \frac{1}{3})$ | $(\frac{1}{3}, \frac{1}{3}, \frac{1}{3})$ | R/P/S | R/P/S |

*Figure 5.6: PSRO for rock-paper-scissors. We show the populations $\Pi_i^k$, distributuons $\delta_i^k$ and best responses $\pi_i'$ for both agents over generations $k = 1 : 5$. (We use the shorthand of R to denote the pure policy that always plays R, and similarly for S and P.) New entries added to the population are shown with an underline. At generation $k = 3$, there are 2 best responses, R and P, so the oracle can select either of them. Similarly, at generation $k = 5$, there are 3 best responses.*

policies in the underyling game $G$. Once we have determined the reward matrix, we can solve for some kind of equilibrium solution (e.g., Nash equilibrium), using a **meta-strategy solver**. We can then extract the probability distributions over policies (aka strategy) $\delta_i^k$ for each agent. To ensure this distribution is diverse, we can enforce a lower bound that $\delta_i^k(\pi_i) > \epsilon$.

We can now expand the set of policies for each agent by using an oracle to compute a new policy $\pi_i'$ and adding it to $\Pi_i^k$ to create the set $\Pi_i^{k+1}$. For example, the oracle can compute a best response

$$\pi_i' \in \underset{\pi_i}{\operatorname{argmax}} \mathbb{E}_{\boldsymbol{\pi}_{-i} \sim \boldsymbol{\delta}_{-i}^k} \left[ U_i((\pi_i, \boldsymbol{\pi}_{-i})) \right] \tag{5.52}$$

where $\boldsymbol{\delta}_{-i}^k(\boldsymbol{\pi}_{-i}) = \prod_{j \neq i} \delta_j^k(\pi_j)$. We can compute $\pi_i'$ by using a single agent RL algorithm in the underlying game $G$, where in each episode the policies of the other agents $j \neq i$ are sampled from $\pi_j \sim \delta_j^k$.

It can be shown that, if PSRO uses a meta-solver that computes exact Nash equilibria for the meta-game, and if the oracle computes the exact best-response policies in the unerlying game $G$, then the distributions $\{\delta_i^k\}_{i \in \mathcal{I}}$ converge to a Nash equilibrium of $G$. See Figure 5.6 for an example.

Note that PSRO can also be applied to general-sum, imperfect information games. For example, [Li+23a] uses (information set) MCTS, together with a learned world model, to compute the best response policy $\pi_i'$ at each step of PSRO (see Section 5.5.3 for details on this kind of online planning).

#### 5.4.5.2 AlphaStar

The **AlphaStar** system of [Vin+19] used a PSRO-like method, combined with the (single agent) A2C RL algorithm, to achieve grandmaster status in the challenging real-time strategy game known as StarCraft II.[2] In particular, it used the following steps: Build a pool of agents that represent different playstyles and skill levels (known as a league); Compute best responses to existing strategies; Update a meta-strategy to mix agents in a way that approximates a Nash equilibrium; select opponents from the Nash mixture to ensure robustness; and train a new agent against the weighted mixture of past opponents. See the paper for more details.

[2] In StarCraft II, the AI agent controls an entire army, and must defeat a human opponent, making this a zero-sum, two-player game, which can be solved using deep RL with self-play. This is different from the StarCraft Multi-Agent Challenge (**SMAC**) [Sam+19], which is a cooperative, partially observed multi-agent game, where the agents (corresponding to individual units) must work together as a team to defeat a fixed AI opponent in certain predefined battles.

## 5.5 Model-based MARL algorithms

In this section, we discuss how to use world models to help improve the sample efficiency of MARL. We mostly focus on methods that are applicable to general-sum partially-observed Markov games. Many of the issues for the single agent model-based RL setting described in Chapter 4 apply here, but there are additional factors to consider, as we discuss below.

### 5.5.1 Model learning

If we are in the fully observed CTDE setting, we have access to the underlying state $s_t$ and the joint actions $\boldsymbol{a}_t$. Hence we can fit a Markovian world model of the form $p(s_{t+1}|s_t, \boldsymbol{a}_t)$ using any kind of supervised learning technique (e.g., maximum likelihood training of a conditional generative model).

Note that a world model is a kind of causal model, since it specifies the effects of different kinds of actions, one per agent [GSP21]. However, if we don't get to observe the other agent's actions, then identifying the true causal model becomes very difficult (this is related to the issue of latent confounders in the causal inference literature).

If we don't get to see the underlying world state, but instead just see the joint observation stream, then we can still fit a joint predictive model of the form $p(\boldsymbol{o}_{t+1}|\boldsymbol{o}_{1:t}, \boldsymbol{a}_{1:t}) = p(\boldsymbol{o}_{t+1}|\boldsymbol{h}_t, \boldsymbol{a}_t)$, where $\boldsymbol{h}_t = (\boldsymbol{o}_0, \boldsymbol{a}_1, \boldsymbol{o}_1, \ldots, \boldsymbol{o}_{t-1}, \boldsymbol{a}_{t-1}, \boldsymbol{o}_t)$ is the observed history. This can be sufficient for learning a simulator that can be used for background planning in the CTDE paradigm. However, if we want to support online planning in a decentralized (per-agent) fashion, each agent needs its own local world model (just as it needs its own local policy). That is, each agent needs to learn a model of the form

$$p_i(o^i_{t+1}|o^i_{1:t}, a^i_{1:t}) = p(o^i_{t+1}|\boldsymbol{h}^i_t, a^i_t) \tag{5.53}$$

This can be solved as a set of $n$ independent supervised learning problems. If the observations are high dimensional, the agent may choose to use local latent variables $z^i_t$ to simplify the modeling problem, as discussed in Section 4.4.1.2.

An alternative approach is for each agent to try to learn the true data generating process, which is defined by a shared hidden latent state $s_t$, the underlying world model $\mathcal{T}$, the agent-specific observation functions $\mathcal{O}_i$, and the agent-specific policies $\pi_i$. This can be done maximizing the marginal likelihood given by Equation (5.4). This requires that each agent computes its belief state $p(s_t|\boldsymbol{h}^i_t)$, and somehow marginalize out the latent variables $s_t$ to compute the objective function.

Even if we are able to fit a predictive model to some trajectory data, we also need to decide what data to collect to power the learning. This requires solving the exploration-exploitation tradeoff. One approach to this is to use optimism in the face of uncertainty or a Thompson sampling like method. For example, at the start of each episode, we can sample a particular model (from the belief state over models), and then plan using that model, as in PSRL Section 7.1.3.2. See e.g., [SKK22] for an example of this approach.

### 5.5.2 Background (offline) planning

Once we have learned a world model, we can use it (together with an agent model) to generate synthetic trajectories by "rolling out in imagination". This data can then be used to perform policy optimization, by plugging any model-free MARL algorithm into Algorithm 10. (Unlike the single agent case, we typically do not use off-policy updates, due to non-stationarity induced by the changing agent policies; thus Dyna-like methods are less relevant.)

### 5.5.3 Decision-time (online) planning

An alternative way to use a world model is to perform online planning at decision time. In the partially observed setting, each agent needs to maintain a belief state, $b^i_t = p(s_t|\boldsymbol{h}^i_t)$. This can be approximated using particle filtering (see e.g., [NLS19]). To do planning, we can sample a ground state from the belief state, and then treat this as the root node of a search tree. We can then use MCTS (or one of the other algorithms discussed in Section 4.2) to pick the next best action (assuming we know (or have learned) the latent world model). This combination of methods (particle filtering plus MCTS) is known as the **POMCP** algorithm [SV10].[3]

To speed up posterior inference, we can use various learning methods. For example, in the CTDE paradigm, where ground truth states are paired with observations, it is possible to train an inference network to approximate the belief state $p(s_t|\boldsymbol{h}_t)$. This can be used as a data-driven proposal distribution for a particle filter, similar to the wake-sleep algorithm. For related work, see [Hu+21b; Hu+21a; Sok+22; Sok+23; Li+23b].

If the agent cannot afford to compute a belief state, and/or it does not know the shared latent world model, then it can still perform online planning by rolling out trajectories in its own local latent state space, using its own local dynamics (given by Equation (5.53)), The agent also needs a model of the other agents, to predict how they will respond. In a symmetric zero-sum game, we can use the self-play method discussed in Section 4.2.2.1, in which the agent assumes its opponent uses the same policy as itself. This is the approach used by the MuZero method (see Section 4.2.2.2).

[3] There is a closely related method from the game theory literature known as **Information Set MCTS** of [CPW12]. This is defined in terms of extensive form games, rather than the partially observed stochastic game framework that we are assuming.

# Chapter 6

# LLMs and RL

In this section, we discuss connections between RL and **foundation models**, also called **large language models** (**LLMs**). These are generative models (usually transformers) which are trained on large amounts of text and image data (see e.g., [Bur25]).[1]

## 6.1 RL for LLMs

In this section, we discuss how to use RL to improve the performance of LLMs. This is a fast growing field, so we only briefly mention a few highlights. For more details, see e.g. and https://github.com/WindyLab/LLM-RL-Papers.

LLMs are usually trained with behavior cloning, i.e., MLE on a fixed dataset, such as a large text corpus scraped from the web. This is called **pre-training**. We can then improve their performance using various **post-training** methods, which are designed to improve their capabilities and **alignment** with human preferences (as opposed to just being generative models of the data seen on the web). A simple way to perform post-training is to use **instruction fine tuning**, also called **supervised fine-tuning** (or **SFT**), in which we collect human demonstrations of (prompt, response) pairs, and fine-tune the model on them. However, it is very difficult to collect sufficient quantities of such data. Therefore there is a lot of interest in using RL to further improve model performance; this is called **reinforcement learning fine-tuning** or **RLFT**.

### 6.1.1 Multi-turn RL

To use RL to train LLMs, we view the LLM as an agent/policy which interacts with an external environment (e.g., a user and/or an external tool, such as a web browser). The action space of the agent is a sequence of tokens, and the state space of the environment is also a sequence of tokens.[2] Let $s_t$ be the environment state at round / turn $t$ of the interaction, and let $\boldsymbol{a}_t = (a_t^1, a_t^2, \ldots, a_t^{1:N_t})$ be the token (action) sequence generated by the agent, step by step, in response. Optionally the environment can then transition to its next state, modeled by $p(s_{t+1}|s_t, \boldsymbol{a}_t)$.

We can view this as a nested process, similar to a semi-MDP, in which the agent the agent performs a (variable length) sequence of primitive actions before the state gets updated, as illustrated in Figure 6.1. However, for notational simplicity, we "flatten" this nested structure into a single stream of tokens, $o_1, o_2, \ldots$. (We can insert special tags to demarcate the start/end of an environment interaction.)

[1] LLMs that consume and/or generate modalities besides text (such as images, video and audio) are sometimes called large multimodal models, but we stick to the term LLM for simplicity.

[2] We use the term "token" instead of "word" since when using VLMs, the "words" are a tokenized representation of the visual input and/or output. Even when using language, the elementary components are sub-words (which allows for generalization to novel words), not words.

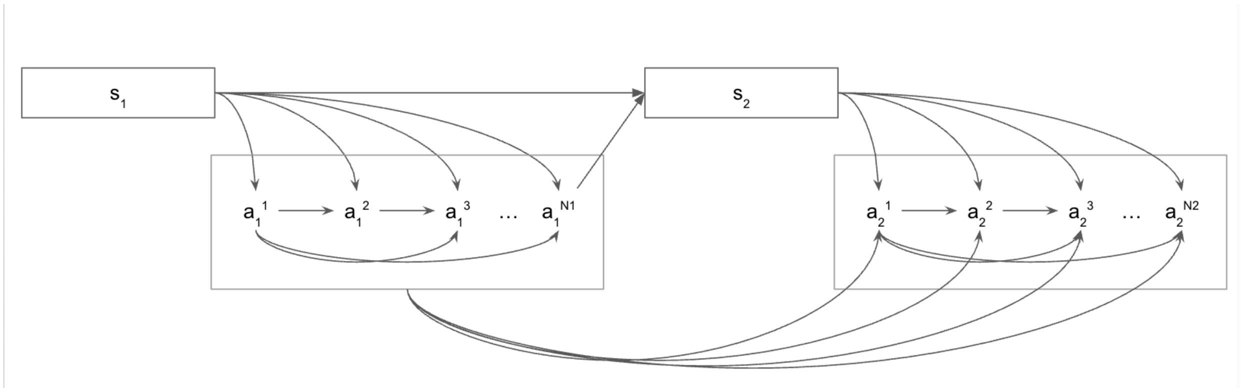


*Figure 6.1: Multi-turn dialog between environment (with states $s_t$) and agent (generating actions $a_t^{1:N}$).*

Since the policy is an LLM, which is usually a transformer, it attends to all previous tokens, rather than being Markovian. We denote the internal state of the agent by $h_t = \boldsymbol{o}_{1:t-1}$, which represents the entire history of previous tokens. The LLM acts like a policy that generates the next token

$$a_t \sim \pi_{llm}(\cdot|h_t) \tag{6.1}$$

The agent state then gets deterministically updated to give

$$p(h_{t+1}|h_t, a_t) = \delta(h_t = \text{concat}(h_t, a_t)) \tag{6.2}$$

(For notational simplicity, we ignore the fact that some of the tokens are generated by the environment, not by the agent.)

Training a model to work well in this context requires **multi-turn RL** (see e.g., [Zho+24c]). However, many current applications (especially on math and reasoning benchmarks) focus on the single-turn setting, where the agent generates a sequence of actions $\boldsymbol{a}_t = \boldsymbol{a}_t^{1:M}$ in response to a prompt, $\boldsymbol{s}_t = \boldsymbol{s}_t^{1:N}$, receives a terminal reward, and then stops. This is more like a contextual bandit problem (with sequence-valued actions) than a true RL problem, since the actions do not affect the external environment (i.e., the next question/prompt $\boldsymbol{s}_{t+1}$ from the user is assumed to be independent of the actions $\boldsymbol{a}_t$.) However, agents that engage in dialog, or which use external tools, require solving the full multi-turn problem.

### 6.1.2 Agents which "think"

In this section, we discuss how to leverage the power of LLMs to create agents that "think" before they act.

#### 6.1.2.1 Chain of thought

The agent generates a sequence of tokens, but not all of them need to be returned to the environment (shown to the user). For example, consider solving a math problem. The agent may want to generate a a "**Chain of Thought**" [Wei+22], representing intermediate internal calculations, before returning the final answer (e.g., "42"). Models that act like this are often said to be doing "**reasoning**" or "**thinking**", although in less anthropomorphic terms, we can think of them as just policies with dynamically unrolled computational graphs.

Although thinking models are usually only applied in the single-turn (contextual bandit) setting (e.g., computing an answer to a question on some leaderboard), they can be extended to the multi-turn RL setting, in order to define policies that can both think internally and act externally. For example, consider the **RAGEN** system of [Wan+25], which is illustrated in Figure 6.2. Here we define define $A_t = (m_t^{1:N}, a_t)$ as a sequence of $N$ internal "mental tokens" $m_t^i$, followed by the external action token $a_t$ (with suitable delimeters, such as `<think>` and `<ans>` added to the output sequence as necessary). The policy is just an LLM of the form

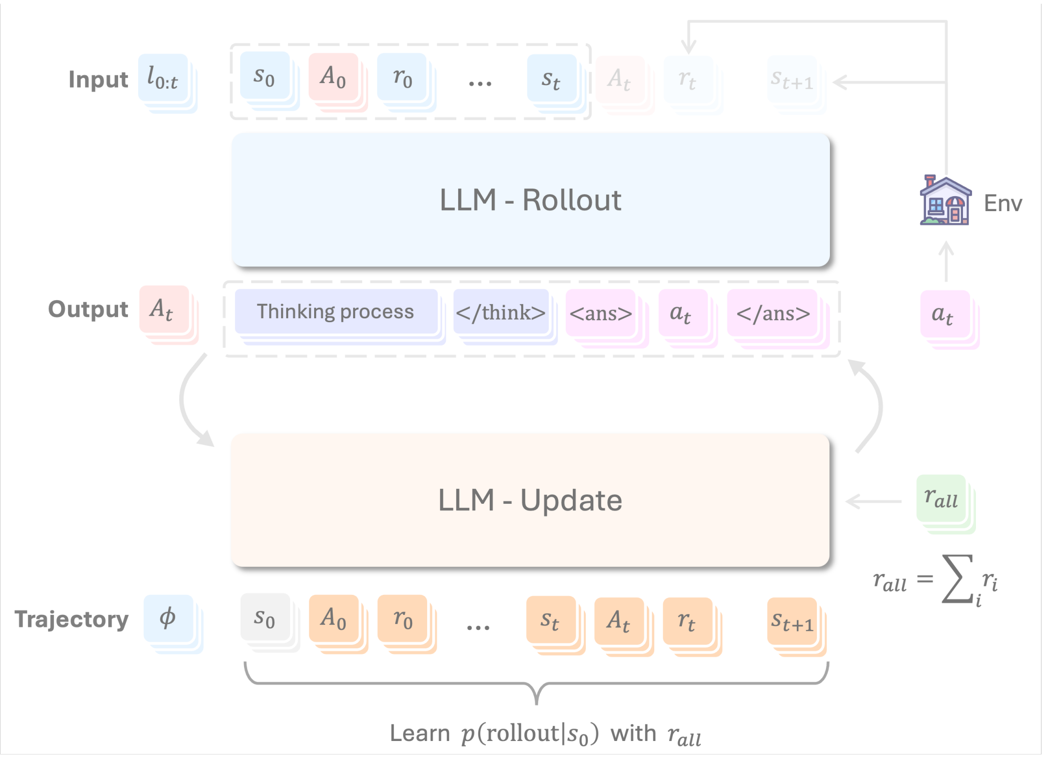


*Figure 6.2: Illustration of how to train an LLM to both "think" internally and "act" externally. From [Wan+25]. Used with kind permission of Zihan Wang.*

$\pi(A_t|s_t, h_{0:t-1})$, where $s_t$ is the current environment state, and the history $h_{0:t}$ contains any initial prompt, plus previous states $s_{0:t-1}$, external actions $a_{0:t-1}$ and rewards $r_{0:t-1}$. The final action $a_t$ is extracted from $A_t$ and passed to the environment to get $(s_{t+1}, r_t) = \text{env.step}(s_t, a_t)$. (Note that the reward only depends on the external action $a_t$, not on the internal thoughts $\boldsymbol{m}_t$.) The policy network is trained to generate action sequences $A_{0:t}$ (including internal thinking actions) based on $K$ MC rollouts $\tau^k = (s_0^k, A_0^k, r_0^k, s_1^k, A_1^k, r_1^k, \ldots)$, which are passed to some kind of policy gradient algorithm, as we discuss below.

#### 6.1.2.2 DeepSeek-R1, ChatGPT-o1, Gemini-Thinking, etc

We can train a thinking model, just like any other policy, provided we have a reliable reward function, as is the case in math and coding problems. (If we don't know the reward function, we may be able to learn it from data, as we discuss in Section 6.1.3.1.) This was recently demonstrated by the **DeepSeek-R1-Zero** system [Dee25] (released by a Chinese company in January 2025). They started with a strong LLM base model, known as **DeepSeek-V3-Base** [Dee24], which was pre-trained (using standard SFT) on a large variety of data (including Chains of Thought). They then used a variant of PPO, known as GRPO (see Section 6.1.2.3) to do RLFT, using a set math and coding benchmarks where the ground truth answer is known. (In [Lam+24], they call this "**RL with verifiable rewards**", as opposed to the learned rewards we discuss in Section 6.1.3.1.) The resulting system got excellent performance on math and coding benchmarks. Furthermore, during the training process, it exhibited some "emergent abilities", such as generating increasingly long sequence of thoughts, and using self-reflection to refine its thinking, before generating the final answer.[3]

Although DeepSeek-R1-Zero exhibited excellent performance on math and coding benchmarks, it did not work as well on more general reasoning benchmarks. So their final system, called DeepSeek-R1, combined RL training with more traditional SFT (on synthetically generated CoTs). They also released a smaller, distilled version of their model, which is more efficient to run.

The closed-source models **ChatGPT-o1** and **ChatGPT-o3** from OpenAI[4] and the **Gemini 2.0 Flash Thinking** model from Google Deepmind[5] are believed to follow similar principles to DeepSeek-R1, although the details are not public.[6] For a very recent review of these methods. see e.g., [Xu+25]

#### 6.1.2.3 GRPO

The **GRPO** algorithm of [Sha+24], which was used to train DeepSeek-R1-Zero, is a variant of PPO which replaces the critic network with a Monte Carlo estimate of the value function, obtained by rolling out multiple action sequences, and averaging their terminal rewards. This is done to avoid the need to have two copies of the LLM, one for the actor and one for the critic, to save memory. In addition, they use the low-variance MC estimator of KL divergence proposed in `http://joschu.net/blog/kl-approx.html`, which has the form $D_{\mathbb{KL}}[Q, P] = E[r - \log r - 1]$, where $r = P(a)/Q(a)$, $P(a)$ is the reference policy $\pi_{\text{ref}}$ (e.g., the SFT base model), $Q(a)$ is the policy which is being optimized $\pi_{\boldsymbol{\theta}}$, and the expectations are wrt $Q(a)$. Thus the final GRPO objective (to be maximized) is $J = J_{ppo} - \beta J_{kl}$, where

$$J_{ppo} = E_q E_{o_i \sim \pi_{\boldsymbol{\theta}_{\text{old}}}(\cdot|q)} \min\left(\frac{\pi_{\boldsymbol{\theta}}(o_i|q)}{\pi_{\boldsymbol{\theta}_{\text{old}}}(o_i|q)} A_i, \text{clip}(\frac{\pi_{\boldsymbol{\theta}}(o_i|q)}{\pi_{\boldsymbol{\theta}_{\text{old}}}(o_i|q)}) A_i\right) \tag{6.3}$$

$$J_{kl} = E_q E_{o_i \sim \pi_{\boldsymbol{\theta}}(\cdot|q)} [r_i - \log r_i - 1] \tag{6.4}$$

$$r_i = \frac{\pi_{\text{ref}}(o_i|q)}{\pi_{\boldsymbol{\theta}}(o_i|q)} \tag{6.5}$$

[3] Note that the claim that RL "caused" these emergent abilities has been disputed by many authors (see e.g., [Liu+25]); instead, the general concensus is that the base model itself was alrady trained on datasets that contained some COT-style reasoning patterns. This is consistent with the findings in [Gan+25a], which showed that applying RL to a base model that had not been pre-trained on reasoning patterns (such as self-reflection) did not result in a final model that could exhibit such behaviors, but RL can "expose" or "amplify" such abilities in a basemodel if they are already present to a certain extent.

[4] See `https://openai.com/index/learning-to-reason-with-llms/`.

[5] See `https://deepmind.google/technologies/gemini/flash-thinking`.

[6] However, shortly after the release of R1, the CRO of Open AI (Mark Chen) confirmed that o1 uses some of the same core ideas as R1: `https://x.com/markchen90/status/1884303237186216272?s=46&t=Vx_O-TgDXth-Mt_kw6ggqw`.

where $q$ is a sampled question and $o_i$ is a sampled output (answer). In practice, Eq. 1 of [Dee25] approximates the $J_{kl}$ term by sampling from $o_i \sim \pi_{\boldsymbol{\theta}_{\text{old}}}(\cdot|q)$.[7]

### 6.1.3 Reward models for LLMs

The main obstacle in using RL methods is defining the reward function. We discuss some methods below.

#### 6.1.3.1 RLHF

To train LLMs to do well in general tasks (beyond just math and coding), it is common to use **reinforcement learning from human feedback** or **RLHF**. The basic idea is as follows. We first generate a large number of (context, answer0, answer1) tuples, either by a human or an LLM. Then human raters are asked if they prefer answer 0 or answer 1. Let $y = 0$ denote the event that they prefer answer 0, and $y = 1$ the event that they prefer answer 1. We can then fit a **Bradley Terry choice model** of the form

$$p(y = 0|a_0, a_1, s) = \frac{\exp(\phi(s, a_0))}{\exp(\phi(s, a_0)) + \exp(\phi(s, a_1))} \tag{6.6}$$

by minizing the binary cross entropy loss wrt $\phi$, where $\phi(s, a)$ is some function that returns a scalar, representing the logit. (Typically $\phi(s, a)$ is a shallow MLP on top of the last layer of a pretrained LLM.)

After training, we define the reward function as $R(s, a) = \phi(s, a)$, and then use this reward to fine-tune the LLM using standard RL methods, such as PPO (see [Hua+24]). It is also possible to optimize the preferences directly, without fitting a reward model, using the **DPO** (Direct Preference Optimization) method of [Raf+23].

For more details on RLHF, see `https://rlhfbook.com/`.

#### 6.1.3.2 Other kinds of reward models

Besides verifiable rewards and RLHF, it is possible to design various other kind of reward function. If we use a frozen prompted LLM as the reward function, the approach is called **RLAIF** (RL from AI feedback) or **RLMF** (RL from machine feedback). We can also use execution feedback (from running a program) [Geh+24], which is known as **RLEF**. For more details, see e.g., [Kau+23; Lam25].

#### 6.1.3.3 Outcome vs process reward

An **Outcome Reward Model** (ORM) is a function of the form $R(s, A) = R(s, (m_{1:N}, a)) = R(s, a)$, which only rewards the final action, rather than the intermediate thought tokens. This can result in very sparse feedback. Better results can sometimes be obtained if we convert the sparse ORM reward into a dense per-step reward; this sometimes called a **Process Reward Model** or PRM.

### 6.1.4 Assistance game

In general, any objective-maximizing agent may suffer from reward hacking (Section 1.3.6.2), even if the reward has been learned using lots of RLHF data. In [Rus19], Stuart Russell proposed a clever solution to this problem. Specifically, the human and machine are both treated as agents in a two-player cooperative game, called an **assistance game**, where the machine's goal is to maximize the user's utility (reward) function, which is inferred based on the human's behavior using inverse RL. That is, instead of trying to learn a point estimate of the reward function using RLHF, and then optimizing that, we treat the reward function as an unknown part of the environment. If we adopt a Bayesian perspective on this, we can maintain a posterior belief over the model parameters. This will incentivize the agent to perform information gathering actions. For example, if the machine is uncertain about whether something is a good idea or not, it will proceed

[7] Note that this is biased, as pointed out in `https://x.com/NandoDF/status/1884038052877680871`. However, the bias is likely small if $\boldsymbol{\theta}_{\text{old}}$ is close to $\boldsymbol{\theta}$. If it is a problem, it is easy to fix using importance sampling.

cautiously (e.g., by asking the user for their preference), rather than blindly solving the wrong problem. For more details on this framework, see [Sha+20].

## 6.2 LLMs for RL

In this section, we discuss how to use LLMs to help create agents that themselves may or may not use language. The LLMs can be used for their prior knowledge, their ability to generate code, their "reasoning" ability, and their ability to perform **in-context learning**. The survey in [Cao+24] groups the literature into four main categories: LLMs for pre-processing the inputs, LLMs for rewards, LLMs for world models, and LLMs for decision making or policies. In our brief presentation below, we follow this categorization. See also e.g., [Spi+24; Hu+24; Pte+24] for more information.

### 6.2.1 LLMs for pre-processing the input

If the input observations $\boldsymbol{o}_t$ sent to the agent are in natural language (or some other textual representation, such as JSON), it is natural to use an LLM to process them, in order to compute a more compact representation, $\boldsymbol{s}_t = \boldsymbol{\phi}(\boldsymbol{o}_t)$, where $\boldsymbol{\phi}$ can the hidden state of the last layer of an LLM. This encoder can either be frozen, or fine-tuned with the policy network. Note that we can also pass in the entire past observation history, $\boldsymbol{o}_{1:t}$, as well as static "side information", such as instruction manuals or human hints; these can all be concatenated to form the LLM prompt.

For example, the **AlphaProof** system[8] uses an LLM (called the "formalizer network") to translate an informal specification of a math problem into the formal Lean representation, which is then passed to an agent (called the "solver network") which is trained, using the AlphaZero method (see Section 4.2.2.1), to generate proofs inside the Lean theorem proving environment. In this environment, the reward is 0 or 1 (proof is correct or not), the state space is a structured set of previously proved facts and the current goal, and the action space is a set of proof tactics. The agent itself is a separate transformer policy network (distinct from the formalizer network) that is a pre-trained LLM, that is fine-tuned on math, Lean and code, and then further trained using RL.

If the observations are images, it it is traditional to use a CNN to proccess the input, so $\boldsymbol{s}_t \in \mathbb{R}^N$ would be an embedding vector. However, we could alternatively use a VLM to compute a structured representation, where $\boldsymbol{s}_t$ might be a set of tokens describing the scene at a high level. We then proceed as in the text case.

Note that the information that is extracted will heavily depend on the prompt that is used. Thus we should think of an LLM/VLM as an **active sensor** that we can control via prompts. Choosing how to control this sensor requires expanding the action space of the agent to include computational actions [Che+24d]. Note also that these kinds of "sensors" are very expensive to invoke, so an agent with some limits on its time and compute (which is all practical agents) will need to reason about the value of information and the cost of computation. This is called **metareasoning** [RW91]. Devising good ways to train agents to perform both computational actions (e.g., invoking an LLM or VLM) and environment actions (e.g., taking a step in the environment or calling a tool) is an open research problem.

### 6.2.2 LLMs for rewards

It is difficult to design a reward function to cause an agent to exhibit some desired behavior, as we discussed in Section 1.3.6. Fortunately LLMs can often help with this task. We discuss a few approaches below.

In [Kli+24], they present the **Motif** system, that uses an LLM in lieu of a human to provide preference judgements to an RLHF system. In more detail, a pre-trained policy is used to collect trajectories, from which pairs of states, $(\boldsymbol{o}, \boldsymbol{o}')$, are selected at random. The LLM is then asked which state is preferable, thus generating $(\boldsymbol{o}, \boldsymbol{o}', y)$ tuples, which can be used to train a binary classifier from which a reward model is extracted, as in Section 6.1.3.1. In [Kli+24], the observations $\boldsymbol{o}$ are text captions generated by the NetHack game, but the same method could be applied to images if we used a VLM instead of an LLM for learning

[8] See `https://deepmind.google/discover/blog/ai-solves-imo-problems-at-silver-medal-level/`.

the reward. The learned reward model is then used as a shaping function (Section 1.3.6.4) when training an agent in the NetHack environment, which has very sparse reward. In [Zhe+24] they extend this work to the online setting, avoiding the need for an informative offline trajectory dataset.

In [Ma+24], they present the **Eureka** system, that learns the reward using bilevel optimization, with RL on the inner loop and LLM-powered evolutionary search on the outer loop. In particular, in the inner loop, given a candidate reward function $R_i$, we use PPO to train a policy, and then return a scalar quality score $S_i = S(R_i)$. In the outer loop, we ask an LLM to generate a new set of reward functions, $R'_i$, given a population of old reward functions and their scores, $(R_i, S_i)$, which have been trained and evaluated in parallel on a fleet of GPUs. The prompt also includes the source code of the environment simulator. Each generated reward function $R_i$ is represented as a Python function, that has access to the ground truth state of the underlying robot simulator. The resulting system is able to learn a complex reward function that is sufficient to train a policy (using PPO) that can control a simulated robot hand to perform various dexterous manipulation tasks, including spinning a pen with its finger tips. In [Li+24], they present a somewhat related approach and apply it to Minecraft.

In [Ven+24], they propose **code as reward**, in which they prompt a VLM with an initial and goal image, and ask it to describe the corresponding sequence of tasks needed to reach the goal. They then ask the LLM to synthesize code that checks for completion of each subtask (based on processing of object properties, such as relative location, derived from the image). These reward functions are then "verified" by applying them to an offline set of expert and random trajectories; a good reward function should allocate high reward to the expert trajectories and low reward to the random ones. Finally, the reward functions are used as auxiliary rewards inside an RL agent.

There are of course many other ways an LLM could be used to help learn reward functions, and this remains an active area of research.

### 6.2.3 LLMs for world models

There are many papers that use transformers or diffusion models to represent the world model $p(s'|s, a)$, as we discussed in Section 4.4. Here we focus our attention on ways to use pre-trained foundation models as world models (WM).

[Yan+24] presents **UniSim**, which is an action-conditioned video diffusion model trained on large amounts of robotics and visual navigation data. Combined with a VLM reward model, this can be used for decision-time planning as follows: sample candidate action trajectories from a proposal, generate the corresponding images, feed them to the reward model, score the rollouts, and then pick the best action from this set. (Note that this is just standard MPC in image space with a diffusion WM and a random shooting planning algorithm.)

[TKE24] presents **WorldCoder**, which takes a very different approach. It prompts a frozen LLM to generate code to represent the WM $p(s'|s, a)$, which it then uses inside of a planning algorithm. The agent then executes this in the environment, and passes back failed predictions to the LLM, asking it to improve the WM. (This is related to the Eureka reward-learning system mentioned in Section 6.2.2.)

There are of course many other ways an LLM could be used to help learn world models, and this remains an active area of research.

### 6.2.4 LLMs for policies

Finally we turn to LLMs as policies.

More recently it has become popular to leverage pre-trained LLMs that are trained on web data, and then to repurpose them as "agents" using in-context learning. We can then sample an action from the policy $\pi(a_t|p_t, o_t, h_{t-1})$, where $p_t$ is a manually chosen prompt. This approach is used by the **ReAct** paper [Yao+22] which works by prompting the LLM to "think step-by-step" ("reasoning") and then to predict an action ("acting"). This approach can be extended by prompting the LLM to first retrieve relevant past examples from an external "memory", rather than explicitly storing the entire history $h_t$ in the context (this is called **retrieval augmented generation** or **RAG**); see Figure 6.3 for an illustration. Note that no explicit

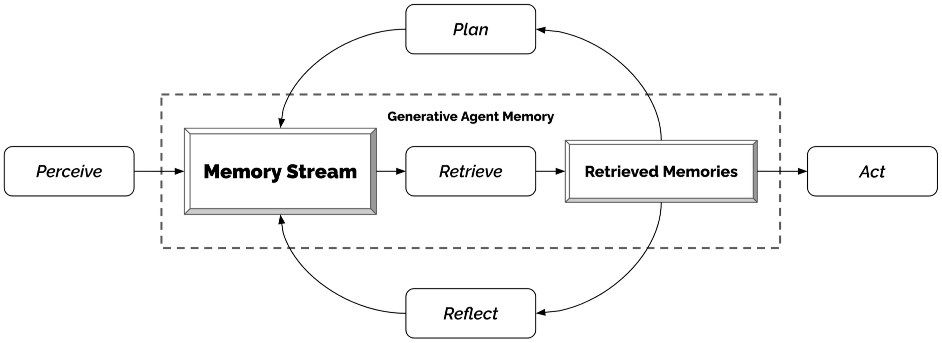


*Figure 6.3: Illustration of how to use a pretrained LLM (combined with RAG) as a policy. From Figure 5 of [Par+23]. Used with kind permission of Joon Park.*

learning (in the form of parametric updates) is performed in these systems; instead they rely entirely on in-context learning (and prompt engineering).

An alternative approach is to enumerate all possible discrete actions, and use the LLM to score them in terms of their likelihoods given the goal, and their suitability given a learned value function applied to the current state, i.e. $\pi(a_t = k|g, p_t, o_t, h_t) \propto \text{LLM}(w_k|g_t, p_t, h_t)V_k(o_t)$, where $g_t$ is the current goal, $w_k$ is a text description of action $k$, and $V_k$ is the value function for action $k$. This is the approach used in the robotics **SayCan** approach [Ich+23], where the primitive actions $a_k$ are separately trained goal-conditioned policies.

The above approaches do not train the LLM, but instead rely on in-context learning in order to adapt the policy. Better results can be obtained by using RL finetuning, as we discussed in Section 6.1.1. This can be even be used to train the agent to "think" before it acts.

Calling the LLM at every step is very slow, so an alternative is to use the LLM to generate code that represents (parts of) the policy. For example, the **Voyager** system in [Wan+24a] builds up a reusable skill library (represented as Python functions), by alternating between environment exploration and prompting the (frozen) LLM to generate new tasks and skills, given the feedback collected so far.

There are of course many other ways an LLM could be used to help learn policies, and this remains an active area of research.

Chapter 7

# Other topics in RL

In this section, we briefly mention some other important topics in RL.

## 7.1 Exploration-exploitation tradeoff revisited

In this section, we discuss solutions to the exploration-exploitation tradeoff that go beyond the simple heuristics introduced in Section 1.3.5.

### 7.1.1 Methods based on the belief state MDP

We can compute an optimal solution to the exploration-exploitation tradeoff by adopting a Bayesian approach to the problem. We start by computing the belief state MDP, as discussed in Section 1.2.5. We then compute the optimal policy, as we explain below.

#### 7.1.1.1 Bandit case (Gittins indices)

Suppose we have a way to compute the recursively compute the belief state over model parameters, $p(\boldsymbol{\theta}_t|\mathcal{D}_{1:t})$. How do we use this to solve for the policy in the resulting belief state MDP?

In the special case of context-free bandits with a finite number of arms, the optimal policy of this belief state MDP can be computed using dynamic programming. The result can be represented as a table of action probabilities, $\pi_t(a_1, \ldots, a_K)$, for each step; this are known as **Gittins indices** [Git89] (see [PR12; Pow22] for a detailed explanation). However, computing the optimal policy for general contextual bandits is intractable [PT87].

#### 7.1.1.2 MDP case (Bayes Adaptive MDPs)

We can extend the above techniques to the MDP case by constructing a **BAMDP**, which stands for "Bayes-Adaptive MDP" [Duf02]. However, this is computationally intractable to solve, so various approximations are made (see e.g., [Zin+21; AS22; Mik+20]).

### 7.1.2 Upper confidence bounds (UCBs)

The optimal solution to explore-exploit is intractable. However, an intuitively sensible approach is based on the principle known as "**optimism in the face of uncertainty**" (OFU). The principle selects actions greedily, but based on optimistic estimates of their rewards. The optimality of this approach is proved in the **R-Max** paper of [Ten02], which builds on the earlier **E3** paper of [KS02].

The most common implementation of this principle is based on the notion of an **upper confidence bound** or **UCB**. We will initially explain this for the bandit case, then extend to the MDP case.

#### 7.1.2.1 Basic idea

To use a UCB strategy, the agent maintains an optimistic reward function estimate $\tilde{R}_t$, so that $\tilde{R}_t(s_t, a) \geq R(s_t, a)$ for all $a$ with high probability, and then chooses the greedy action accordingly:

$$a_t = \operatorname*{argmax}_a \tilde{R}_t(s_t, a) \tag{7.1}$$

UCB can be viewed a form of **exploration bonus**, where the optimistic estimate encourages exploration. Typically, the amount of optimism, $\tilde{R}_t - R$, decreases over time so that the agent gradually reduces exploration. With properly constructed optimistic reward estimates, the UCB strategy has been shown to achieve near-optimal regret in many variants of bandits [LS19]. (We discuss regret in Section 1.1.2.)

The optimistic function $\tilde{R}$ can be obtained in different ways, sometimes in closed forms, as we discuss below.

#### 7.1.2.2 Bandit case: Frequentist approach

A frequentist approach to computing a confidence bound can be based on a **concentration inequality** [BLM16] to derive a high-probability upper bound of the estimation error: $|\hat{R}_t(s, a) - R_t(s, a)| \leq \delta_t(s, a)$, where $\hat{R}_t$ is a usual estimate of $R$ (often the MLE), and $\delta_t$ is a properly selected function. An optimistic reward is then obtained by setting $\tilde{R}_t(s, a) = \hat{R}_t(s, a) + \delta_t(s, a)$.

As an example, consider again the context-free Bernoulli bandit, $R(a) \sim \text{Ber}(\mu(a))$. The MLE $\hat{R}_t(a) = \hat{\mu}_t(a)$ is given by the empirical average of observed rewards whenever action $a$ was taken:

$$\hat{\mu}_t(a) = \frac{N_t^1(a)}{N_t(a)} = \frac{N_t^1(a)}{N_t^0(a) + N_t^1(a)} \tag{7.2}$$

where $N_t^r(a)$ is the number of times (up to step $t-1$) that action $a$ has been tried and the observed reward was $r$, and $N_t(a)$ is the total number of times action $a$ has been tried:

$$N_t(a) = \sum_{s=1}^{t-1} \mathbb{I}(a_t = a) \tag{7.3}$$

Then the **Chernoff-Hoeffding inequality** [BLM16] leads to $\delta_t(a) = c/\sqrt{N_t(a)}$ for some constant $c$, so

$$\tilde{R}_t(a) = \hat{\mu}_t(a) + \frac{c}{\sqrt{N_t(a)}} \tag{7.4}$$

#### 7.1.2.3 Bandit case: Bayesian approach

We can also derive an upper confidence about using Bayesian inference. If we use a beta prior, we can compute the posterior in closed form, as shown in Equation (1.22). The posterior mean is $\hat{\mu}_t(a) = \mathbb{E}[\mu(a)|\boldsymbol{h}_t] = \frac{\alpha_t^a}{\alpha_t^a + \beta_t^a}$, and the posterior standard deviation is approximately

$$\hat{\sigma}_t(a) = \sqrt{\mathbb{V}[\mu(a)|\boldsymbol{h}_t]} \approx \sqrt{\frac{\hat{\mu}_t(a)(1 - \hat{\mu}_t(a))}{N_t(a)}} \tag{7.5}$$

We can use similar techniques for a Gaussian bandit, where $p_R(R|a, \boldsymbol{\theta}) = \mathcal{N}(R|\mu_a, \sigma_a^2)$, $\mu_a$ is the expected reward, and $\sigma_a^2$ the variance. If we use a conjugate prior, we can compute $p(\mu_a, \sigma_a|\mathcal{D}_t)$ in closed form. Using an uninformative version of the conjugate prior, we find $\mathbb{E}[\mu_a|\boldsymbol{h}_t] = \hat{\mu}_t(a)$, which is just the empirical mean of rewards for action $a$. The uncertainty in this estimate is the standard error of the mean, i.e., $\sqrt{\mathbb{V}[\mu_a|\boldsymbol{h}_t]} = \hat{\sigma}_t(a)/\sqrt{N_t(a)}$, where $\hat{\sigma}_t(a)$ is the empirical standard deviation of the rewards for action $a$.

Once we have computed the mean and posterior standard deviation, we define the optimistic reward estimate as

$$\tilde{R}_t(a) = \hat{\mu}_t(a) + c\hat{\sigma}_t(a) \tag{7.6}$$

for some constant $c$ that controls how greedy the policy is. See Figure 7.1 for an illustration. We see that this is similar to the frequentist method based on concentration inequalities, but is more general.

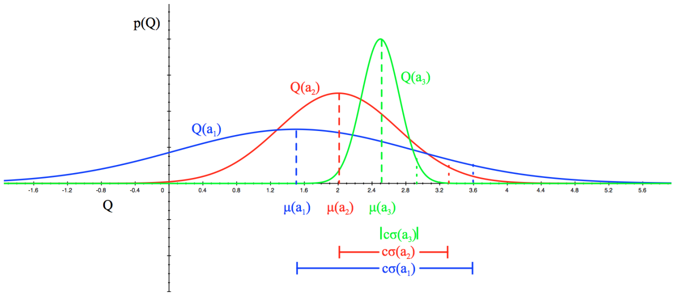


*Figure 7.1: Illustration of the reward distribution $Q(a)$ for a Gaussian bandit with 3 different actions, and the corresponding lower and upper confidence bounds. We show the posterior means $Q(a) = \mu(a)$ with a vertical dotted line, and the scaled posterior standard deviations $c\sigma(a)$ as a horizontal solid line. From [Sil18]. Used with kind permission of David Silver.*

#### 7.1.2.4 MDP case

The UCB idea (especially in its frequentist form) has been extended to the MDP case in several works. (The Bayesian version is discussed in Section 7.1.3.) For example, [ACBF02] proposes to combine UCB with Q learning, by defining the policy as

$$\pi(a|s) = \mathbb{I}\left(a = \underset{a'}{\operatorname{argmax}}\, Q(s,a') + c\sqrt{\log(t)/N_t(s,a')}\right) \tag{7.7}$$

[AJO08] presents the more sophisticated **UCRL2** algorithm, which computes confidence intervals on all the MDP model parameters at the start of each episode; it then computes the resulting **optimistic MDP** and solves for the optimal policy, which it uses to collect more data.

### 7.1.3 Thompson sampling

A common alternative to UCB is to use **Thompson sampling** [Tho33], also called **probability matching** [Sco10]. We start by describing this in the bandit case, then extend to the MDP case. For more details, see [Rus+18]. (See also [Ger18] for some evidence that humans use Thompson-sampling like mechanisms.)

#### 7.1.3.1 Bandit case

In Thompson sampling, we define the policy at step $t$ to be $\pi_t(a|s_t, \boldsymbol{h}_t) = p_a$, where $p_a$ is the probability that $a$ is the optimal action. This can be computed using

$$p_a = \Pr(a = a_*|s_t, \boldsymbol{h}_t) = \int \mathbb{I}\left(a = \underset{a'}{\operatorname{argmax}}\, R(s_t, a'; \boldsymbol{\theta})\right) p(\boldsymbol{\theta}|\boldsymbol{h}_t) d\boldsymbol{\theta} \tag{7.8}$$

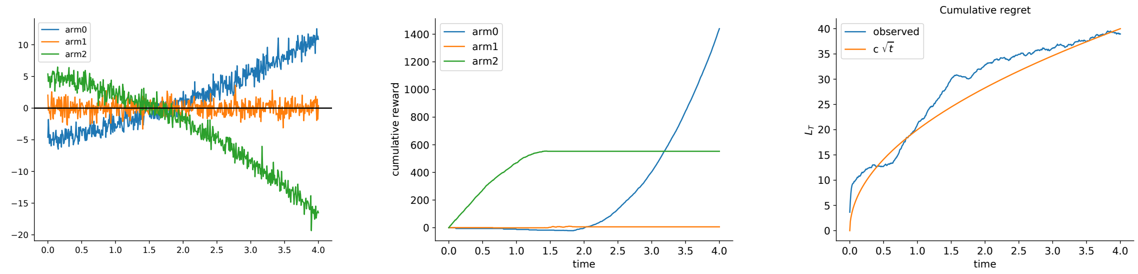
If the posterior is uncertain, the agent will sample many different actions, automatically resulting in exploration. As the uncertainty decreases, it will start to exploit its knowledge.

To see how we can implement this method, note that we can compute the expression in Equation (7.8) by using a single Monte Carlo sample $\tilde{\boldsymbol{\theta}}_t \sim p(\boldsymbol{\theta}|\boldsymbol{h}_t)$. We then plug in this parameter into our reward model, and greedily pick the best action:

$$a_t = \underset{a'}{\operatorname{argmax}}\, R(s_t, a'; \tilde{\boldsymbol{\theta}}_t) \tag{7.9}$$

This sample-then-exploit approach will choose actions with exactly the desired probability, since

$$p_a = \int \mathbb{I}\left(a = \underset{a'}{\operatorname{argmax}}\, R(s_t, a'; \tilde{\boldsymbol{\theta}}_t)\right) p(\tilde{\boldsymbol{\theta}}_t|\boldsymbol{h}_t) = \Pr_{\tilde{\boldsymbol{\theta}}_t \sim p(\boldsymbol{\theta}|\boldsymbol{h}_t)} (a = \underset{a'}{\operatorname{argmax}}\, R(s_t, a'; \tilde{\boldsymbol{\theta}}_t)) \tag{7.10}$$



(a)

(b)

(c)

*Figure 7.2: Illustration of Thompson sampling applied to a linear-Gaussian contextual bandit. The context has the form $\boldsymbol{s}_t = (1, t, t^2)$. (a) True reward for each arm vs time. (b) Cumulative reward per arm vs time. (c) Cumulative regret vs time. Generated by thompson_sampling_linear_gaussian.ipynb.*

Despite its simplicity, this approach can be shown to achieve optimal regret (see e.g., [Rus+18] for a survey). In addition, it is very easy to implement, and hence is widely used in practice [Gra+10; Sco10; CL11].

In Figure 7.2, we give a simple example of Thompson sampling applied to a linear regression bandit. The context has the form $\boldsymbol{s}_t = (1, t, t^2)$. The true reward function has the form $R(\boldsymbol{s}_t, a) = \boldsymbol{w}_a^\mathsf{T} \boldsymbol{s}_t$. The weights per arm are chosen as follows: $\boldsymbol{w}_0 = (-5, 2, 0.5)$, $\boldsymbol{w}_1 = (0, 0, 0)$, $\boldsymbol{w}_2 = (5, -1.5, -1)$. Thus we see that arm 0 is initially worse (large negative bias) but gets better over time (positive slope), arm 1 is useless, and arm 2 is initially better (large positive bias) but gets worse over time. The observation noise is the same for all arms, $\sigma^2 = 1$. See Figure 7.2(a) for a plot of the reward function. We use a conjugate Gaussian-gamma prior and perform exact Bayesian updating. Thompson sampling quickly discovers that arm 1 is useless. Initially it pulls arm 2 more, but it adapts to the non-stationary nature of the problem and switches over to arm 0, as shown in Figure 7.2(b). In Figure 7.2(c), we show that the empirical cumulative regret in blue is close to the optimal lower bound in red.

#### 7.1.3.2 MDP case (posterior sampling RL)

We can generalize Thompson sampling to the (episodic) MDP case by maintaining a posterior over all the model parameters (reward function and transition model), sampling an MDP from this belief state at the start of each episode, solving for the optimal policy corresponding to the sampled MDP, using the resulting policy to collect new data, and then updating the belief state at the end of the episode. This is called **posterior sampling RL** [Str00; ORVR13; RR14; OVR17; WCM24].

As a more computationally efficient alternative, it is also possible to maintain a posterior over policies or $Q$ functions instead of over world models; see e.g., [Osb+23a] for an implementation of this idea based on **epistemic neural networks** [Osb+23b], and **epistemic value estimation** [SSTVH23] for an implementation based on Laplace approximation. Another approach is to use successor features (Section 4.5.4), where the $Q$ function is assumed to have the form $Q^\pi(s, a) = \boldsymbol{\psi}^\pi(s, a)^\mathsf{T} \boldsymbol{w}$. In particular, [Jan+19b] proposes **Sucessor Uncertainties**, in which they model the uncertainty over $\boldsymbol{w}$ as a Gaussian, $p(\boldsymbol{w}) = \mathcal{N}(\boldsymbol{\mu}_{\boldsymbol{w}}, \boldsymbol{\Sigma}_{\boldsymbol{w}})$. From this they can derive the posterior distribution over $Q$ values as

$$p(Q(s, a)) = \mathcal{N}(\boldsymbol{\Psi}^\pi \boldsymbol{\mu}_{\boldsymbol{w}}, \boldsymbol{\Psi}^\pi \boldsymbol{\Sigma}_{\boldsymbol{w}} (\boldsymbol{\Psi}^\pi)^\mathsf{T}) \tag{7.11}$$

where $\boldsymbol{\Psi}^\pi = [\boldsymbol{\psi}^\pi(s, a)]^\mathsf{T}$ is a matrix of features, one per state-action pair.

## 7.2 Distributional RL

The **distributional RL** approach of [BDM17; BDR23], predicts the distribution of (discounted) returns, not just the expected return. More precisely, let $Z^\pi = \sum_{t=0}^{T} \gamma^t r_t$ be a random variable representing the reward-to-

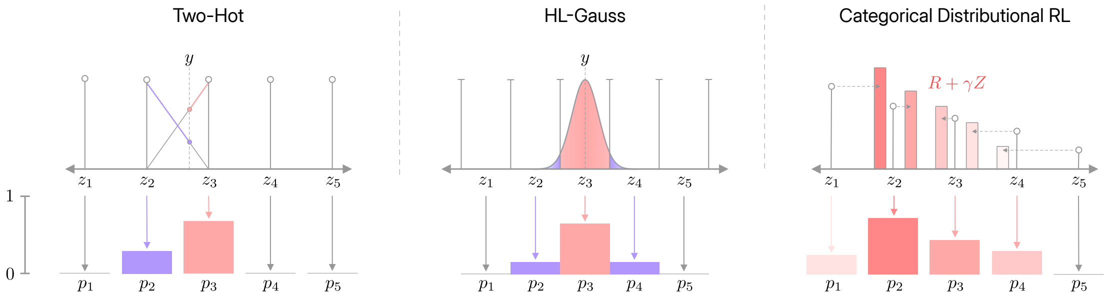


*Figure 7.3: Illustration of how to encode a scalar target $y$ or distributional target $Z$ using a categorical distribution. From Figure 1 of [Far+24]. Used with kind permission of Jesse Farebrother.*

go. The standard value function is defined to compute the expectation of this variable: $V^\pi(s) = \mathbb{E}[Z^\pi | s_0 = s]$. In DRL, we instead attempt to learn the full distribution, $p(Z^\pi | s_0 = s)$. For a general review of distributional regression, see [KSS23]. Below we briefly mention a few algorithms in this class that have been explored in the context of RL.

### 7.2.1 Quantile regression methods

An alternative to predicting a full distribution is to predict a fixed set of quantiles. This is called quantile regression, and has been used with DQN in [Dab+17] to get **QR-DQN**, and with SAC in [Wur+22] to get **QR-SAC**. (The latter was used in Sony's **GTSophy** Gran Turismo AI racing agent.)

### 7.2.2 Replacing regression with classification

An alternative to quantile regression is to approximate the distribution over returns using a histogram, and then fit it using cross entropy loss (see Figure 7.3). This approach was first suggested in [BDM17], who called it **categorical DQN**. (In their paper, they use 51 discrete categories (atoms), giving rise to the name **C51**.)

An even simpler approach is to replace the distributional target with the standard scalar target (representing the mean), and then discretize this target and use cross entropy loss instead of squared error.[1] Unfortunately, this encoding is lossy. In [Sch+20], they proposed the **two-hot** transform, that is a lossless encoding of the target based on putting appropriate weight on the nearest two bins (see Figure 7.3). In [IW18], they proposed the **HL-Gauss** histogram loss, that convolves the target value $y$ with a Gaussian, and then discretizes the resulting continuous distribution. This is more symetric than two-hot encoding, as shown in Figure 7.3. Regardless of how the discrete target is chosen, predictions are made using $\hat{y}(s; \boldsymbol{\theta}) = \sum_k p_k(s) b_k$, where $p_k(s)$ is the probability of bin $k$, and $b_k$ is the bin center.

In [Far+24], they show that the HL-Gauss trick works much better than MSE, two-hot and C51 across a variety of problems (both offline and online), especially when they scale to large networks. They conjecture that the reason it beats MSE is that cross entropy is more robust to noisy targets (e.g., due to stochasticity) and nonstationary targets. They also conjecture that the reason HL works better than two-hot is that HL is closer to ordinal regression, and reduces overfitting by having a softer (more entropic) target distribution (similiar to label smoothing in classification problems).

## 7.3 Intrinsic reward

When the extrinsic reward is sparse, it can be useful to (also) reward the agent for solving "generally useful" tasks, such as learning about the world. This is called **intrinsically motivated RL** [AMH23; Lin+19;

[1] Technically speaking, this is no longer a distributional RL method, since the prediction target is the mean, but the mechanism for predicting the mean leverages a distribution, for robustness and ease of optimization.

Ami+21; Yua22; Yua+24; Col+22]. It can be thought of as a special case of reward shaping, where the shaping function is dynamically computed.

We can classify these methods into two main types: **knowledge-based intrinsic motivation**, or **artificial curiosity**, where the agent is rewarded for learning about its environment; and **competence-based intrinsic motivation**, where the agent is rewarded for achieving novel goals or mastering new skills.

### 7.3.1 Knowledge-based intrinsic motivation

One simple approach to knowledge-based intrinsic motivation is to add to the extrinsic reward an intrinsic **exploration bonus** $R_t^i(s_t)$, which is high when the agent visits novel states. For tabular environments, we can just count the number of visits to each state, $N_t(s)$, and define $R_t^i(s) = 1/N_t(s)$ or $R_t^i(s) = 1/\sqrt{N_t(s)}$, which is similar to the UCB heuristic used in bandits (see Section 7.1.2). We can extend exploration bonuses to high dimensional states (e.g. images) using density models [Bel+16]. Alternatively, [MBB20] propose to use the $\ell_1$ norm of the successor feature (Section 4.5.4) representation as an alternative to the visitation count, giving rise to an intrinsic reward of the form $R^i(s) = 1/||\boldsymbol{\psi}^\pi(s)||_1$. Recently [Yu+23] extended this to combine SFs with *predecessor* representations, which encode retrospective information about the previous state (c.f., inverse dynamics models, mentioned below). This encourages exploration towards bottleneck states.

Another approach is the **Random Network Distillation** or **RND** method of [Bur+18]. This uses a fixed random neural network feature extractor $\boldsymbol{z}_t = f(\boldsymbol{s}_t; \boldsymbol{\theta}^*)$ to define a target, and then trains a predictor $\hat{\boldsymbol{z}}_t = f(\boldsymbol{s}_t; \hat{\boldsymbol{\theta}}_t)$ to predict these targets. If $\boldsymbol{s}_t$ is similar to previously seen states, then the trained model will have low prediction error. We can thus define the intrinsic reward as proportional to the squared error $||\hat{\boldsymbol{z}}_t - \boldsymbol{z}_t||_2^2$. The **BYOL-Explore** method of [Guo+22] goes beyond RND by learning the target representation (for the next state), rather than using a fixed random projection, but is still based on prediction error.

We can also define an intrinsic reward in terms of the information theoretic **surprise** of the next state given the current one:

$$R(\boldsymbol{s}, \boldsymbol{a}, \boldsymbol{s}') = -\log q(\boldsymbol{s}'|\boldsymbol{s}, \boldsymbol{a}) \tag{7.12}$$

This is the same as methods based on rewarding states for prediction error. Unfortunately such methods can suffer from the **noisy TV problem** (also called a **stochastic trap**), in which an agent is attracted to states which are intrinsically to predict. To see this, note that by averaging over future states we see that the above reward reduces to

$$R(\boldsymbol{s}, \boldsymbol{a}) = -\mathbb{E}_{p^*(\boldsymbol{s}'|\boldsymbol{s},\boldsymbol{a})}\left[\log q(\boldsymbol{s}'|\boldsymbol{s}, \boldsymbol{a})\right] = \mathbb{H}_{ce}(p^*, q) \tag{7.13}$$

where $p^*$ is the true model and $q$ is the learned dynamics model, and $\mathbb{H}_{ce}$ is the cross -entropy. As we learn the optimal model, $q = p^*$, this reduces to the conditional entropy of the predictive distribution, which can be non-zero for inherently unpredictable states.

To help filter out such random noise, [Pat+17] proposes an **Intrinsic Curiosity Module**. This first learns an **inverse dynamics model** of the form $a = f(\boldsymbol{s}, \boldsymbol{s}')$, which tries to predict which action was used, given that the agent was in $\boldsymbol{s}$ and is now in $\boldsymbol{s}'$. The classifier has the form $\text{softmax}(g(\phi(\boldsymbol{s}), \phi(s'), a))$, where $\boldsymbol{z} = \phi(\boldsymbol{s})$ is a representation function that focuses on parts of the state that the agent can control. Then the agent learns a forwards dynamics model in $\boldsymbol{z}$-space. Finally it defines the intrinsic reward as

$$R(\boldsymbol{s}, \boldsymbol{a}, \boldsymbol{s}') = -\log q(\phi(\boldsymbol{s}')|\phi(\boldsymbol{s}), a) \tag{7.14}$$

Thus the agent is rewarded for visiting states that lead to unpredictable consequences, where the difference in outcomes is measured in a (hopefully more meaningful) latent space.

Another solution is to replace the cross entropy with the KL divergence, $R(\boldsymbol{s}, \boldsymbol{a}) = D_{\mathbb{KL}}(p||q) = \mathbb{H}_{ce}(p, q) - \mathbb{H}(p)$, which goes to zero once the learned model matches the true model, even for unpredictable states. This has the desired effect of encouraging exploration towards states which have epistemic uncertainty (reducible noise) but not aleatoric uncertainty (irreducible noise) [MP+22]. The **BYOL-Hindsight** method of [Jar+23] is one recent approach that attempts to use the $R(\boldsymbol{s}, \boldsymbol{a}) = D_{\mathbb{KL}}(p||q)$ objective. Unfortunately, computing the $D_{\mathbb{KL}}(p||q)$ term is much harder than the usual variational objective of $D_{\mathbb{KL}}(q||p)$. A related

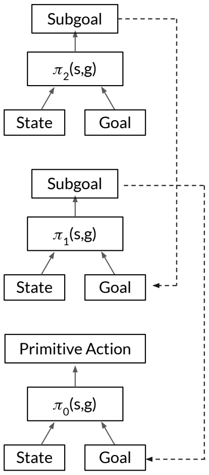


*Figure 7.4: Illustration of a 3 level hierarchical goal-conditioned controller. From* `http://bigai.cs.brown.edu/2019/09/03/hac.html`*. Used with kind permission of Andrew Levy.*

idea, proposed in the RL context by [Sch10], is to use the **information gain** as a reward. This is defined as $R_t(\boldsymbol{s}_t, \boldsymbol{a}_t) = D_{\mathbb{KL}}(q(\boldsymbol{s}_t|\boldsymbol{h}_t, \boldsymbol{a}_t, \boldsymbol{\theta}_t)||q(\boldsymbol{s}_t|\boldsymbol{h}_t, \boldsymbol{a}_t, \boldsymbol{\theta}_{t-1})$, where $\boldsymbol{h}_t$ is the history of past observations, and $\boldsymbol{\theta}_t = \text{update}(\boldsymbol{\theta}_{t-1}, \boldsymbol{h}_t, \boldsymbol{a}_t, \boldsymbol{s}_t)$ are the new model parameters. This is closely related to the BALD (Bayesian Active Learning by Disagreement) criterion [Hou+11; KAG19], and has the advantage of being easier to compute, since it is does not reference the true distribution $p$.

### 7.3.2 Goal-based intrinsic motivation

We will discuss goal-conditioned RL in Section 7.4.1. If the agent creates its own goals, then it provides a way to explore the environment. The question of when and how an agent to switch to pursuing a new goal is studied in [Pis+22] (see also [BS23]). Some other key work in this space includes the **scheduled auxiliary control** method of [Rie+18], and the **Go Explore** algorithm in [Eco+19; Eco+21] and its recent LLM extension [LHC24].

## 7.4 Hierarchical RL

So far we have focused on MDPs that work at a single time scale. However, this is very limiting. For example, imagine planning a trip from San Francisco to New York: we need to choose high level actions first, such as which airline to fly, and then medium level actions, such as how to get to the airport, followed by low level actions, such as motor commands. Thus we need to consider actions that operate multiple levels of **temporal abstraction**. This is called **hierarchical RL** or **HRL**. This is a big and important topic, and we only brief mention a few key ideas and methods. Our summary is based in part on [Pat+22]. (See also Section 4.5 where we discuss multi-step predictive models; by contrast, in this section we focus on model-free methods.)

### 7.4.1 Feudal (goal-conditioned) HRL

In this section, we discuss an approach to HRL known as **feudal RL** [DH92]. Here the action space of the higher level policy consists of **subgoals** that are passed down to the lower level policy. See Figure 7.4 for an illustration. The lower level policy learns a **universal policy** $\pi(a|s, g)$, where $g$ is the goal passed into it [Sch+15a]. This policy optimizes an MDP in which the reward is define as $R(s, a|g) = 1$ iff the goal state is achieved, i.e., $R(s, a|s) = \mathbb{I}(s = g)$. (We can also define a dense reward signal using some state abstraction function $\phi$, by definining $R(s,a|g) = \text{sim}(\phi(s), \phi(g))$ for some similarity metric.) This approach to RL is known as **goal-conditioned RL** [LZZ22].

#### 7.4.1.1 Hindsight Experience Relabeling (HER)

In this section, we discuss an approach to efficiently learning goal-conditioned policies, in the special case where the set of goal states $\mathcal{G}$ is the same as the set of original states $\mathcal{S}$. We will extend this to the hierarchical case below.

The basic idea is as follows. We collect various trajectores in the environment, from a starting state $s_0$ to some terminal state $s_T$, and then define the goal of each trajectory as being $g = s_T$; this trajectory then serves as a demonstration of how to achieve this goal. This is called **hindsight experience relabeling** or **HER** [And+17]. This can be used to relabel the trajectories stored in the replay buffer. That is, if we have $(s, a, R(s|g), s', g)$ tuples, we replace them with $(s, a, R(s|g'), g')$ where $g' = s_T$. We can then use any off-policy RL method to learn $\pi(a|s,g)$. In [Eys+20], they show that HER can be viewed as a special case of maximum-entropy inverse RL, since it is estimating the reward for which the corresponding trajectory was optimal.

#### 7.4.1.2 Hierarchical HER

We can leverage HER to learn a hierarchical controller in several ways. In [Nac+18] they propose **HIRO** (Hierarchical Reinforcement Learning with Off-policy Correction) as a way to train a two-level controller. (For a two-level controller, the top level is often called the **manager**, and the low level the **worker**.) The data for the manager are transition tuples of the form $(s_t, g_t, \sum r_{t:t+c}, s_{t+c})$, where $c$ is the time taken for the worker to reach the goal (or some maximum time), and $r_t$ is the main task reward function at step $t$. The data for the worker are transition tuples of the form $(s_{t+i}, g_t, a_{t+i}, r_{t+i}^{g_t}, s_{t+i+1})$ for $i = 0 : c$, where $r_t^g$ is the reward wrt reaching goal $g$. This data can be used to train the two policies. However, if the worker fails to achieve the goal in the given time limit, all the rewards will be 0, and no learning will take place. To combat this, if the worker does not achieve $g_t$ after $c$ timesteps, the subgoal is relabeled in the transition data with another subgoal $g'_t$ which is sampled from $p(g|\tau)$, where $\tau$ is the observed trajectory. Thus both policies treat $g'_t$ as the goal in hindsight, so they can use the actually collected data for training

The **hierarchical actor critic** (HAC) method of [Lev+18] is a simpler version of HIRO that can be extended to multiple levels of hierarchy, where the lowest level corresponds to primitive actions (see Figure 7.4). In the HAC approach, the output subgoal in the higher level data, and the input subgoal in the lower-level data, are replaced with the actual state that was achieved in hindsight. This allows the training of each level of the hierarchy independently of the lower levels, by assuming the lower level policies are already optimal (since they achieved the specified goal). As a result, the distribution of $(s, a, s')$ tuples experienced by a higher level will be stable, providing a stationary learning target. By contrast, if all policies are learned simultaneously, the distribution becomes **non-stationary**, which makes learning harder. For more details, see the paper, or the corresponding blog post (with animations) at `http://bigai.cs.brown.edu/2019/09/03/hac.html`.

#### 7.4.1.3 Learning the subgoal space

In the previous approaches, the subgoals are defined in terms of the states that were achieved at the end of each trajectory, $g' = s_T$. This can be generalized by using a state abstraction function to get $g' = \phi(s_T)$. The methods in Section 7.4.1.2) assumed that $\phi$ was manually specified. We now mention some ways to learn $\phi$.

In [Vez+17], they present **Feudal Networks** for learning a two level hierarchy. The manager samples subgoals in a learned latent subgoal space. The worker uses distance to this subgoal as a reward, and is trained in the usual way. The manager uses the "transition gradient" as a reward, which is derived from the task reward as well as the distance between the subgoal and the actual state transition made by the worker. This reward signal is used to learn the manager policy and the latent subgoal space.

Feudal networks do not guarantee that the learned subgoal space will result in optimal behavior. In [Nac+19], they present a method to optimize the policy and $\phi$ function so as to minimize a bound on the suboptimality of the hierarchical policy. This approach is combined with HIRO (Section 7.4.1.2) to tackle the non-stationarity issue.

## 7.4.2 Options

The feudal approach to HRL is somewhat limited, since not all subroutines or skills can be defined in terms of reaching a goal state (even if it is a partially specified one, such as being in a desired location but without specifying the velocity). For example, consider the skill of "driving in a circle", or "finding food". The **options** framework is a more general framework for HRL first proposed in [SPS99]. We discuss this below.

### 7.4.2.1 Definitions

An option $\omega = (I, \pi, \beta)$ is a tuple consisting of: the **initiation set** $I_\omega \subset S$, which is a subset of states that this option can start from (also called the **affordances** of each state [Khe+20]); the **subpolicy** $\pi_\omega(a|s) \in [0,1]$; and the **termination condition** $\beta_\omega(s) \in [0,1]$, which gives the probability of finishing in state $s$. (This induces a geometric distribution over option durations, which we denote by $\tau \sim \beta_\omega$.) The set of all options is denoted $\Omega$.

To execute an option at step $t$ entails choosing an action using $a_t = \pi_\omega(s_t)$ and then deciding whether to terminate at step $t+1$ with probability $1 - \beta_\omega(s_{t+1})$ or to continue following the option at step $t+1$. (This is an example of a **semi-Markov decision process** [Put94].) If we define $\pi_\omega(s) = a$ and $\beta_\omega(s) = 0$ for all $s$, then this option corresponds to primitive action $a$ that terminates in one step. But with options we can expand the repertoire of actions to include those that take many steps to finish.

To create an MDP with options, we need to define the reward function and dynamics model. The reward is defined as follows:

$$R(s,\omega) = \mathbb{E}\left[R_1 + \gamma R^2 + \cdots + \gamma^{\tau-1} R_\tau | S_0 = s, A_{0:\tau-1} \sim \pi_\omega, \tau \sim \beta_\omega\right] \tag{7.15}$$

The dynamics model is defined as follows:

$$p_\gamma(s'|s,\omega) = \sum_{k=1}^{\infty} \gamma^k \Pr\left(S_k = s', \tau = k | S_0 = s, A_{0:k-1} \sim \pi_\omega, \tau \sim \beta_\omega\right) \tag{7.16}$$

Note that $p_\gamma(s'|s,\omega)$ is not a conditional probability distribution, because of the $\gamma^k$ term, but we can usually treat it like one. Note also that a dynamics model that can predict multiple steps ahead is sometimes called a **jumpy model** (see also Section 4.5.3.2).

We can use these definitions to define the value function for a hierarchical policy using a generalized Bellman equation, as follows:

$$V_\pi(s) = \sum_{\omega \in \Omega(s)} \pi(\omega|s)\left[R(s,\omega) + \sum_{s'} p_\gamma(s'|s,\omega) V_\pi(s')\right] \tag{7.17}$$

We can compute this using value iteration. We can then learn a policy using policy iteration, or a policy gradient method. In other words, once we have defined the options, we can use all the standard RL machinery.

Note that GCRL can be considered a special case of options where each option corresponds to a different goal. Thus the reward function has the form $R(s,\omega) = \mathbb{I}(s = \omega)$, the termination function is $\beta_\omega(s) = \mathbb{I}(s = \omega)$, and the initiation set is the entire state space.

### 7.4.2.2 Learning options

The early work on options, including the **MAXQ** approach of [Die00], assumed that the set of options was manually specified. Since then, many methods for learning options have been proposed. We mention a few of these below.

The first set of methods for option learning rely on two stage training. In the first stage, exploration methods are used to collect trajectories. Then this data is analysed, either by inferring hidden segments using EM applied to a latent variable model [Dan+16], or by using the **skill chaining** method of [KB09], which uses classifiers to segment the trajectories. The labeled data can then be used to define a set of options, which can be trained using standard methods.

The second set of methods for option learning use end-to-end training, i.e., the options and their policies are jointly learned online. For example, [BHP17] propose the **option-critic** architecture. The number of options is manually specified, and all policies are randomly initialized. Then they are jointly trained using policy gradient methods designed for semi-MDPs. (See also [RLT18] for a hierarchical extension of option-critic to support options calling options.) However, since the learning signal is just the main task reward, the method can work poorly in problems with sparse reward compared to subgoal methods (see discussion in [Vez+17; Nac+19]).

Another problem with option-critic is that it requires specialized methods that are designed for optimizing semi-MDPs. In [ZW19], they propose **double actor critic**, which allows the use of standard policy gradient methods. This works by defining two parallel **augmented MDPs**, where the state space of each MDP is the cross-product of the original state space and the set of options. The manager learns a policy over options, and the worker learns a policy over states for each option. Both MDPs just use task rewards, without subgoals or subtask rewards.

It has been observed that option learning using option-critic or double actor-critic can fail, in the sense that the top level controller may learn to switch from one option to the next at almost every time step [ZW19; Har+18]. The reason is that the optimal policy does not require the use of temporally extended options, but instead can be defined in terms of primitive actions (as in standard RL). Therefore in [Har+18] they propose to add a regularizer called the **deliberation cost**, in which the higher level policy is penalized whenever it switches options. This can speed up learning, at the cost of a potentially suboptimal policy.

Another possible failure mode in option learning is if the higher level policy selects a single option for the entire task duration. To combat this, [KP19] propose the **Interest Option Critic**, which learns the initiation condition $I_\omega$ so that the option is selected only in certain states of interest, rather than the entire state space.

In [Mac+23], they discuss how the successor representation (discussed in Section 4.5) can be used to define options, using a method they call the **Representation-driven Option Discovery** (ROD) cycle.

In [Lin+24b] they propose to represent options as programs, which are learned using LLMs.

## 7.5 Imitation learning

In previous sections, an RL agent is to learn an optimal sequential decision making policy so that the total reward is maximized. **Imitation learning** (IL), also known as **apprenticeship learning** and **learning from demonstration** (LfD), is a different setting, in which the agent does not observe rewards, but has access to a collection $\mathcal{D}_{\text{exp}}$ of trajectories generated by an expert policy $\pi_{\text{exp}}$; that is, $\boldsymbol{\tau} = (s_0, a_0, s_1, a_1, \dots, s_T)$ and $a_t \sim \pi_{\text{exp}}(s_t)$ for $\boldsymbol{\tau} \in \mathcal{D}_{\text{exp}}$. The goal is to learn a good policy by imitating the expert, in the absence of reward signals. IL finds many applications in scenarios where we have demonstrations of experts (often humans) but designing a good reward function is not easy, such as car driving and conversational systems. (See also Section 7.6, where we discuss the closely related topic of offline RL, where we also learn from a collection of trajectories, but no longer assume they are generated by an optimal policy.)

### 7.5.1 Imitation learning by behavior cloning

A natural method is **behavior cloning**, which reduces IL to supervised learning; see [Pom89] for an early application to autonomous driving. It interprets a policy as a classifier that maps states (inputs) to actions (labels), and finds a policy by minimizing the imitation error, such as

$$\min_{\pi} \mathbb{E}_{p^{\gamma}_{\pi_{\text{exp}}}(s)} \left[ D_{\mathbb{KL}} \left( \pi_{\text{exp}}(s) \parallel \pi(s) \right) \right] \tag{7.18}$$

where the expectation wrt $p^\gamma_{\pi_{\text{exp}}}$ may be approximated by averaging over states in $\mathcal{D}_{\text{exp}}$. A challenge with this method is that the loss does not consider the sequential nature of IL: future state distribution is not fixed but instead depends on earlier actions. Therefore, if we learn a policy $\hat{\pi}$ that has a low imitation error under distribution $p^\gamma_{\pi_{\text{exp}}}$, as defined in Equation (7.18), it may still incur a large error under distribution $p^\gamma_{\hat{\pi}}$ (when the policy $\hat{\pi}$ is actually run). This problem has been tackled by the offline RL literature, which we discuss in Section 7.6.

### 7.5.2 Imitation learning by inverse reinforcement learning

An effective approach to IL is **inverse reinforcement learning** (IRL) or **inverse optimal control** (IOC). Here, we first infer a reward function that "explains" the observed expert trajectories, and then compute a (near-)optimal policy against this learned reward using any standard RL algorithms studied in earlier sections. The key step of reward learning (from expert trajectories) is the opposite of standard RL, thus called inverse RL [NR00].

It is clear that there are infinitely many reward functions for which the expert policy is optimal, for example by several optimality-preserving transformations [NHR99]. To address this challenge, we can follow the maximum entropy principle, and use an energy-based probability model to capture how expert trajectories are generated [Zie+08]:

$$p(\boldsymbol{\tau}) \propto \exp\big(\sum_{t=0}^{T-1} R_{\boldsymbol{\theta}}(s_t, a_t)\big) \tag{7.19}$$

where $R_{\boldsymbol{\theta}}$ is an unknown reward function with parameter $\boldsymbol{\theta}$. Abusing notation slightly, we denote by $R_{\boldsymbol{\theta}}(\boldsymbol{\tau}) = \sum_{t=0}^{T-1} R_{\boldsymbol{\theta}}(s_t, a_t))$ the cumulative reward along the trajectory $\boldsymbol{\tau}$. This model assigns exponentially small probabilities to trajectories with lower cumulative rewards. The partition function, $Z_{\boldsymbol{\theta}} \triangleq \int_{\boldsymbol{\tau}} \exp(R_{\boldsymbol{\theta}}(\boldsymbol{\tau}))$, is in general intractable to compute, and must be approximated. Here, we can take a sample-based approach. Let $\mathcal{D}_{\text{exp}}$ and $\mathcal{D}$ be the sets of trajectories generated by an expert, and by some known distribution $q$, respectively. We may infer $\boldsymbol{\theta}$ by maximizing the likelihood, $p(\mathcal{D}_{\text{exp}}|\boldsymbol{\theta})$, or equivalently, minimizing the negative log-likelihood loss

$$\mathcal{L}(\boldsymbol{\theta}) = -\frac{1}{|\mathcal{D}_{\text{exp}}|} \sum_{\boldsymbol{\tau} \in \mathcal{D}_{\text{exp}}} R_{\boldsymbol{\theta}}(\boldsymbol{\tau}) + \log \frac{1}{|\mathcal{D}|} \sum_{\boldsymbol{\tau} \in \mathcal{D}} \frac{\exp(R_{\boldsymbol{\theta}}(\boldsymbol{\tau}))}{q(\boldsymbol{\tau})} \tag{7.20}$$

The term inside the log of the loss is an importance sampling estimate of $Z$ that is unbiased as long as $q(\boldsymbol{\tau}) > 0$ for all $\boldsymbol{\tau}$. However, in order to reduce the variance, we can choose $q$ adaptively as $\boldsymbol{\theta}$ is being updated. The optimal sampling distribution, $q_*(\boldsymbol{\tau}) \propto \exp(R_{\boldsymbol{\theta}}(\boldsymbol{\tau}))$, is hard to obtain. Instead, we may find a policy $\hat{\pi}$ which induces a distribution that is close to $q_*$, for instance, using methods of maximum entropy RL discussed in Section 3.6.4. Interestingly, the process above produces the inferred reward $R_{\boldsymbol{\theta}}$ as well as an approximate optimal policy $\hat{\pi}$. This approach is used by **guided cost learning** [FLA16], and found effective in robotics applications.

### 7.5.3 Imitation learning by divergence minimization

We now discuss a different, but related, approach to IL. Recall that the reward function depends only on the state and action in an MDP. It implies that if we can find a policy $\pi$, so that $p^\gamma_\pi(s,a)$ and $p^\gamma_{\pi_{\text{exp}}}(s,a)$ are close, then $\pi$ receives similar long-term reward as $\pi_{\text{exp}}$, and is a good imitation of $\pi_{\text{exp}}$ in this regard. A number of IL algorithms find $\pi$ by minimizing the divergence between $p^\gamma_\pi$ and $p^\gamma_{\pi_{\text{exp}}}$. We will largely follow the exposition of [GZG19]; see [Ke+19] for a similar derivation.

Let $f$ be a convex function, and $\mathrm{D_f}$ be the corresponding $f$-divergence [Mor63; AS66; Csi67; LV06; CS04]. From the above intuition, we want to minimize $\mathrm{D_f}\left(p^\gamma_{\pi_{\text{exp}}} \middle\| p^\gamma_\pi\right)$. Then, using a variational approximation of $\mathrm{D_f}$ [NWJ10], we can solve the following optimization problem for $\pi$:

$$\min_\pi \max_{\boldsymbol{w}} \mathbb{E}_{p^\gamma_{\pi_{\text{exp}}}(s,a)}\left[T_{\boldsymbol{w}}(s,a)\right] - \mathbb{E}_{p^\gamma_\pi(s,a)}\left[f^*(T_{\boldsymbol{w}}(s,a))\right] \tag{7.21}$$

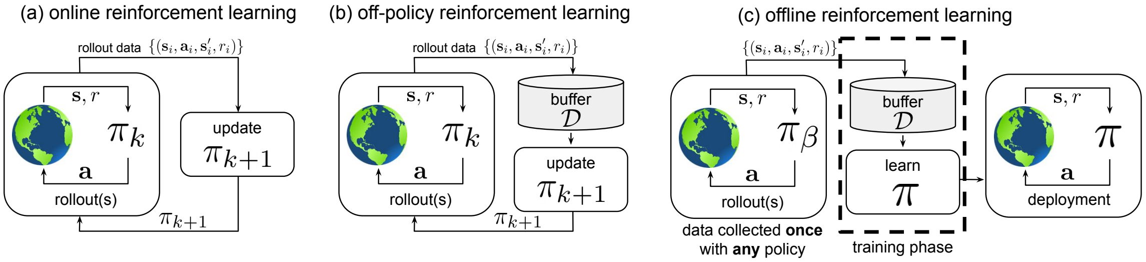

(a) online reinforcement learning
rollout data $\{(\mathbf{s}_i, \mathbf{a}_i, \mathbf{s}'_i, r_i)\}$
$\mathbf{s}, r$
$\pi_k$
$\mathbf{a}$
rollout(s)
update
$\pi_{k+1}$
$\pi_{k+1}$
(b) off-policy reinforcement learning
rollout data $\{(\mathbf{s}_i, \mathbf{a}_i, \mathbf{s}'_i, r_i)\}$
$\mathbf{s}, r$
$\pi_k$
$\mathbf{a}$
rollout(s)
buffer $\mathcal{D}$
update
$\pi_{k+1}$
$\pi_{k+1}$
(c) offline reinforcement learning
$\{(\mathbf{s}_i, \mathbf{a}_i, \mathbf{s}'_i, r_i)\}$
$\mathbf{s}, r$
$\pi_\beta$
$\mathbf{a}$
rollout(s)
data collected **once** with **any** policy
buffer $\mathcal{D}$
learn
$\pi$
training phase
$\mathbf{s}, r$
$\pi$
$\mathbf{a}$
deployment

*Figure 7.5: Comparison of online on-policy RL, online off-policy RL, and offline RL. From Figure 1 of [Lev+20a]. Used with kind permission of Sergey Levine.*

where $f^*$ is the convex conjugate of $f$, and $T_{\boldsymbol{w}} : \mathcal{S} \times \mathcal{A} \to \mathbb{R}$ is some function parameterized by $\boldsymbol{w}$. We can think of $\pi$ as a generator (of actions) and $T_{\boldsymbol{w}}$ as an adversarial critic that is used to compare the generated $(s, a)$ pairs to the real ones. Thus the first expectation can be estimated using $\mathcal{D}_{\text{exp}}$, as in behavior cloning, and the second can be estimated using trajectories generated by policy $\pi$. Furthermore, to implement this algorithm, we often use a parametric policy representation $\pi_{\boldsymbol{\theta}}$, and then perform stochastic gradient updates to find a saddle-point to Equation (7.21). With different choices of the convex function $f$, we can obtain many existing IL algorithms, such as **generative adversarial imitation learning** (**GAIL**) [HE16] and **adversarial inverse RL** (**AIRL**) [FLL18], etc.

## 7.6 Offline RL

**Offline reinforcement learning** (also called **batch reinforcement learning** [LGR12]) is concerned with learning a reward maximizing policy from a fixed, static dataset, collected by some existing policy, known as the **behavior policy**. Thus no interaction with the environment is allowed (see Figure 7.5). This makes policy learning harder than the online case, since we do not know the consequences of actions that were not taken in a given state, and cannot test any such "counterfactual" predictions by trying them. (This is the same problem as in off-policy RL, which we discussed in Section 3.5.) In addition, the policy will be deployed on new states that it may not have seen, requiring that the policy generalize out-of-distribution, which is the main bottleneck for current offline RL methods [Par+24b].

A very simple and widely used offline RL method is known as behavior cloning or BC. This amounts to training a policy to predict the observed output action $a_t$ associated with each observed state $s_t$, so we aim to ensure $\pi(s_t) \approx a_t$, as in supervised learning. This assumes the offline dataset was created by an expert, and so falls under the umbrella of imitation learning (see Section 7.5.1 for details). By contrast, offline RL methods can leverage suboptimal data. We give a brief summary of some of these methods below. For more details, see e.g., [Lev+20b; Che+24b; Cet+24]. For some offline RL benchmarks, see DR4L [Fu+20], RL Unplugged [Gul+20], OGBench (Offline Goal-Conditioned benchmark) [Par+24a], and D5RL [Raf+24].

### 7.6.1 Offline model-free RL

In principle, we can tackle offline RL using the off-policy methods that we discussed in Section 3.5. These use some form of importance sampling, based on $\pi(a|s)/\pi_b(a|s)$, to reweight the data in the replay buffer $\mathcal{D}$, which was collected by the behavior policy, towards the current policy (the one being evaluated/ learned). Unfortunately, such methods only work well if the behavior policy is is close to the new policy. In the online RL case, this can be ensured by gradually updating the new policy away from the behavior policy, and then sampling new data from the updated policy (which becomes the new behavior policy). Unfortunately, this is not an option in the offline case. Thus we need to use other strategies to control the discrepancy between the behavior policy and learned policy, as we discuss below. (Besides the algorithmic techniques we discuss, another reliable way to get better offline RL performance is to train on larger, more diverse datasets, as shown in [Kum+23].)

#### 7.6.1.1 Policy constraint methods

In the **policy constraint** method, we use a modified form of actor-critic, which, at iteration $k$, uses an update of the form

$$Q^\pi_{k+1} \leftarrow \operatorname*{argmin}_Q \mathbb{E}_{(s,a,s')\sim\mathcal{D}}\left[\left(Q(s,a) - (R(s,a) + \gamma \mathbb{E}_{\pi_k(a'|s')}\left[Q^\pi_k(s',a')\right])\right)^2\right] \tag{7.22}$$

$$\pi_{k+1} \leftarrow \operatorname*{argmax}_\pi \mathbb{E}_{s\sim\mathcal{D}}\left[\mathbb{E}_{\pi(a|s)}\left[Q^\pi_{k+1}(s,a)\right]\right] \quad \text{s.t.} \quad D(\pi,\pi_b) \leq \epsilon \tag{7.23}$$

where $D(\pi(\cdot|s), \pi_b(\cdot|s))$ is a divergence measure on distributions, such as KL divergence or another $f$-divergence. This ensures that we do not try to evaluate the $Q$ function on actions $a'$ that are too dissimilar from those seen in the data buffer (for each sampled state $s$), which might otherwise result in artefacts similar to an adversarial attack.

As an alternative to adding a constraint, we can add a penalty of $\alpha D(\pi(\cdot|s), \pi_b(\cdot|s))$ to the target $Q$ value and the actor objective, resulting in the following update:

$$Q^\pi_{k+1} \leftarrow \operatorname*{argmin}_Q \mathbb{E}_{(s,a,s')\sim\mathcal{D}}\left[\left(Q(s,a) - (R(s,a) + \gamma \mathbb{E}_{\pi_k(a'|s')}\left[Q^\pi_k(s',a') - \alpha D(\pi_k(\cdot|s'), \pi_b(\cdot|s'))\right])\right)^2\right] \tag{7.24}$$

$$\pi_{k+1} \leftarrow \operatorname*{argmax}_\pi \mathbb{E}_{s\sim\mathcal{D}}\left[\mathbb{E}_{\pi(a|s)}\left[Q^\pi_{k+1}(s,a)\right] - \alpha D(\pi(\cdot|s'), \pi_b(\cdot|s'))\right] \tag{7.25}$$

One problem with the above method is that we have to fit a parametric model to $\pi_b(a|s)$ in order to evaluate the divergence term. Fortunately, in the case of KL, the divergence can be enforced implicitly, as in the **advantage weighted regression** or **AWR** method of [Pen+19], the **reward weighted regression** method of [PS07], the **advantage weighted actor critic** or **AWAC** method of [Nai+20], the **advantage weighted behavior model** or **ABM** method of [Sie+20], In this approach, we first solve (nonparametrically) for the new policy under the KL divergence constraint to get $\overline{\pi}_{k+1}$, and then we project this into the required policy function class via supervised regression, as follows:

$$\overline{\pi}_{k+1}(a|s) \leftarrow \frac{1}{Z}\pi_b(a|s)\exp\left(\frac{1}{\alpha}Q^\pi_k(s,a)\right) \tag{7.26}$$

$$\pi_{k+1} \leftarrow \operatorname*{argmin}_\pi D_{\mathbb{KL}}\left(\overline{\pi}_{k+1} \parallel \pi\right) \tag{7.27}$$

In practice the first step can be implemented by weighting samples from $\pi_b(a|s)$ (i.e., from the data buffer) using importance weights given by $\exp\left(\frac{1}{\alpha}Q^\pi_k(s,a)\right)$, and the second step can be implemented via supervised learning (i.e., maximum likelihood estimation) using these weights.

It is also possible to replace the KL divergence with an integral probability metric (IPM), such as the maximum mean discrepancy (MMD) distance, which can be computed from samples, without needing to fit a distribution $\pi_b(a|s)$. This approach is used in [Kum+19]. This has the advantage that it can constrain the support of the learned policy to be a subset of the behavior policy, rather than just remaining close to it. To see why this can be advantageous, consider the case where the behavior policy is uniform. In this case, constraining the learned policy to remain close (in KL divergence) to this distribution could result in suboptimal behavior, since the optimal policy may just want to put all its mass on a single action (for each state).

#### 7.6.1.2 Behavior-constrained policy gradient methods

Recently a class of methods has been developed that is simple and effective: we first learn a baseline policy $\pi(a|s)$ (using BC) and a Q function (using Bellman minimization) on the offline data, and then update the policy parameters to pick actions that have high expected value according to $Q$ and which are also likely under the BC prior. An early example of this is the $Q^\dagger$ algorithm of [Fuj+19]. In [FG21], they present the **DDPG+BC** method, which optimizes

$$\max_\pi J(\pi) = \mathbb{E}_{(s,a)\sim\mathcal{D}}\left[Q(s, \mu^\pi(s)) + \alpha \log \pi(a|s)\right] \tag{7.28}$$

where $\mu^\pi(s) = \mathbb{E}_{\pi(a|s)}[a]$ is the mean of the predicted action, and $\alpha$ is a hyper-parameter. As another example, the **DQL** method of [WHZ23] optimizes a diffusion policy using

$$\min_\pi \mathcal{L}(\pi) = \mathcal{L}_{\text{diffusion}}(\pi) + \mathcal{L}_q(\pi) = \mathcal{L}_{\text{diffusion}}(\pi) - \alpha \mathbb{E}_{s\sim\mathcal{D}, a\sim\pi(\cdot|s)}\left[Q(s, a)\right] \tag{7.29}$$

where the second term is a penalty derived from Conservative Q Learning (Section 7.6.1.4), that ensures the Q values do no tget too small. Finally, [Aga+22b] discusses how to transfer the policy from a previous agent to a new agent by combining BC with Q learning.

#### 7.6.1.3 Uncertainty penalties

An alternative way to avoid picking out-of-distribution actions, where the $Q$ function might be unreliable, is to add a penalty term to the $Q$ function based on the estimated epistemic uncertainty, given the dataset $\mathcal{D}$, which we denote by $\text{Unc}(P_D(Q^\pi))$, where $P_D(Q^\pi)$ is the distribution over $Q$ functions, and Unc is some metric on distributions. For example, we can use a deep ensemble to represent the distribution, and use the variance of $Q(s, a)$ across ensemble members as a measure of uncertainty. This gives rise to the following policy improvement update:

$$\pi_{k+1} \leftarrow \underset{\pi}{\text{argmax}}\, \mathbb{E}_{s\sim\mathcal{D}}\left[\mathbb{E}_{\pi(a|s)}\left[\mathbb{E}_{P_D(Q^\pi_{k+1})}\left[Q^\pi_{k+1}(s, a)\right]\right] - \alpha \text{Unc}(P_D(Q^\pi_{k+1}))\right] \tag{7.30}$$

For examples of this approach, see e.g., [An+21; Wu+21; GGN22].

#### 7.6.1.4 Conservative Q-learning and pessimistic value functions

An alternative to explicitly estimating uncertainty is to add a **conservative penalty** directly to the $Q$-learning error term. That is, we minimize the following wrt $\boldsymbol{w}$ using each batch of data $\mathcal{B}$:

$$\overline{\mathcal{E}}(\mathcal{B}, \boldsymbol{w}) = \alpha \mathcal{C}(\mathcal{B}, \boldsymbol{w}) + \mathcal{E}(\mathcal{B}, \boldsymbol{w}) \tag{7.31}$$

where $\mathcal{E}(\mathcal{B}, \boldsymbol{w}) = \mathbb{E}_{(s,a,s')\in\mathcal{B}}\left[(Q_{\boldsymbol{w}}(s, a) - (r + \gamma \max_{a'} Q_{\boldsymbol{w}}(s', a')))^2\right]$ is the usual loss for $Q$-learning, and $\mathcal{C}(\mathcal{B}, \boldsymbol{w})$ is some conservative penalty. In the **conservative Q learning** or **CQL** method of [Kum+20], we use the following penalty term:

$$\mathcal{C}(\mathcal{B}, \boldsymbol{w}) = \mathbb{E}_{s\sim\mathcal{B}, a\sim\pi(\cdot|s)}\left[Q_{\boldsymbol{w}}(s, a)\right] - \mathbb{E}_{(s,a)\sim\mathcal{B}}\left[Q_{\boldsymbol{w}}(s, a)\right] \tag{7.32}$$

If $\pi$ is the behavior policy, this penalty becomes 0.

### 7.6.2 Offline model-based RL

In Chapter 4, we discussed model-based RL, which can train a dynamics model given a fixed dataset, and then use this to generate synthetic data to evaluate and then optimize different possible policies. However, if the model is wrong, the method may learn a suboptimal policy, as we discussed in Section 4.3.3. This problem is particularly severe in the offline RL case, since we cannot recover from any errors by collecting more data. Therefore various conservative MBRL algorithms have been developed, to avoid exploiting model errors. For example, [Kid+20] present the **MOREL** algorithm, and [Yu+20a] present the **MOPO** algorithm. Unlike the value function uncertainty method of Section 7.6.1.3, or the conservative value function method of Section 7.6.1.4, these model-based methods add a penalty for visiting states where the model is likely to be incorrect.

In more detail, let $u(s,a)$ be an estimate of the uncertainty of the model's predictions given input $(s,a)$. In MOPO, they define a conservative reward using $\overline{R}(s,a) = R(s,a) - \lambda u(s,a)$, and in MOREL, they modify the MDP so that the agent enters an absorbing state with a low reward when $u(s,a)$ is sufficiently large. In both cases, it is possible to prove that the model-based estimate of the policy's performance under the modified reward or dynamics is a lower bound of the performance of the policy's true performance in the real MDP, provided that the uncertainty function $u$ is an error oracle, which means that is satisfies $D(M_{\boldsymbol{\theta}}(s'|s,a), M^*(s'|s,a)) \leq u(s,a)$, where $M^*$ is the true dynamics, and $M_{\boldsymbol{\theta}}$ is the estimated dynamics.

For more information on offline MBRL methods, see [Che+24c].

### 7.6.3 Offline RL using reward-conditioned sequence modeling

Recently an approach to offline RL based on sequence modeling has become very popular. The basic idea — known as **upside down RL** [Sch19] or **RvS** (RL via Supervised learning) [KPL19; Emm+21] — is to train a generative model over future states and/or actions conditioned on the observed reward, rather than predicting the reward given a state-action trajectory. At test time, the conditioning is changed to represent the desired reward, and futures are sampled from the model. The implementation of this idea then depends on what kind of generative model to use, as we discuss below.

The **trajectory transformer** method of [JLL21] learns a joint model of the form $p(\boldsymbol{s}_{1:T}, \boldsymbol{a}_{1:T}, \boldsymbol{r}_{1:T})$ using a transformer, and then samples from this using beam search, selecting the ones with high reward (similar to MPC, Section 4.2.4). The **decision transformer** [Che+21b] is related, but just generates action sequences, and conditions on the past observations and the future reward-to-go. That is, it fits

$$\underset{\boldsymbol{\theta}}{\operatorname{argmax}}\, \mathbb{E}_{p_{\mathcal{D}}} \left[\log \pi_{\boldsymbol{\theta}}(a_t | s_{0:t}, a_{0:t-1}, \text{RTG}_{0:t})\right] \tag{7.33}$$

where $\text{RTG}_t = \sum_{k=t}^{T} r_t$ is the return to go. (For a comparison of decision transformers to other offline RL methods, see [Bha+24].)

The **diffuser** method of [Jan+22] is a diffusion version of trajectory transformer, so it fits $p(\boldsymbol{s}_{1:T}, \boldsymbol{a}_{1:T}, \boldsymbol{r}_{1:T})$ using diffusion, where the action space is assumed to be continuous. They also replace beam search with classifier guidance. The **decision diffuser** method of [Aja+23] extends diffuser by using classifer-free guidance, where the conditioning signal is the reward-to-go, simlar to decision transformer. However, unlike diffuser, the decision diffuser just models the future state trajectories (rather than learning a joint distribution over states and actions), and infers the actions using an **inverse dynamics model** $a_t = \pi(s_t, s_{t+1})$, which is trained using supervised learning.

One problem with the above approaches is that conditioning on a desired return and taking the predicted action can fail dramatically in stochastic environments, since trajectories that result in a return may have only achieved that return due to chance [PMB22; Yan+23; Bra+22; Vil+22]. (This is related to the optimism bias in the control-as-inference approach discussed in Section 3.6.)

### 7.6.4 Hybrid offline/online methods

Despite the progress in offline RL, it is fundamentally more limited in what it can learn compared to online RL [OCD21]. Therefore, various hybrids of offline and online RL have been proposed, such as [Bal+23] and [Nak+23].

For example, [Nak+23] suggest pre-training with offline RL (specifically CQL) followed by online finetuning. Naively this does not work that well, because CQL can be too conservative, requiring the online learning to waste some time at the beginning fixing the pessimism. So they propose a small modification to CQL, known as **calibrated Q learning**. This simply prevents CQL from being too conservative, by replacing the CQL regularizer in Equation (7.32) with a slightly modified expression. Then online finetuning is performed in the usual way.

## 7.7 General RL, AIXI and universal AGI

The term "**general RL**" (see e.g., [Hut05; LHS13; HQC24; Maj21]) refers to the setup in which an agent receives a stream of observations $o_1, o_2, \ldots$ and rewards $r_1, r_2, \ldots$, and performs a sequence of actions in response, $a_1, a_2, \ldots$, but where we do not make any Markovian (or even stationarity) assumptions about the environment that generates the observation stream. Instead, we assume that the environment is a computable function or program $p^*$, which generated the observations $o_{1:t}$ and $r_{1:t}$ seen so far in response to the actions taken, $a_{1:t-1}$. We denote this by $U(p^*, \boldsymbol{a}_{1:t}) = (o_1 r_1 \cdots o_t r_t)$, where $U$ is a universal Turing machine. If we use the receeding horizon control strategy (see Section 4.2.4), the optimal action at each step is the one that maximizes the posterior expected reward-to-go (out to some horizon $m$ steps into the future). If we assume the agent represents the unknown environment as a program $p \in \mathcal{M}$, then the optimal action is given by the following **expectimax** formula:

$$a_t = \underset{a_t}{\operatorname{argmax}} \sum_{o_t, r_t} \cdots \max_{a_m} \sum_{o_m, r_m} [r_t + \cdots + r_m] \sum_{p : U(p, \boldsymbol{a}_{1:m}) = (o_1 r_1 \cdots o_m r_m)} \Pr(p) \tag{7.34}$$

where $\Pr(p)$ is the prior probability of $p$, and we assume the likelihood is 1 if $p$ can generate the observations given the actions, and is 0 otherwise.

One important question is: what is a reasonable prior over programs? In [Hut05], Marcus Hutter proposed to apply the idea of **Solomonoff induction** [Sol64] to the case of an online decision making agent. This amounts to using the prior $\Pr(p) = 2^{-\ell(p)}$, where $\ell(p)$ is the length of program $p$. This prior favors shorter programs, and the likelihood filters out programs that cannot explain the data. The resulting agent is known as **AIXI**, where "AI" stands for "Artificial Intelligence" and "XI" referring to the Greek letter $\xi$ used in Solomonoff induction. The AIXI agent has been called the "most intelligent general-purpose agent possible" [HQC24], and can be viewed as the theoretical foundation of (universal) **artificial general intelligence** or **AGI**.

Unfortunately, the AIXI agent is intractable to compute, for two main reasons: (1) it relies on Solomonoff induction and Kolmogorov complexity, both of which are intractable; and (2) the expectimax computation is intractable. Fortunately, various tractable approximations have been devised. In lieu of Kolmogorov complexity, we can use measures like MDL (minimum description length), and for Solomonoff induction, we can use various local search or optimization algorithms through suitable function classes. For the expectimax computation, we can use MCTS (see Section 4.2.2) to approximate it. Alternatively, [GM+24] showed that it is possible to use meta learning to train a generic sequence predictor, such as a transformer or LSTM, on data generated by random Turing machines, so that the transformer learns to approximate a universal predictor. Another approach is to learn a policy (to avoid searching over action sequences) using TD-learning (Section 2.3.2); the weighting term in the policy mixture requires that the agent predict its own future actions, so this approach is known as **self-AIXI** [Cat+23].

Note that AIXI is a normative theory for optimal agents, but is not very practical, since it does not take computational limitations into account. In [Aru+24a; Aru+24b], they describe an approach which extends the above Bayesian framework, while also taking into account the data budget (due to limited environment interactions) that real agents must contend with (which prohibits modeling the entire environment or finding the optimal action). This approach, known as **Capacity-Limited Bayesian RL** (CBRL), combines Bayesian inference, RL, and rate distortion theory, and can be seen as a normative theoretical foundation for computationally bounded rational agents.

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