An Introduction to Reinforcement Learning

From theory to algorithms

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Contents

Foreword

As of Fall 2024, this document contains lecture notes from a course given in Master 2 in *Université Paris–Saclay*. These are highly incomplete and constantly updated as the lectures are given.

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Introduction

Reinforcement learning deals with problems where an agent sequentially interacts with a dynamic environement, which yields a sequence of rewards. We aim at finding the decision rule for the agent which yields the highest cumulative reward. We first study the case where characteristics of the environements are known, and then turn to techniques for dealing with unknown environements, which must then be progressively learnt through repeated interaction.

Reinforcement learning achives great success in various applications: super-human algorithm for Go, robotics, finance, protein structure prediction, to name a few. Because it is so sucessful in practice, many resources are practice-oriented.

In these lectures, we first aim at a very rigorous presentation of the basic notions and tools. These building blocks will then be used to define algorithms, and establish theoretical guarantees for some of them.

Chapter 1

Markov decision processes

The framework for reinforcement learning is the Markov Decision process, which is a repeated interaction between an agent and a dynamic environment, which can be informally described as follows.

We are given three finite nonempty sets $\mathcal{S}$, $\mathcal{A}$ and $\mathcal{R}$, the latter being a subset of $\mathbb{R}$. The environment chooses an initial *state* $S_0 \in \mathcal{S}$ and reveals it to the agent. The agent then chooses an *action* $A_0 \in \mathcal{A}$, possibly at random. The environment then draws $(R_1, S_1) \in \mathcal{R} \times \mathcal{S}$ according to a probability distribution that depends on S_0 and A_0. The *reward* R_1 and the new state S_1 are revealed to the agent. The agent then chooses action $A_2 \in \mathcal{A}$, possibly at random. The environment then draws $(R_2, S_2) \in \mathcal{R} \times \mathcal{S}$ according to a probability distribution which depends on S_0 and A_0, and so on.

The total reward of the agent is defined as $\sum_{t=1}^{+\infty} \gamma^{t-1} R_t$, where $0 < \gamma < 1$ is a given *discount factor*. The goal is to find the decision rule for the agent that yields the highest expected total reward.

Note that at stage $t \geqslant 1$, the choice of actions A_t by the agent may depend on all previously observed information, meaning $(S_0, A_0, R_1, \dots, R_t, S_t)$.

Depending on the problem, the dynamics of the environment (which maps a state-action pair to a probability distribution over reward-state pairs) may be known or not.

This chapter presents basic notions regarding MDPs, in a formal fashion.

For a finite set I, we denote $\Delta(I)$ the corresponding unit simplex in $\mathbb{R}^I$:

$$\Delta(I) = \left\{ x \in \mathbb{R}_+^I,\ \sum_{i \in I} x_i = 1 \right\}$$

and interpret it as set the probability distributions over I. For $i \in I$, the corresponding Dirac measure is denoted δ_i.

1.1 Formal definition

Definition 1.1.1. A *finite Markov Decision Process* (MDP) is a 4-tuple $(\mathcal{S}, \mathcal{A}, \mathcal{R}, p)$ where $\mathcal{S}, \mathcal{A}, \mathcal{R}$ are nonempty finite sets and $\mathcal{R} \subset \mathbb{R}$, and $p : \mathcal{S} \times \mathcal{A} \times \mathcal{S} \times \mathcal{R} \to [0, 1]$ is such that for all $s, a \in \mathcal{S} \times \mathcal{A}$,

$$\sum_{(r,s') \in \mathcal{R} \times \mathcal{S}} p(s, a, r, s') = 1.$$

The elements of $\mathcal{S}$, $\mathcal{A}$ and $\mathcal{S}$ are respectively called *states*, *actions* and *rewards*. The following notation will be used:

$$p(r, s'|s, a) = p(s, a, r, s'), \quad (s, a, r, s') \in \mathcal{S} \times \mathcal{A} \times \mathcal{R} \times \mathcal{S}.$$

The knowledge of $\mathcal{S}$ and $\mathcal{A}$ is always assumed, but $\mathcal{R}$ and p may not be known, depending on the context.

From now on, we assume that a finite MDP is given.

Remark 1.1.2. For fixed values $(s, a) \in \mathcal{S} \times \mathcal{A}$, $p(s, a, \cdot\,)$ defines a probability distribution on $\mathcal{R} \times \mathcal{S}$, which justifies notation $p(\,\cdot\,|s, a)$.

Definition 1.1.3. Let $t \geqslant 1$. A *history of length t* is a finite sequence of the form

$$(s_0, a_0, r_1, s_1, a_1, r_2, s_2, a_2, \ldots, s_{t-1}, a_{t-1}, r_t, s_t) \in (\mathcal{S} \times \mathcal{A} \times \mathcal{R})^t \times \mathcal{S}.$$

By convention, a history of length 0 is an element $s_0 \in \mathcal{S}$. $\mathcal{H}^{(t)}$ denotes the set of histories of length t and $\mathcal{H}^{\infty} = (\mathcal{S} \times \mathcal{A} \times \mathcal{R})^{\mathbb{N}}$ the set of infinite histories.

Remark 1.1.4. Histories of length t correspond to the information observed by the agent at step t before choosing its action.

1.2 Policies

We now define policies, which are the formalization of decision rules for the agent. We first consider general policies, which allow for random decisions, as well as decision rules that depend on all available information (from the beginning of the interaction to the present state).

Definition 1.2.1. A *policy* is a sequence of maps $\pi = (\pi^{(t)})_{t \geqslant 0}$ where $\pi^{(t)} : \mathcal{H}^{(t)} \to \Delta(\mathcal{A})$. For each $t \geqslant 0$ and $h^{(t)} \in \mathcal{H}^{(t)}$, denote

$$\pi^{(t)}(a|h^{(t)}) := \pi^{(t)}(h^{(t)})_a.$$

Π denotes the set of all policies.

Remark 1.2.2. When using policy π, $\pi^{(t)}(a|h^{(t)})$ is interpreted as the probability of the agent choosing action a at time t after having observed history $h^{(t)}$.

Definition 1.2.3. A policy $\pi = (\pi^{(t)})_{t \geqslant 0}$ is

- *deterministic* if for each $t \geqslant 0$ and $h^{(t)} \in \mathcal{H}^{(t)}$, there exists $a \in \mathcal{A}$ such that $\pi^{(t)}(h^{(t)})$ is the Dirac distribution in a;
- *Markovian* if for each $t \geqslant 0$, $\pi^{(t)}$ is constant in all its variables but the last: in other words for a fixed value $s_t \in \mathcal{S}$, the map $\pi^{(t)}(\,\cdot\,, s_t)$ is constant; $\pi^{(t)}$ can then be represented as $\pi^{(t)} : \mathcal{S} \to \Delta(\mathcal{A})$;
- *stationary* if it is Markovian and if for all $t \geqslant 0$, $\pi^{(t)} = \pi^{(t)}$; π can then be represented as $\pi : \mathcal{S} \to \Delta(\mathcal{A})$ and denoted $\pi(a|s) = \pi(s)_a$ for $(s, a) \in \mathcal{S} \times \mathcal{A}$.

Denote Π_0 (resp. $\Pi_{0,d}$) the set of stationary policies (resp. stationary and deterministic policies). A stationary and deterministic policy can be represented as $\pi : \mathcal{S} \to \mathcal{A}$.

In the next chapter, we will establish that there exists a stationary and deterministic optimal policy, and focus on stationary policies. We will however continue working with non-deterministic strategies, as they will later prove handy for *exploring* an unknown environment.

1.3 Induced probability distributions over histories

As soon as an MDP, a policy π, and an initial state distribution μ are given, the interaction produces random variables $S_0, A_0, R_1, S_1, A_0, R_2, \ldots$. This is formalized by the proposition below.

We first introduce the following notation. For $T \geqslant 0$ and $h^{(T)} = (s_0, a_0, r_1, \ldots r_T, s_T)$, we consider the following associated subset of $\mathcal{H}^\infty$:

$$\operatorname{Cyl} h^{(T)} = \{s_0\} \times \{a_0\} \times \{r_1\} \times \cdots \times \{r_T\} \times \{s_T\} \times (\mathcal{A} \times \mathcal{R} \times \mathcal{S})^{\mathbb{N}}.$$

Proposition 1.3.1. *Let $\mu \in \Delta(\mathcal{S})$ and a policy π. There exists a unique probability measure $\mathbb{P}_{\mu,\pi}$ on $\mathcal{H}^\infty = (\mathcal{S} \times \mathcal{A} \times \mathcal{R})^{\mathbb{N}}$ (equipped with the product σ-algebra) such that for all $T \geqslant 0$, and all $h^{(T)} = (s_0, a_0, r_1, \ldots, r_T, s_T) \in \mathcal{H}^{(T)}$,*

$$\mathbb{P}_{\mu,\pi}\left(\operatorname{Cyl} h^{(T)}\right) = \mu(s_0) \prod_{t=0}^{T-1} \pi^{(t)}(a_t|h^{(t)})\, p(r_{t+1}, s_{t+1}|s_t, a_t).$$

where for each $0 \leqslant t \leqslant T$, $h^{(t)} = (s_0, a_0, r_1, \ldots, s_{t-1}, a_{t-1}, r_t, s_t)$.

Sketch of proof. The above expression defines associates a value for each set of the form $\mathrm{Cyl}\, h^{(T)}$ for $T \geqslant 0$ and $h^{(T)} \in \mathcal{H}^{(T)}$. The map $\mathbb{P}_{\mu,\pi}$ can then be extended to so-called cylinder sets of the form

$$\prod_{t=0}^{T} (\mathcal{S}_t \times \mathcal{A}_t \times \mathcal{R}_{t+1}) \times \mathcal{S}_{T+1} \times (\mathcal{A} \times \mathcal{R} \times \mathcal{S})^{\mathbb{N}},$$

where $\mathcal{S}_0, \ldots, \mathcal{S}_{T+1} \subset \mathcal{S}$, $\mathcal{A}_0, \ldots, \mathcal{A}_T \subset \mathcal{A}$ and $\mathcal{R}_1, \ldots, \mathcal{R}_{T+1} \subset \mathcal{R}$ by summing as follows:

$$\begin{aligned}
&\mathbb{P}_{\mu,\pi}\left(\prod_{t=0}^{T} (\mathcal{S}_t \times \mathcal{A}_t \times \mathcal{R}_{t+1}) \times \mathcal{S}_{T+1} \times (\mathcal{A} \times \mathcal{R} \times \mathcal{S})^{\mathbb{N}}\right) \\
&\quad = \sum_{\substack{s_0 \in \mathcal{S}_0 \\ \vdots \\ s_{T+1} \in \mathcal{S}_{T+1}}} \sum_{\substack{a_0 \in \mathcal{A}_0 \\ \vdots \\ a_T \in \mathcal{A}_T}} \sum_{\substack{r_1 \in \mathcal{R}_1 \\ \vdots \\ r_{T+1} \in \mathcal{R}_{T+1}}} \mu(s_0) \prod_{t=0}^{T} \pi^{(t)}(a_t | h^{(t)})\, p(s_{t+1}, r_{t+1} | s_t, a_t).
\end{aligned}$$

$\mathbb{P}_{\mu,\pi}$ can then be seen to satisfy the assumptions of Kolmogorov's extension theorem which assures that $\mathbb{P}_{\mu,\pi}$ can be extended to a unique probability measure on $\mathcal{H}^{\infty}$. □

Remark 1.3.2. In particular, Proposition 1.3.1 implies that a measure on $\mathcal{H}^{\infty}$ coincide with $\mathbb{P}_{\mu,\pi}$ as soon as they coincide on sets of the form $\mathrm{Cyl}\, h^{(T)}$. This will be used in the proofs of Propositions 1.3.4 and 1.3.5 below.

Definition 1.3.3. Let $\mu \in \Delta(\mathcal{S})$, $\pi \in \Pi$, $s \in \mathcal{S}$ and $a \in \mathcal{A}$.

(i) $\mathbb{P}_{\mu,\pi}$ from Proposition 1.3.1 is called the *probability distribution over histories* induced by initial state distribution μ and policy π.

(ii) We write $\mathbb{P}_{s,\pi}$ instead of $\mathbb{P}_{\delta_s,\pi}$, which is called the probability distribution over histories induced by initial state s and policy π.

(iii) Let $\tilde{\pi} = (\tilde{\pi}^{(t)})_{t \geqslant 0}$ be defined as

$$\begin{aligned}
\tilde{\pi}^{(t)}(s) &= \delta_a, \\
\tilde{\pi}^{(t)}(s') &= \pi^{(t)}(s') \quad \text{for } s' \neq s \\
\tilde{\pi}^{(t)} &= \pi^{(t)} \quad \text{for } t \geqslant 1.
\end{aligned}$$

$\mathbb{P}_{s,\tilde{\pi}}$ is then called the probability distribution induced by initial state s, initial action a, and policy π, and is denoted $\mathbb{P}_{s,a,\pi}$.

The following shorthands will be used:

$$\begin{aligned}
\mathbb{E}_{\mu,\pi}[\,\cdot\,] &= \mathbb{E}_{(S_0,A_0,R_1,\ldots)\sim\mathbb{P}_{\mu,\pi}}[\,\cdot\,] \\
\mathbb{E}_{s,\pi}[\,\cdot\,] &= \mathbb{E}_{(S_0,A_0,R_1,\ldots)\sim\mathbb{P}_{s,\pi}}[\,\cdot\,] \\
\mathbb{E}_{s,a,\pi}[\,\cdot\,] &= \mathbb{E}_{(S_0,A_0,R_1,\ldots)\sim\mathbb{P}_{s,a,\pi}}[\,\cdot\,].
\end{aligned}$$

$\mathbb{P}_{s,a,\pi}$ corresponds to the interaction where the initial state is s, initial action is a (deterministically), and decision rule is given by π only for $t \geqslant 1$. In general, it cannot be defined as $\mathbb{P}_{s,a}$ conditioned on the event $\{A_0 = a\}$ because the probability $\pi(a|s)$ of this event may be zero.

Proposition 1.3.4. *Let $\pi = (\pi^{(t)})_{t\geqslant 0}$ be a policy and $s \in \mathcal{S}$. Then,*

$$\mathbb{P}_{s,\pi} = \sum_{a\in\mathcal{A}} \pi^{(0)}(a|s) \cdot \mathbb{P}_{s,a,\pi}.$$

Proof. It is sufficient to prove the identity between those two measures on the sets $\operatorname{Cyl} h^{(T)}$ that appear in the statement of Proposition 1.3.1, because they would then uniquely extend to all measurable subsets of $\mathcal{H}^\infty$.

Let $T \geqslant 0$ and $h^{(T)} = (s_0, a_0, r_1, \dots, r_T, s_T) \in \mathcal{H}^{(T)}$, and denote $h^{(t)} := (s_0, a_0, r_1, \dots, r_r, s_t)$ for $0 \leqslant t \leqslant T$. If $s_0 \neq s$, then the measures of the identity are zero when evaluated at $\operatorname{Cyl} h^{(T)}$. We now assume $s_0 = s$.

Fix $a \in \mathcal{A}$ and consider $\tilde{\pi}$ defined as in Definition 1.3.3. Then,

$$\begin{aligned}
\pi^{(0)}(a|s) \cdot \mathbb{P}_{s,a,\pi}\left(\operatorname{Cyl} h^{(T)}\right) &= \pi^{(0)}(a|s) \prod_{t=0}^{T-1} \tilde{\pi}^{(t)}(a_t|h^{(t)})\, p(r_{t+1}, s_{t+1}|s_t, a_t) \\
&= \mathbb{1}\left\{s_0 = s\right\} \prod_{t=0}^{T-1} \pi^{(t)}(a_t|h^{(t)})\, p(r_{t+1}, s_{t+1}|s_t, a_t) \\
&= \mathbb{1}\left\{a_0 = a\right\} \cdot \mathbb{P}_{s,\pi}\left(\operatorname{Cyl} h^{(T)}\right).
\end{aligned}$$

Summing over $a \in \mathcal{A}$ then gives

$$\sum_{a\in\mathcal{A}} \pi^{(0)}(a|s) \cdot \mathbb{P}_{s,a,\pi}\left(\operatorname{Cyl} h^{(T)}\right) = \mathbb{P}_{s,\pi}\left(\operatorname{Cyl} h^{(T)}\right).$$

□

The following proposition demonstrates that a given stationary policy induces a distribution over histories that has a Markov property in the following sense: for all $t \geqslant 0$, the distribution of $(S_t, A_t, R_{t+1}, \dots)$ conditionnally on $\{S_t = s\}$ has the same is the same as the distribution of $(S_0, A_0, R_1, \dots)$ when the latter has initial state s.

Proposition 1.3.5 (Markov property)**.** *Let $s, s' \in \mathcal{S}$, $a, a' \in \mathcal{A}$, π a stationary policy, $f : \mathcal{H}^\infty \to \mathbb{R}$ a bounded measurable function (with respect to the product σ-algebra), random variables $(S'_0, A'_0, R'_1, S'_2, A'_2, R'_2, \dots)$ with distribution $\mathbb{P}_{s,\pi}$ or $\mathbb{P}_{s,a,\pi}$, and $t \geqslant 0$.*

(i) If $\mathbb{P}\left[S'_t = s'\right] > 0$, the distribution of $(S'_t, A'_t, R'_{t+1}, S'_{t+1}, \dots)$ conditionnaly on $\{S'_t = s'\}$ is $\mathbb{P}_{s',\pi}$.

(ii) Almost-surely,

$$\mathbb{E}_{S'_t,\pi}\left[f(S_0, A_0, R_1, \dots)\right] = \mathbb{E}\left[f(S'_t, A'_t, R'_{t+1}, \dots) \,\middle|\, S'_t\right].$$

(iii) If $\mathbb{P}\left[S'_t = s',\ A'_t = a'\right] > 0$*, the distribution of* $(S'_t, A'_t, R_{t+1}, S'_{t+1}, \dots)$ *conditionnaly on* $\{S'_t = s',\ A'_t = a'\}$ *is* $\mathbb{P}_{s',a',\pi}$*.*

(iv) Almost-surely,

$$\mathbb{E}_{S'_t,A'_t,\pi}\left[f(S_0, A_0, R_1, \dots)\right] = \mathbb{E}\left[f(S'_t, A'_t, R'_{t+1}, \dots) \,\middle|\, S'_t, A'_t\right].$$

Proof. Let us assume $\mathbb{P}\left[S'_t = s'\right] > 0$. To prove (i), thanks to Proposition 1.3.1, it is enough to prove that $\mathbb{P}\left[\,\cdot \mid S'_t = s'\right]$ and $\mathbb{P}_{s',\pi}$ coincide on sets on the form $\mathrm{Cyl}\, h^{(T)}$. Let $T \geqslant t$ and $(s_t, a_t, r_{t+1}, \dots, r_T, s_T) \in \mathcal{H}^{(T-t)}$. Using the expression from the statement of Proposition 1.3.1,

$$\begin{aligned}
&\mathbb{P}\left[S'_t = s_t,\ A'_t = a_t,\ R'_{t+1} = r_{t+1}, \dots, R_T = r_T,\ S_T = s_T \,\middle|\, S'_t = s'\right] \\
&= \frac{\mathbb{P}\left[S'_t = s',\ S'_t = s_t,\ A'_t = a_t,\ R'_{t+1} = r_{t+1}, \dots, R_T = r_T,\ S_T = s_T\right]}{\mathbb{P}\left[S'_t = s'\right]} \\
&= \frac{\mathbb{1}_{\{s_0 = s'\}} \times \displaystyle\sum_{(s_0,\dots,s_{t-1})\in\mathcal{S}^t} \delta_s(s_0) \prod_{\tau=0}^{T-1} \pi(a_\tau)\, p(r_{\tau+1}, s_{\tau+1} | s_\tau, a_\tau)}{\displaystyle\sum_{(s_0,\dots,s_{t-1})\in\mathcal{S}^t} \delta_s(s_0) \prod_{t=0}^{T-1} \pi(a_\tau)\, p(r_{\tau+1}, s_{\tau+1} | s_\tau, a_\tau)} \\
&= \mathbb{1}_{\{s_0 = s'\}} \times \prod_{\tau=t}^{T-1} \pi(a_\tau)\, p(r_{\tau+1}, s_{\tau+1} | s_\tau, a_\tau) \\
&= \mathbb{P}_{s',\pi}\left[S_0 = s_t,\ A_0 = a_t,\ R_1 = r_{t+1}, \dots, R_{T-t} = r_T,\ S_{T-t} = s_T\right],
\end{aligned}$$

and (i) follows.

We now turn to (ii). By definition of the conditionnal expectation, $\mathbb{E}\left[f(S'_t, A'_t, R'_{t+1}, \dots) \,\middle|\, S'_t\right]$ designates any random variable, measurable with respect to S'_t and with expectation equal to $\mathbb{E}\left[f(S'_t, A'_t, R'_{t+1}, \dots)\right]$. Let us prove that $\mathbb{E}_{S'_t,\pi}\left[f(S_0, A_0, R_1, \dots)\right]$ indeed satisfy those properties. It is obviously measurable with respect to S'_t, as a deterministic function of the value of S'_t. Regarding the expectation, we can write

$$\begin{aligned}
\mathbb{E}\left[\mathbb{E}_{S_t,\pi}\left[f(S_0, A_0, R_1, \dots)\right]\right] &= \sum_{s'\in\mathcal{S}} \mathbb{P}\left[S'_t = s'\right] \times \mathbb{E}_{s',\pi}\left[f(S_0, A_0, R_1, \dots)\right] \\
&= \sum_{\substack{s'\in\mathcal{S} \\ \mathbb{P}[S'_t = s'] > 0}} \mathbb{P}\left[S'_t = s'\right] \times \mathbb{E}\left[f(S'_t, A'_t, R'_{t+1}, \dots) \,\middle|\, S'_t = s'\right] \\
&= \mathbb{E}\left[f(S'_t, A'_t, R'_{t+1}, \dots)\right].
\end{aligned}$$

(iii) and (iv) are proved similarly. □

1.4 Value functions

We now introduce value functions which are fundamental tools for solving MDPs. The *optimal* value function, defined in the next chapter, associates to each state the best possible average reward than can be obtained starting from that state. Almost all algorithms aim at getting close to the optimal value function through iterative updates.

Definition 1.4.1. (i) A *state-value function* (aka *V-function*) is a function $v : \mathcal{S} \to \mathbb{R}$ or equivalently a vector $v = (v(s))_{s\in\mathcal{S}} \in \mathbb{R}^{\mathcal{S}}$.

(ii) An *action-value function* (aka *Q-function*) is a function $q : \mathcal{S} \times \mathcal{A} \to \mathbb{R}$ or equivalently a vector $q = (q(s,a))_{(s,a)\in\mathcal{S}\times\mathcal{A}} \in \mathbb{R}^{\mathcal{S}\times\mathcal{A}}$.

We equip both spaces with the ℓ^∞ norm:

$$\|v\|_\infty = \max_{s\in\mathcal{S}} |v(s)|\,, \qquad \|q\|_\infty = \max_{(s,a)\in\mathcal{S}\times\mathcal{A}} |q(s,a)|\,,$$

and with component-wise inequalities:

$$v \leqslant v' \iff \forall s \in \mathcal{S},\ v(s) \leqslant v'(s),$$
$$q \leqslant q' \iff \forall (s,a) \in \mathcal{S}\times\mathcal{A},\ q(s,a) \leqslant q'(s,a).$$

Lemma 1.4.2. *Let $(R_t)_{t\geqslant 1}$ be a sequence of random variables with values in $\mathcal{R}$ and $\gamma \in (0,1)$. Then, the series $\sum_{t\geqslant 1} \gamma^{t-1} R_t$ converges almost-surely, and its sum is integrable.*

Proof. $\mathcal{R}$ being a finite subset of $\mathbb{R}$, it holds that $\max_{r\in\mathcal{R}} |r| < +\infty$. Then,

$$\left|\gamma^{t-1} R_t\right| \leqslant \gamma^{t-1} \max_{r\in\mathcal{R}} |r|\,, \quad \text{a.s.}$$

The result follows from the dominated convergence theorem. □

Definition 1.4.3. Let $\pi \in \Pi$ and $\gamma \in (0,1)$.

(i) The *state-value function of policy* π with discount factor γ is defined as

$$v_\pi^{(\gamma)}(s) = \mathbb{E}_{s,\pi}\left[\sum_{t=1}^{+\infty} \gamma^{t-1} R_t\right], \quad s \in \mathcal{S}.$$

(ii) The *action-value function of policy* π with discount factor γ is defined as

$$q_\pi^{(\gamma)}(s,a) = \mathbb{E}_{s,a,\pi}\left[\sum_{t=1}^{+\infty} \gamma^{t-1} R_t\right], \quad (s,a) \in \mathcal{S}\times\mathcal{A}.$$

We may denote $v_\pi = v_\pi^{(\gamma)}$ and $q_\pi = q_\pi^{(\gamma)}$ when γ is clear from the context.

Remark 1.4.4. $v_\pi(s)$ corresponds to the expected total reward starting from state s and following policy π.

Chapter 2

Bellman operators & optimality

This chapter introduces Bellman operators, which are the fundamental tools for solving MDPs. We then define optimal value functions and policies, and characterize them with the help of the Bellman operators.

We assume that $\gamma \in (0, 1)$ in given. The image of an element $x \in X$ by a map $F : X \to Y$ will often be denoted Fx instead of $F(x)$.

2.1 Bellman operators

Definition 2.1.1. Let π be a stationary policy. We define the following operators.

(i) $D^{(\gamma)} : \mathbb{R}^{\mathcal{S}} \to \mathbb{R}^{\mathcal{S}\times\mathcal{A}}$ as

$$(D^{(\gamma)}v)(s, a) = \sum_{(r,s')\in\mathcal{S}\times\mathcal{R}} p(r, s'|s, a)(r + \gamma v(s')), \quad s \in \mathcal{S},\ a \in \mathcal{A}.$$

(ii) $E_\pi : \mathbb{R}^{\mathcal{S}\times\mathcal{A}} \to \mathbb{R}^{\mathcal{S}}$ as

$$(E_\pi q)(s) = \sum_{a\in\mathcal{A}} \pi(s|a)q(s, a), \quad s \in \mathcal{S}.$$

(iii) $E_* : \mathbb{R}^{\mathcal{S}\times\mathcal{A}} \to \mathbb{R}^{\mathcal{S}}$ as

$$(E_* q)(s) = \max_{a\in\mathcal{A}} q(s, a), \quad s \in \mathcal{S}.$$

(iv) $B_\pi^{(V,\gamma)} = E_\pi \circ D^{(\gamma)}$ (Bellman expectation operator for state-value functions)

(v) $B_*^{(V,\gamma)} = E_* \circ D^{(\gamma)}$ (Bellman optimality operator for state-value functions)

(vi) $B_\pi^{(Q,\gamma)} = D^{(\gamma)} \circ E_\pi$ (Bellman expectation operator for action-value functions)

(vii) $B_*^{(Q,\gamma)} = D^{(\gamma)} \circ E_*$ (Bellman optimality operator for action-value functions)

We will use lighter notation $D, E_\pi, E_*, B_\pi, B_*$ as soon as context prevents confusion. The following expressions follow from the definitions.

$$\begin{tikzcd}
\mathbb{R}^{\mathcal{S}} \arrow[loop left, "B_*^{(V)}"] \arrow[loop right, "B_\pi^{(V)}"] \arrow[rr, bend left, "D"] & & \mathbb{R}^{\mathcal{S}\times\mathcal{A}} \arrow[loop left, "B_\pi^{(Q)}"] \arrow[loop right, "B_*^{(Q)}"] \arrow[ll, bend left, "E_\pi"] \arrow[ll, bend left=60, "E_*"]
\end{tikzcd}$$

Figure 2.1: Operators $D, E_\pi, E_*, B_\pi^{(V)}, B_*^{(V)}, B_\pi^{(Q)}$ and $B_*^{(Q)}$.

Proposition 2.1.2 (Explicit expression of Bellman operators)**.** *Let $v \in \mathbb{R}^{\mathcal{S}}$, $q \in \mathbb{R}^{\mathcal{S}\times\mathcal{A}}$, and π a stationary policy. Then, the following expressions hold.*

$$(B_\pi v)(s) = \sum_{(a,r,s')\in\mathcal{A}\times\mathcal{S}\times\mathcal{R}} \pi(a|s)\, p(r,s'|s,a) \left(r + \gamma v(s')\right), \quad s \in \mathcal{S},$$

$$(B_* v)(s) = \max_{a\in\mathcal{A}} \sum_{(r,s')\in\mathcal{S}\times\mathcal{R}} p(r,s'|s,a)(r+\gamma v(s')), \quad s \in \mathcal{S},$$

$$(B_\pi q)(s,a) = \sum_{(r,s',a')\in\mathcal{S}\times\mathcal{R}\times\mathcal{A}} p(r,s'|s,a) \left(r + \gamma\pi(a'|s')q(s',a')\right), \quad (s,a) \in \mathcal{S}\times\mathcal{A},$$

$$(B_* q)(s,a) = \sum_{(r,s')\in\mathcal{S}\times\mathcal{R}} p(r,s'|s,a) \left(r + \gamma \max_{a'\in\mathcal{A}} q(s',a')\right), \quad (s,a) \in \mathcal{S}\times\mathcal{A}.$$

Proof. Immediate from the definitions. $\square$

Proposition 2.1.3 (Bellman operators as expectations)**.** *Let $v \in \mathbb{R}^{\mathcal{S}}$, $q \in \mathbb{R}^{\mathcal{S}\times\mathcal{A}}$, π a policy, $s \in \mathcal{S}$, $a \in \mathcal{A}$. Then,*

(i) $(Dv)(s,a) = \mathbb{E}_{s,a,\pi}\left[R_1 + \gamma v(S_1)\right]$,

and if π is stationary,

(ii) $(E_\pi q)(s) = \mathbb{E}_{s,\pi}\left[q(s, A_0)\right]$,

(iii) $(B_\pi v)(s) = \mathbb{E}_{s,\pi}\left[R_1 + \gamma v(S_1)\right]$,

(iv) $(B_\pi q)(s, a) = \mathbb{E}_{s,a,\pi}\left[R_1 + \gamma q(S_1, A_1)\right]$.

(v) $(B_* v)(s) = \max_{a \in \mathcal{A}} \mathbb{E}_{s,a,\pi}\left[R_1 + \gamma v(S_1)\right]$,

(vi) $(B_* q)(s, a) = \mathbb{E}_{s,a,\pi}\left[R_1 + \gamma \max_{a' \in \mathcal{A}} q(S_1, a')\right]$.

Proof. Let us prove (i). Let π' the policy associated with (s, a) used in Definition 1.3.3 to define $\mathbb{P}_{s,a,\pi}$. Using the definition of the probability measure $\mathbb{P}_{s,\pi}$ (see Proposition 1.3.1),

$$
\begin{aligned}
\mathbb{E}_{s,a,\pi}\left[R_1 + \gamma v(S_1)\right] &= \mathbb{E}_{s,\pi'}\left[R_1 + \gamma v(S_1)\right] \\
&= \sum_{(r,s') \in \mathcal{R} \times \mathcal{S}} (r + \gamma v(s')) \\
&\qquad \times \mathbb{P}_{s,\pi'}\left(\mathcal{S} \times \mathcal{A} \times \{r\} \times \left\{s'\right\} \times (\mathcal{R} \times \mathcal{S} \times \mathcal{A})^{\mathbb{N}}\right) \\
&= \sum_{(r,s') \in \mathcal{R} \times \mathcal{S}} p(r, s'|s, a)(r + \gamma v(s')) \\
&= (Dv)(s, a)
\end{aligned}
$$

We now turn to (ii).

$$
\begin{aligned}
E_{s,\pi}\mathbb{E}\left[q(s, A_0)\right] &= \sum_{a \in \mathcal{A}} q(s, a) \times \mathbb{P}_{s,a}\left(\mathcal{S} \times \{a\} \times (\mathcal{R} \times \mathcal{S} \times \mathcal{A})^{\mathbb{N}}\right) \\
&= \sum_{a \in \mathcal{A}} q(s, a)\pi(a|s) = (E_\pi q)(s).
\end{aligned}
$$

We now deduce (iii) using Proposition 1.3.4:

$$
\begin{aligned}
(B_\pi v)(s) = (E_\pi(Dv))(s) &= \sum_{a \in \mathcal{A}} \pi(a|s)\mathbb{E}_{s,a,\pi}\left[R_1 + \gamma v(S_1)\right] \\
&= \mathbb{E}_{s,\pi}\left[R_1 + \gamma v(S_1)\right].
\end{aligned}
$$

For (iv), we combine (i) and (ii) with the help of the Markov property from Proposition 1.3.5; let $(S'_0, A'_0, R'_1, \dots) \sim \mathbb{P}_{s,a,\pi}$, then

$$
\begin{aligned}
(B_\pi q)(s, a) = (D(E_\pi q))(s, a) &= \mathbb{E}\left[R'_1 + \gamma(E_\pi q)(S'_1)\right] \\
&= \mathbb{E}\left[R'_1 + \gamma \cdot \mathbb{E}_{S'_1,\pi}\left[q(S_0, A_0)\right]\right] \\
&= \mathbb{E}\left[R'_1 + \gamma \cdot \mathbb{E}\left[q(S'_1, A'_1) \mid S'_1\right]\right] \\
&= \mathbb{E}\left[R'_1 + \gamma \cdot q(S'_1, A'_1)\right].
\end{aligned}
$$

Finally, (v) and (vi) follow by composition. □

Remark 2.1.4. If for each $s \in \mathcal{S}$, $v(s)$ is interpreted as an estimate of the total reward obtained starting from state s and using policy π, $(B_\pi v)(s)$ is then an alternative estimate, as it is the expectation, when starting from state s of the actual first reward R_1, *plus* $\lambda v(S_1)$ which is an estimate of remaining discounted rewards, as estimated by v. A similar interpretation holds for $B_\pi q$. We will see that the latter estimate is in some sense better: the Bellman operators will thus be used to iteratively *update* the estimates.

Definition 2.1.5. Let $d, n \geqslant 1$ integers. A map $F : \mathbb{R}^d \to \mathbb{R}^n$ is *monotone* if for all $x, x' \in \mathbb{R}^d$, $x \leqslant x'$ implies $Fx \leqslant Fx'$, where the inequalities are to be understood component-wise.

Proposition 2.1.6. *Let π be a stationary policy. Then, operators D, E_π, $B_\pi^{(V)}$ and $B_\pi^{(Q)}$ are affine with nonnegative coefficients. E_π is moreover linear. In particular, they are monotone.*

Proof. Immediate from the definitions. □

Proposition 2.1.7. *Let $v \in \mathbb{R}^{\mathcal{S}}$, $q \in \mathbb{R}^{\mathcal{S}\times\mathcal{A}}$, $s \in \mathcal{S}$ and $a \in \mathcal{A}$. Then,*

(i) $(E_* q)(s) = \max_{\pi\in\Pi_0} (E_\pi q)(s) = \max_{\pi\in\Pi_{0,d}} (E_\pi q)(s)$,

(ii) $(B_* v)(s) = \max_{\pi\in\Pi_0} (B_\pi v)(s) = \max_{\pi\in\Pi_{0,d}} (B_\pi v)(s)$,

(iii) $(B_* q)(s, a) = \max_{\pi\in\Pi_0} (B_\pi q)(s, a) = \max_{\pi\in\Pi_{0,d}} (B_\pi q)(s, a)$.

Proof. (i) Let $s \in \mathcal{S}$ and $\pi \in \Pi_0$.

$$\begin{aligned}(E_\pi q)(s) &= \sum_{a\in\mathcal{A}} \pi(a|s)\, q(s,a) \leqslant \sum_{a\in\mathcal{A}} \pi(a|s)\, \max_{a\in\mathcal{A}} q(s,a) \\ &= (E_* q)(s) \sum_{a\in\mathcal{A}} \pi(a|s) = (E_* q)(s).\end{aligned}$$

Taking the supremum over $\pi \in \Pi_0$ yields

$$\sup_{\pi\in\Pi_0} (E_\pi q)(s) \leqslant (E_* q)(s).$$

Besides, for each $s \in \mathcal{S}$, there exists a maximizer of $q(s, \cdot)$ (because the number of values is finite). Let $\pi_{0,d}(\cdot|s)$ be a Dirac at one of the maximizers. This defines a stationary and deterministic policy $\pi_{0,d}$, which satisfies $(E_{\pi_0} q)(s) = \max_{a\in\mathcal{A}} q(s,a)$ for all $s \in \mathcal{S}$. We then write for $s \in \mathcal{S}$,

$$\begin{aligned}\sup_{\pi\in\Pi_0} (E_\pi q)(s) &\leqslant (E_* q)(s) = \max_{a\in\mathcal{A}} q(s,a) = (E_{\pi_{0,d}} q)(s) \\ &\leqslant \sup_{\pi\in\Pi_{0,d}} (E_\pi q)(s) \leqslant \sup_{\pi\in\Pi_0} (E_\pi q)(s).\end{aligned}$$

The above lowest and highest quantities are the same. Therefore, all inequalities are equalities, and the supremums are maximums because they are attained by $\pi_{0,d}$.

Then (ii) and (iii) follow from the monotonicity from Proposition 2.1.6. □

2.2 Bellman equations

Definition 2.2.1. Let X be a set and $F : X \to X$. An element $x \in X$ is a *fixed point* of F is $Fx = x$.

The fixed points of Bellman operators will be of particular interest. They are often written in the form of the so-called Bellman equations: for a given stationary policy π, a state-value function $v \in \mathbb{R}^{\mathcal{S}}$ is a fixed point of $B_\pi^{(V)}$ if, and only if:

$$v(s) = \sum_{(a,r,s') \in \mathcal{A} \times \mathcal{S} \times \mathcal{R}} \pi(a|s)\, p(r, s'|s, a) \left(r + \gamma v(s')\right), \quad s \in \mathcal{S}.$$

The above is called the *Bellman expectation equation* for state-value functions. Similarly, v is the fixed point of $B_*^{(V)}$ if, and only if:

$$v(s) = \max_{a \in \mathcal{A}} \sum_{(r,s') \in \mathcal{S} \times \mathcal{R}} p(r, s'|s, a)(r + \gamma v(s')), \quad s \in \mathcal{S},$$

which is called the Bellman *optimality equation*. The corresponding equations for action-value functions are similarly defined. We establish below that these equations have unique solutions and that they correspond respectively to v_π and v_*, where v_* is the value function associated with an optimal policy.

Definition 2.2.2. Let (X, d) and (Y, d') be a metric spaces. A map $F : X \to Y$ is a γ-contraction if $\gamma \in [0, 1)$ and F is a γ-contraction.

Theorem 2.2.3 (Banach's fixed point theorem)**.** *Let $0 \leqslant \gamma < 1$, (X, d) a complete metric space, and $F : X \to X$ a γ-contraction. Then, F has a unique fixed point $x_* \in X$ and for all sequence $(x_k)_{k \geqslant 0}$ satisfying $x_{k+1} = Fx_k$ $(k \geqslant 0)$, it holds that*

$$d(x_k, x_*) \leqslant \gamma^k d(x_0, x_*), \quad k \geqslant 0,$$

and thus $x_k \longrightarrow x_*$ as $k \to +\infty$.

Proof. For all $k \geqslant 1$, using the Lipschitz continuity of F,

$$d(x_{k+1}, x_k) = d(Fx_k, Fx_{k-1}) \leqslant \gamma\, d(x_k, x_{k-1}),$$

which by a simple induction implies

$$d(x_{k+1}, x_k) \leqslant \gamma^k\, d(x_1, x_0),$$

from which we deduce that $(x_k)_{k\geqslant 0}$ is a Cauchy sequence and thus admits a limit $x_* \in X$. Map F is continuous because of its Lipschitz property, and taking the limit in the identity $x_{k+1} = Fx_k$ yields $x_* = Fx_*$, in other words, x_* is indeed of fixed point of F. If $x_{**} \in X$ is also a fixed point, it holds that

$$d(x_*, x_{**}) = d(Fx_*, Fx_{**}) \leqslant \gamma\, d(x_*, x_{**}),$$

which, because $0 \leqslant \gamma < 1$, is only possible when $x_* = x_{**}$. The fixed point is therefore unique.

Besides, for all $k \geqslant 0$,

$$d(x_{k+1}, x_*) = d(Fx_k, Fx_*) \leqslant \gamma\, d(x_k, x_*),$$

which by a simple induction yields

$$d(x_k, x_*) \leqslant \gamma^k\, d(x_0, x_*).$$

□

Remark 2.2.4. The above convergence is guaranteed *regardless* of the initial point x_0.

Proposition 2.2.5. *Let π be a stationary policy. With respect to the norms $\|\cdot\|_\infty$ in $\mathbb{R}^{\mathcal{S}}$ and $\mathbb{R}^{\mathcal{S}\times\mathcal{A}}$,*

(i) $D^{(\gamma)}$ *is a γ-contraction,*

(ii) E_π *is 1-Lipschitz continuous,*

(iii) E_* *is 1-Lipschitz continuous,*

(iv) $B_\pi^{(V,\gamma)}$*,* $B_*^{(V,\gamma)}$*,* $B_\pi^{Q,\gamma}$ *and* $B_*^{(Q,\gamma)}$ *are γ-contractions and admit unique fixed points.*

Proof. Let $v, v' \in \mathbb{R}^{\mathcal{S}}$.

$$\begin{aligned}
\left\|Dv' - Dv\right\|_\infty &= \max_{(s,a)\in\mathcal{S}\times\mathcal{A}} \left|Dv'(s,a) - Dv(s,a)\right| \\
&= \max_{(s,a)\in\mathcal{S}\times\mathcal{A}} \left| \sum_{(r,s')\in\mathcal{R}\times\mathcal{S}} p(r,s'|s,a)\gamma(v'(s') - v(s)) \right| \\
&\leqslant \max_{(s,a)\in\mathcal{S}\times\mathcal{A}} \gamma \left\|v' - v\right\|_\infty \sum_{(r,s')\in\mathcal{R}\times\mathcal{S}} p(r,s'|s,a) \\
&= \gamma \left\|v' - v\right\|_\infty,
\end{aligned}$$

where the last inequality follows from $p(\,\cdot\,|s,a)$ being a probability distribution over $\mathcal{R}\times\mathcal{S}$, which proves (i).

Let $q, q' \in \mathbb{R}^{\mathcal{S}\times\mathcal{A}}$ and π a stationary policy.

$$\begin{aligned}\left\|E_\pi q' - E_\pi q\right\|_\infty &= \max_{s\in\mathcal{A}}\left|\sum_{a\in\mathcal{A}}\pi(a|s)\left|q'(s,a)-q(s,a)\right|\right| \\ &\leqslant \max_{s\in\mathcal{A}}\sum_{a\in\mathcal{A}}\pi(a|s)\left\|q'-q\right\|_\infty \\ &= \left\|q'-q\right\|_\infty,\end{aligned}$$

where the last inequality follows from $\pi(\,\cdot\,|s)$ being a probability distribution over $\mathcal{A}$.

Let $s\in\mathcal{S}$. If $(E_* q')(s) \geqslant (E_* q)(s)$, then

$$\begin{aligned}\left|(E_* q')(s) - (E_* q)(s)\right| &= (E_* q')(s) - (E_* q)(s) \\ &= \max_{a'\in\mathcal{A}} q'(s,a') - \max_{a\in\mathcal{A}} q(s,a) \\ &\leqslant \max_{a'\in\mathcal{A}}\left\{q'(s,a')-q(s,a')\right\} \\ &\leqslant \max_{a'\in\mathcal{A}}\left|q'(s,a')-q(s,a')\right| \\ &\leqslant \left\|q'-q\right\|_\infty.\end{aligned}$$

Similarly, if $(E_* q')(s) \leqslant (E_* q)(s)$, then

$$\left|E_* q'(s) - E_* q(s)\right| \leqslant \left\|q'-q\right\|_\infty.$$

Taking the maximum over $s\in\mathcal{S}$ yields (iii):

$$\left\|E_* q' - E_* q\right\|_\infty \leqslant \left\|q'-q\right\|_\infty.$$

The Lipschitz property (iv) of Bellman operators then follow by composition. □

Proposition 2.2.6. *Let π be a stationary policy. Then,*

(i) $v_\pi = E_\pi q_\pi$,

(ii) $q_\pi = D v_\pi$,

(iii) v_π *is the unique fixed point of* $B_\pi^{(V)}$,

(iv) q_π *is the unique fixed point of* $B_\pi^{(Q)}$.

Proof. Let $s \in \mathcal{S}$. We prove (i) using Proposition 1.3.4:

$$\begin{aligned}
(E_\pi q_\pi)(s) &= \sum_{a\in\mathcal{A}} \pi(a|s)\cdot \mathbb{E}_{s,a,\pi}\left[\sum_{t=1}^{+\infty}\gamma^{t-1}R_t\right]\\
&= \mathbb{E}_{s,\pi}\left[\sum_{t=1}^{+\infty}\gamma^{t-1}R_t\right]\\
&= v_\pi.
\end{aligned}$$

We now turn to (ii). Let $a \in \mathcal{A}$. Let $(S'_0, A'_0, R'_1, \dots) \sim \mathbb{P}_{s,a,\pi}$. Then, using the expression of the Bellman operator as an expectation (from Proposition 2.1.3), we write

$$\begin{aligned}
(Dv_\pi)(s,a) &= \mathbb{E}_{s,a,\pi}\left[R_1 + \gamma\, v_\pi(S_1)\right]\\
&= \mathbb{E}\left[R'_1 + \gamma\, v_\pi(S'_1)\right]\\
&= \mathbb{E}\left[R'_1 + \gamma\cdot \mathbb{E}_{S'_1,\pi}\left[\sum_{t=1}^{+\infty}\gamma^{t-1}R_t\right]\right]\\
&= \mathbb{E}\left[R'_1 + \gamma\cdot \mathbb{E}\left[\sum_{t=1}^{+\infty}\gamma^{t-1}R'_{t+1}\,\middle|\, S'_1\right]\right]\\
&= \mathbb{E}\left[\sum_{t=1}^{+\infty}\gamma^{t-1}R_t\right] = v_\pi,
\end{aligned}$$

where for the fourth equality we used the Markov property for $\mathbb{P}_{s,a,\pi}$ from Proposition 1.3.5.

Combining (i) and (ii) together with Banach's fixed point theorem from Theorem (2.2.3) yields (iv) and (iv). □

$$\begin{tikzcd}
\mathbb{R}^{\mathcal{S}} & \mathbb{R}^{\mathcal{S}\times\mathcal{A}} \\
v_\pi \arrow[loop left, "B_\pi^{(V)}"] \arrow[r, bend left, "D"] & q_\pi \arrow[l, bend left, "E_\pi"] \arrow[loop right, "B_\pi^{(Q)}"]
\end{tikzcd}$$

Figure 2.2: Relations between v_π, q_π, D, E_π $B_\pi^{(V)}$ and $B_\pi^{(Q)}$.

Remark 2.2.7. In other words, v_π (resp. q_π) is the unique solution of the Bellman expectation equation for state-value function (resp. action-value functions).

2.3 Greedy policies

Definition 2.3.1. A stationary and deterministic policy $\pi : \mathcal{S} \to \mathcal{A}$ is

(i) a *greedy policy* with respect to an action-value function $q \in \mathbb{R}^{\mathcal{S}\times\mathcal{A}}$ if for all $s \in \mathcal{S}$,

$$\pi(s) \in \operatorname*{Arg\,max}_{a\in\mathcal{A}} q(s, a),$$

where Arg max denotes the set of maximizers.

(ii) a *greedy policy* with respect to an state-value function $v \in \mathbb{R}^{\mathcal{S}}$ if $\pi \in \Pi_g[Dv]$.

$\Pi_g[q]$ denotes the set of greedy policies with respect to q and $\Pi_g[v]$ is a shorthand for $\Pi_g[Dv]$. Notation $\pi_g[q]$ (resp. $\pi_g[v]$) denotes any element from $\Pi_g[q]$ (resp. $\Pi_g[v]$).

Remark 2.3.2. $\pi_g[q]$ corresponds to a policy which selects actions by simply comparing values of the action-value function q. In the case of $\pi_g[v]$, the action selection is based on a *one-step look-ahead*, as it rewrites as follows using Proposition 2.1.3:

$$\pi_g(s) \in \operatorname*{Arg\,max}_{a\in\mathcal{A}} \mathbb{E}_{s,a,\pi}\left[R_1 + \gamma v(S_1)\right].$$

Proposition 2.3.3. *For $v \in \mathbb{R}^{\mathcal{S}}$ (resp. $q \in \mathbb{R}^{\mathcal{S}\times\mathcal{A}}$), $\Pi_g[v]$ (resp. $\Pi_g[q]$) is nonempty.*

Proof. The set of actions $\mathcal{A}$ being finite (and nonempty), $\operatorname{Arg\,max}_{a\in\mathcal{A}} q(s, a)$ is nonempty, and the result follows. □

Proposition 2.3.4. *Let $v \in \mathbb{R}^{\mathcal{S}}$ and $q \in \mathbb{R}^{\mathcal{S}\times\mathcal{A}}$. Then,*

(i) $E_* q = E_{\pi_g[q]} q$,

(ii) $B_* q = B_{\pi_g[q]} q$.

(iii) $B_* v = B_{\pi_g[v]} v$,

Proof. Let $s \in \mathcal{S}$ and $\pi \in \Pi_g[q]$. By definition of a greedy policy,

$$(E_* q)(s) = \max_{a\in\mathcal{A}} q(s, a) = q(s, \pi(s)) = \sum_{a\in\mathcal{A}} \pi(s|a) q(s, a) = (E_\pi q)(s).$$

Then, $B_*^{(Q)} q = D \circ E_* = D \circ E_\pi = B_\pi$ and $B_*^{(V)} q = E_* \circ D = E_\pi \circ D = B_\pi$. □

2.4 Optimal value functions & policies

Definition 2.4.1. Let $\gamma \in (0,1)$. The *optimal state-value* and *actions-value functions* with respect to discount factor γ are respectively defined as

$$v_*^{(\gamma)}(s) = \sup_{\pi \in \Pi} v_\pi^{(\gamma)}(s), \quad s \in \mathcal{S},$$
$$q_*^{(\gamma)}(s,a) = \sup_{\pi \in \Pi} q_\pi^{(\gamma)}(s,a), \quad (s,a) \in \mathcal{S} \times \mathcal{A}.$$

As soon as discount factor γ is clear from the context, we may simply use notation v_* and q_*.

Remark 2.4.2. v_* and q_* are well-defined because v_π and q_π can be easily seen to by bounded by $(1-\gamma)^{-1} \max_{r \in \mathbb{R}} |r|$.

Definition 2.4.3. A policy π_* is *optimal* if $v_{\pi_*} = v_*$.

Theorem 2.4.4. *Let v_0 and q_0 the unique fixed points of $B_*^{(V)}$ and $B_*^{(Q)}$ respectively. Then, $\Pi_g[v_0] = \Pi_g[q_0]$ and for π_g in the latter set,*

(i) $v_* = v_0 = v_{\pi_g}$,

(ii) $q_* = q_0 = q_{\pi_g}$,

(iii) $v_* = E_* q_*$,

(iv) $q_* = D v_*$.

Remark 2.4.5. Some important takeaways from the above theorem are the following:

- v_* (resp. q_*) is the unique fixed point of $B_*^{(V)}$ (resp. $B_*^{(Q)}$), meaning the unique solution to the Bellman optimality equation for state-value function (resp. action-value function);
- there exists a stationary and deterministic optimal policy.

Proof. Let us first prove that $q_0 = Dv_0$ and $v_0 = E_* q_0$. Indeed,

$$Dv_0 = DB_*v_0 = DE_*Dv_0 = B_*(Dv_0),$$

therefore, Dv_0 is the unique fixed point of B_*, in other words $q_0 = Dv_0$. Then,

$$E_*q_0 = E_*Dv_0 = B_*v_0 = v_0.$$

Therefore, $\Pi_g[v_0] = \Pi_g[Dv_0] = \Pi_g[q_0]$. We recall that a set of greedy policies is never empty, as stated in Proposition 2.3.3.

Let $\pi_g \in \Pi_g[v_0]$. Then using the property of greedy policies from Proposition 2.3.4, $v_0 = B_*v_0 = B_{\pi_g}v_0$ and $q_0 = B_*q_0 = B_{\pi_g}q_0$. Value functions v_0

and q_0 are therefore the unique fixed points of $B^{(V)}_{\pi_g}$ and $B^{(Q)}_{\pi_g}$, respectively. In other words $v_0 = v_{\pi_g}$ and $q_0 = q_{\pi_g}$, by Proposition 2.2.6.

Therefore, $v_0 = v_{\pi_g} \leqslant \sup_{\pi\in\Pi_{0,d}} v_\pi$ because $\pi_g \in \Pi_{0,d}$ by definition, and similarly $q_0 \leqslant \sup_{\pi\in\Pi_{0,d}} q_\pi$.

Let us now prove that $v_0 \geqslant \sup_{\pi\in\Pi} v_\pi$. Let $\pi = (\pi^{(t)})_{t\geqslant 0}$ be any policy, $s \in \mathcal{S}$, and consider random variables $(S_0, A_0, R_1, S_2, A_2, R_3, \dots) \sim \mathbb{P}_{s,\pi}$. Let $t \geqslant 0$,

$$v_0(S_t) = (B_* v_0)(S_t) = \max_{a\in\mathcal{A}} (Dv)(S_t, a) \geqslant (Dv)(S_t, A_t).$$

Let us rewrite this last quantity. Let $(s_0, a_0) \in \mathcal{S}$ such that $\mathbb{P}\left[S_t = s_0,\ A_t = a_0\right] > 0$. Then, using the definition of $\mathbb{P}_{s,\pi}$,

$$\begin{aligned}
(Dv)(s_0, a_0) &= \sum_{(r,s')\in\mathcal{R}\times\mathcal{S}} p(r, s'|s_0, a_0)(r + \gamma v(s')) \\
&= \sum_{(r,s')\in\mathcal{R}\times\mathcal{S}} \frac{\mathbb{P}\left[R_{t+1} = r,\ S_{t+1} = s',\ S_t = s_0,\ A_t = a_0\right]}{\mathbb{P}\left[S_t = s_0,\ A_t = a_0\right]}(r + \gamma v(s')) \\
&= \mathbb{E}\left[R_{t+1} + \gamma v(S_{t+1}) \,|\, S_t, A_t\right].
\end{aligned}$$

Therefore,

$$v_0(S_t) \geqslant \mathbb{E}\left[R_{t+1} + \gamma v(S_{t+1}) \,|\, S_t, A_t\right].$$

Then using the expression of $(Bv_0)(s)$ from Proposition 2.1.3, applying the above recursively, we get

$$\begin{aligned}
v_0(s) = (Bv_0)(s) &= \mathbb{E}\left[R_1 + \gamma v_0(S_1)\right] \\
&\geqslant \mathbb{E}\left[R_1 + \gamma \mathbb{E}\left[R_2 + \gamma v(S_2) \,|\, S_1, A_1\right]\right] \\
&\geqslant \dots \geqslant \mathbb{E}_{s,\pi}\left[\sum_{t=1}^{T} \gamma^{t-1} R_t + \gamma^T v(S_T)\right] \\
&\geqslant \mathbb{E}\left[\sum_{t=1}^{+\infty} \gamma^{t-1} R_t\right] = v_\pi(s).
\end{aligned}$$

Therefore,

$$v_* = \sup_{\pi\in\Pi} v_\pi \leqslant v_0 = v_{\pi_g} \leqslant \sup_{\pi\in\Pi_{0,d}} v_\pi \leqslant \sup_{\pi\in\Pi} v_\pi = v_*,$$

and the lower and upper bounds being equal, all inequalities are equalities, and the supremums are maximums because they are attained for $\pi_g \in \Pi_{0,d} \subset \Pi$.

Then, we write

$$\begin{aligned}
q_* = \sup_{\pi\in\Pi} q_\pi &\geqslant \max_{\pi\in\Pi_{0,d}} q_\pi \geqslant q_{\pi_g} = q_0 = Dv_0 \\
&= D\left(\max_{\pi\in\Pi} v_\pi\right) \geqslant \sup_{\pi\in\Pi} Dv_\pi = \sup_{\pi\in\Pi} q_\pi = q_*,
\end{aligned}$$

where the last inequality holds by monotonicity of D from Proposition 2.1.6 (by writing for $\pi \in \Pi$, $D \max_{\pi\in\Pi} v_\pi \geqslant D v_\pi$ and then taking the supremum over $\pi \in \Pi$). Therefore, all inequalities are equalities and all supremums are maximums. $\square$