

Chapter 3

Optimism and Bellman Equations

In the previous chapter, we ran the policy gradient algorithm on two environments: CartPole and Pong. We observed that finding the optimal policy was much easier in CartPole than in Pong. This naturally raises the question: what makes some RL problems easier than others?

By “easy,” we mean problems for which we can design algorithms that are efficient in both sample complexity (the amount of interaction required) and computational complexity (the amount of computation, e.g., GPU hours, needed).

This chapter will focus on: when can we design sample efficient RL algorithms? This chapter introduces two core algorithmic ideas in reinforcement learning theory: *optimism* and *bellman equations*. These principles underlie many sample-efficient algorithms across various settings, including Linear Bellman-Complete MDPs [5], Linear MDPs [6], Deterministic linear Q^* [7], and more. The first attempt to generalize these ideas was made in [8]. A broader overview can be found in [9].

In this chapter, we focus on the simplest such setting—the *linear setting*—where the optimal value functions V^* and Q^* lie in a known linear function class.

Definition 3.1 (Linear V^* and Q^*). *We assume that the optimal value functions admit a known linear feature representation:*

- **Linear Q^* :** *There exists an unknown parameter vector $w^* \in \mathbb{R}^d$ and a known feature map $\phi : S \times A \rightarrow \mathbb{R}^d$ such that*

$$Q^*(s, a) = \langle w^*, \phi(s, a) \rangle \quad \text{for all } (s, a) \in S \times A.$$

- **Linear V^* :** *There exists an unknown parameter vector $\theta^* \in \mathbb{R}^d$ and a known feature map $\phi : S \rightarrow \mathbb{R}^d$ such that*

$$V^*(s) = \langle \theta^*, \phi(s) \rangle \quad \text{for all } s \in S.$$

We use the same notation ϕ for both feature maps, with the meaning clear from context.

We study the problem of learning a near-optimal policy in the finite-horizon linear setting, where the agent interacts with the environment and seeks a *sample-efficient* algorithm: one that learns a good policy using as few episodes as possible.

Definition 3.2 (Goal: Sample-Efficient Algorithm for Linear Setting). *Let $\varepsilon, \delta \in (0, 1)$ be accuracy and confidence parameters. The goal is to design an algorithm which, with probability at least $1 - \delta$, outputs a policy $\hat{\pi}$ such that*

$$V^{\hat{\pi}}(s_0) \geq V^*(s_0) - \varepsilon,$$

where V^* denotes the value of an optimal policy and s_0 is the starting state. The algorithm is *sample efficient* if the number of environment interactions required is polynomial in the feature dimension d , number of actions $|A|$, horizon H , and parameters $\varepsilon^{-1}, \log \delta^{-1}$.

3.1 Bellman Equation

A key observation behind our algorithm is the Bellman equation, which holds for all state-action pairs (s_h, a_h) :

$$Q_h^*(s_h, a_h) = \mathbb{E}_{\substack{s_{h+1} \sim T(s_h, a_h) \\ r_h \sim R(s_h, a_h)}} [r_h + V_{h+1}^*(s_{h+1})]. \quad (3.1)$$

This immediately implies:

$$\mathbb{E}_{\substack{s_{h+1} \sim T(s_h, a_h) \\ r_h \sim R(s_h, a_h)}} [Q_h^*(s_h, a_h) - r_h - V_{h+1}^*(s_{h+1})] = 0. \quad (3.2)$$

We are interested in analyzing this identity under the distribution induced by a policy, which we define next.

Definition 3.3 (Trajectory Distribution d^π). *Let π be a policy. The distribution d_h^π denotes the marginal over (s_h, a_h, r_h, s_{h+1}) at time h under policy π , with the following sampling process:*

- s_0 is the known starting state,
- $a_t \sim \pi(s_t)$, $s_{t+1} \sim T(s_t, a_t)$, and $r_t \sim R(s_t, a_t)$.

We write $d^\pi = \{d_0^\pi, \dots, d_{H-1}^\pi\}$ to denote the full set of marginals over the trajectory.

Taking expectations in Equation (3.2) over any distribution on (s_h, a_h) , including the trajectory distribution d^π induced by a policy π , preserves the identity:

$$\mathbb{E}_{(s_h, a_h, r_h, s_{h+1}) \sim d_h^\pi} [Q^*(s_h, a_h) - r_h - V_{h+1}^*(s_{h+1})] = 0. \quad (3.3)$$

For brevity, henceforth, we will use $\mathbb{E}_{d_h^\pi}$ to denote the above expectation. Finally, note that given a policy π , it is straightforward to sample from d^π by interacting with the environment: simply run π for multiple episodes and collect the tuples (s_h, a_h, r_h, s_{h+1}) at each time step h .

3.2 Algorithm

We now present a sample-efficient algorithm that iteratively constructs policies that are (a) *optimistic*, and (b) *approximately satisfy Bellman equation on past data*. At each iteration t , the algorithm uses data collected under previous policies $\pi_1, \dots, \pi_t$ to construct a new policy π_{t+1} that maximizes estimated value while ensuring that its Bellman residual (Equation (3.3)) is small under the empirical trajectory distributions from earlier policies.

Let $\hat{d}_h^{\pi_k}$ denote the empirical distribution over $n_{\text{emp}} = \text{poly}(d, H)$ transitions (s_h, a_h, r_h, s_{h+1}) collected from executing policy π_k . The number of samples collected per policy n_{emp} and the constraint parameter $\varepsilon_{\text{cons}}$ will be chosen later in the analysis.

Algorithm 2: Optimistic Algorithm

```

{1} for  $t = 1, 2, \dots, n_{\text{rounds}}$  do
{2}   Solve the following optimization problem:

           
$$\begin{aligned} & \max_{\theta, w} \langle \theta, \phi(s_0) \rangle \\ \text{s.t. } & \sum_{k=1}^{t-1} \mathbb{E}_{\hat{d}_h^{\pi_k}} \left[ \langle w, \phi(s_h, a_h) \rangle - r_h - \langle \theta, \phi(s_{h+1}) \rangle \right]^2 \leq \frac{\varepsilon^2}{\text{poly}(d, H)} \end{aligned}$$


           Here,  $\|\theta\|_2, \|w\|_2 \leq 1$  are norm constrained and satisfy
            $\langle \theta, \phi(s) \rangle = \max_a \langle w, \phi(s, a) \rangle$  for all states  $s$ .

{3}   Let  $\theta_t, w_t$  be the resulting parameters. Define  $\pi_t$  as the resulting
       policy defined by  $\pi_t(s) = \text{argmax}_a \langle w_t, \phi(s, a) \rangle$ .

{4}   Execute  $\pi_t$  for  $n_{\text{emp}}$  episodes, and use the collected data to
       construct empirical distributions  $\hat{d}^{\pi_t} = \{\hat{d}_h^{\pi_t}\}_{h=0}^{H-1}$ ;

{5} return the best policy  $\pi_t$  observed so far.;
```

3.3 Optimization Constraint in Linear Form

We begin by rewriting the constraint in our optimization program using the linear representations of the value functions. Recall that we denote the time-indexed value functions as Q_h^π and V_h^π , where $h \in \{0, \dots, H-1\}$. However, to keep notation light, we will suppress the dependence on h in the remainder of

this proof, with the understanding that the analysis applies separately at each time step.

At round t , let θ_t, w_t be the resulting parameters, and define π_t as the resulting policy defined by $\pi_t(s) = \operatorname{argmax}_a \langle w_t, \phi(s, a) \rangle$. Define the concatenated parameter and feature vectors:

$$\begin{aligned} W(\pi_t) &:= [w_t, \theta_t] \in \mathbb{R}^{2d}, \\ X(\pi_t) &:= \mathbb{E}_{d_h^{\pi_t}} [\phi(s_h, a_h), -\phi(s_{h+1})] \in \mathbb{R}^{2d}. \end{aligned}$$

Here, recall the notation $\mathbb{E}_{d_h^{\pi_t}}$ is shorthand for the expectation over samples $(s_h, a_h, s_{h+1}) \sim d_h^{\pi_t}$. The expected Bellman optimality equation for a candidate policy π_t at time step h is:

$$\mathbb{E}_{d^{\pi_t}} [\langle w_t, \phi(s_h, a_h) \rangle - r_h - \langle \theta_t, \phi(s_{h+1}) \rangle] \quad (3.4)$$

$$\begin{aligned} &= \mathbb{E}_{d^{\pi_t}} [\langle w_t, \phi(s_h, a_h) \rangle - \langle \theta_t, \phi(s_{h+1}) \rangle - Q^*(s_h, a_h) + V^*(s_{h+1})] \\ &= \langle W(\pi_t) - W(\pi^*), X(\pi_t) \rangle, \end{aligned} \quad (3.5)$$

where the first equality uses the Bellman identity for the optimal policy (Equation (3.3)) to replace r_h with $Q^*(s_h, a_h) - V^*(s_{h+1})$ in expectation.

3.4 Optimism: Bounding Regret

To analyze the regret, we relate the suboptimality of the current policy π_t to the difference between its parameters and those of the optimal value functions. The key idea is optimism: the algorithm selects θ_t, w_t to maximize $\langle \theta_t, \phi(s_0) \rangle$, which serves as an optimistic estimate of $V^{\pi_t}(s_0)$. Although this estimate may be inaccurate, the algorithm proceeds by acting according to π_t .

Lemma 3.4 (Regret Decomposition via Optimism). *Let the policy π_t , and vectors $W(\pi_t), X(\pi_t) \in \mathbb{R}^{2d}$ be as defined above. Then:*

$$V^*(s_0) - V^{\pi_t}(s_0) \leq \sum_{h=0}^{H-1} |\langle W(\pi_t) - W(\pi^*), X_h(\pi_t) \rangle|.$$

Proof. Throughout, we use that $a_h = \operatorname{argmax}_a \langle w_t, \phi(s_h, a) \rangle$. The claim follows

from:

$$\begin{aligned}
& V^*(s_0) - V^{\pi_t}(s_0) \\
& \leq \langle \theta_t, \phi(s_0) \rangle - V^{\pi_t}(s_0) \quad (\text{follows from optimism}) \\
& = \langle w_t, \phi(s_0, a_0) \rangle - \mathbb{E}_{d^{\pi_t}} \left[\sum_{h=0}^{H-1} r_h \right] \quad (\text{since } \langle \theta_t, \phi(s_0) \rangle = \langle w_t, \phi(s_0, a_0) \rangle) \\
& = \sum_{h=0}^{H-1} \mathbb{E}_{d_h^{\pi_t}} [\langle w_t, \phi(s_h, a_h) \rangle - r_h - \langle w_t, \phi(s_{h+1}, a_{h+1}) \rangle] \quad (\text{by telescoping sum}) \\
& = \sum_{h=0}^{H-1} \mathbb{E}_{d_h^{\pi_t}} [\langle w_t, \phi(s_h, a_h) \rangle - r_h - \langle \theta_t, \phi(s_{h+1}) \rangle] \\
& \quad (\text{since } \langle \theta_t, \phi(s_{h+1}) \rangle = \langle w_t, \phi(s_h, a_h) \rangle) \\
& \leq \sum_{h=0}^{H-1} |\langle W(\pi_t) - W(\pi^*), X_h(\pi_t) \rangle|. \quad (\text{follows from Equation (3.5)})
\end{aligned}$$

□

3.5 Exploration: Bounding the Number of Rounds

The final step is to bound how many rounds n_{rounds} are needed before the algorithm identifies a policy π_t with small suboptimality. We provide a simplified argument, which can be improved to obtain tighter bounds.

The key idea is that for large enough n_{emp} , the empirical distribution $\hat{d}_h^{\pi_k}$ concentrates around the true distribution $d_h^{\pi_k}$. Then, from the regret decomposition lemma above (Lemma 3.4), we know that if the residual term $\langle W(\pi_k) - W(\pi^*), X_h(\pi_k) \rangle$ is zero for all h , then the policy π_k is optimal. Otherwise, a nonzero residual indicates that π_k adds a new constraint that helps eliminate a portion of the hypothesis space.

More precisely, these constraints are linear in the difference vector $W(\pi) - W(\pi^*)$, and each non-redundant policy introduces a constraint that is at least ε -independent (Definition 3.5) of the previous ones. Since the vector space has finite dimension $2d$, only a bounded number of such ε -independent constraints can exist. This implies that the algorithm can only generate a finite number of meaningfully distinct (and suboptimal) policies before it must identify the optimal one.

Thus, it suffices to analyze the following situation: how many times can it happen that

$$\begin{aligned}
& \sum_{k=1}^{t-1} (\langle W(\pi_t) - W(\pi^*), X_h(\pi_k) \rangle)^2 \leq \varepsilon^2 \\
& \quad (\langle W(\pi_t) - W(\pi^*), X_h(\pi_t) \rangle)^2 > \varepsilon^2
\end{aligned}$$

This question—how many times an ε -independent constraint can arise—was first analyzed by Russo and Van Roy [10].

Definition 3.5 (ε -independence). *Let $S_d = \{\theta \in R^d : \|\theta\|_2 \leq 1\}$. We say $x_n \in S_d$ is ε -independent of sequence $\{x_1, x_2, \dots, x_{n-1}\}$ if there exists $\theta, \theta^* \in S_d$ such that*

$$\begin{aligned} \sum_{i=1}^{n-1} (\langle \theta, x_i \rangle - \langle \theta^*, x_i \rangle)^2 &\leq \varepsilon^2 \\ (\langle \theta, x_n \rangle - \langle \theta^*, x_n \rangle)^2 &> \varepsilon^2 \end{aligned}$$

We now bound the number of such ε -independent vectors that can appear in a sequence.

Lemma 3.6 (Bound on Number of ε -Independent Constraints). *Let $\{x_1, \dots, x_n\} \subseteq S_d$ be a sequence such that each x_k is ε -independent of the previous vectors in the sense of Definition 3.5. Then, the number n of such vectors is at most*

$$n = O\left(d \cdot \log\left(\frac{1}{\varepsilon}\right)\right).$$

Proof. More generally, assume that $\|x_k\|_2 \leq B_\phi$ for all k , and that $\|\theta - \theta^*\|_2 \leq 2B_\theta$. In our case, both B_ϕ and B_θ are 1.

Let $V_n := \sum_{i=1}^{n-1} x_i x_i^\top + \lambda I$ for some regularization $\lambda = \varepsilon^2 / (2B_\theta)^2$. If x_n is ε -independent of the previous $x_1, \dots, x_{n-1}$, then there exists θ, θ^* with $\|\theta - \theta^*\|_2 \leq 2B_\theta$ such that:

$$\sum_{i=1}^{n-1} (\langle \theta - \theta^*, x_i \rangle)^2 \leq \varepsilon^2, \quad \text{but} \quad (\langle \theta - \theta^*, x_n \rangle)^2 > \varepsilon^2.$$

This implies:

$$\begin{aligned} \varepsilon &\leq \left\{ (\theta - \theta^*)^\top x_n : (\theta - \theta^*)^\top \left(\sum_{i=1}^{n-1} x_i x_i^\top \right) (\theta - \theta^*) \leq \varepsilon^2 \quad \text{and} \quad (\theta - \theta^*)^\top I (\theta - \theta^*) \leq (2B_\theta)^2 \right\} \\ &\leq \max_{\rho} \left\{ \rho^\top x_n : \rho^\top \left(\sum_{i=1}^{n-1} x_i x_i^\top \right) \rho \leq \varepsilon^2 \quad \text{and} \quad \rho^\top I \rho \leq (2B_\theta)^2 \right\} \\ &\leq \max_{\rho} \left\{ \rho^\top x_n : \rho^\top \left(\sum_{i=1}^{n-1} x_i x_i^\top + \lambda I \right) \rho \leq 2\varepsilon^2 \right\} \\ &= \sqrt{2\varepsilon^2} \|x_n\|_{V_n^{-1}} \end{aligned}$$

And therefore,

$$\|x_n\|_{V_n^{-1}}^2 = x_n^\top V_n^{-1} x_n \geq \frac{1}{2}.$$

We now analyze the growth of $\det(V_n)$ using the matrix determinant lemma:

$$\begin{aligned}\det(V_n) &= \det(V_{n-1}) (1 + x_{n-1}^\top V_{n-1}^{-1} x_{n-1}) \\ &\geq \det(V_{n-1}) \cdot \frac{3}{2}.\end{aligned}$$

Iterating gives:

$$\det(V_n) \geq \det(\lambda I) \cdot \left(\frac{3}{2}\right)^{n-1} = \lambda^d \left(\frac{3}{2}\right)^{n-1}.$$

On the other hand, since $\text{trace}(V_n) \leq nB_\phi^2 + d\lambda$, we apply the AM–GM inequality:

$$\det(V_n) \leq \left(\frac{\text{trace}(V_n)}{d}\right)^d \leq \left(\frac{nB_\phi^2}{d} + \lambda\right)^d.$$

Equating the lower and upper bounds on $\det(V_n)$ gives:

$$\lambda^d \left(\frac{3}{2}\right)^{n-1} \leq \left(\frac{nB_\phi^2}{d} + \lambda\right)^d.$$

Solving this inequality yields the desired bound:

$$n = O\left(d \cdot \log\left(\frac{B_\theta^2 B_\phi^2}{\varepsilon}\right)\right).$$

□