Markov Decision Processes

Infinite-horizon discounted MDPs

An MDP $M = (S, A, P, R, \gamma)$

State space S.

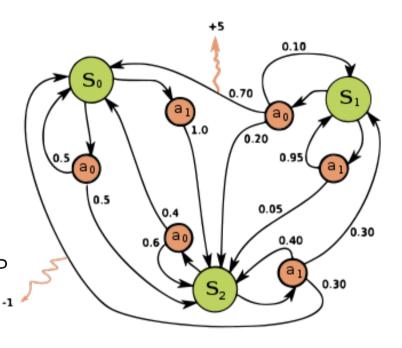
- We will only consider discrete and finite
- Action space A.
- spaces in this course (w/o losing much).
- Transition function $P: S \times A \rightarrow \Delta(S)$. $\Delta(S)$ is the probability simplex over S, i.e., all non-negative vectors of length |S| that sums up to 1
- Reward function $R: S \times A \rightarrow \mathbb{R}$. (deterministic reward function)
- Discount factor $\gamma \in [0,1)$
- The agent starts in some state s_1 , takes action a_1 , receives reward $r_1 = R(s_1, a_1)$, transitions to $s_2 \sim P(s_1, a_1)$, takes action a_2 , so on so forth the process continues **forever**
- Objective: (discounted) expected total reward
 - other terms used: return, value, utility, long-term reward, etc

Additional/alternative notations

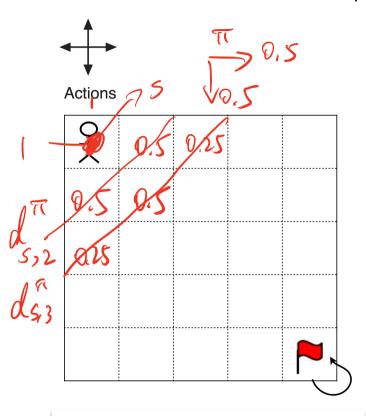
- The probability of transitioning to a particular state: $P(s' \mid s, a)$
- Sometimes reward is random and/or depends on the next-state, e.g., R(s, a, s'), or R(s, a) is a random variable
 - The most general case: given (s, a), (r, s') is drawn from some joint distribution (Sutton & Barto 2nd ed; see link on course website)
 - When we consider random rewards we will assume a simplified case: r and s' are independent conditioned on (s, a)
 - Such differences usually don't matter—we will revisit later
- Sometimes the available actions depend on the state, A_s
 - Again, the theory/algs developed for fixed action spaces usually extend to state-dependent action spaces

Toy Example

- $P(s_0 | s_2, a_0) = 0.4$
- $P(s_1 | s_2, a_0) = 0$
- $P(s_2 | s_2, a_0) = 0.6$
- ...
- If there is only 1 action, the MDP becomes a Markov chain (associated with a reward function)
- As another special case, if there are multiple actions but transition is deterministic, the MDP becomes a directed graph



Example: Gridworld



"Absorbing state": emulate the termination of a task in infinite-horizon MDPs

- State: grid No. (or integer x, y coordinates)
- Action: N, S, E, W
- Dynamics:
 - Deterministic transitions to the adjacent grid in the direction of action in most cases.
 - Keep in the current state if moving towards wall or having reached goal
- Reward: 0 in the goal state and -1 everywhere else
- Discount factor γ: 0.99

Why discounting?

- When defining the MDP (esp. the reward function & the discount factor/horizon), you should make sure that the total expected reward of a policy precisely reflects how you like that policy. Don't worry about learning yet.
 - e.g., in the grid world example, if there is no discounting (γ = 1), the total expected reward is the negative expected number of steps before reaching the goal
 - After you've learned a policy, you should evaluate the policy using this reward function / horizon
- So why discounting?
 - In the previous example, $\gamma=1$ allows some strategies to obtain - ∞ expected return—we don't like infinities

Why discounting? (cont.)

As a mathematical convenience...

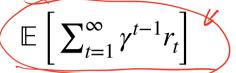
- We introduce a discount factor close to (but smaller than) 1, so that even the agent moves in circles, the expected total reward is still finite.
- On the other hand, for most reasonable policies (esp. the nearoptimal ones), the total reward is still approximately the negative total number of steps—our training objective closely tracks what we really care about
- Reason 2: discounting + infinite horizon = stationary optimal policy & value functions, again a mathematical convenience
- Reason 3: heavy discounting (small γ) yields faster planning / learning (we will see)
- Discounting does have economic interpretations, but they are seldom relevant in RL

Homework

- Homework 0 (handled via Gradescope; more info to come on Campuswire)
 - Due 1 week from now, before class starts
 - Main purpose: remind you some maths & set the expectation about how mathy this course will be
 - Does not count towards final grades but (1) we will look at it, and (2) you have to submit in time otherwise you use up your change to drop the lowest score for homework (see late policy)
- Reading: Sutton & Barto, Chap 3
 - Note difference in notations
 - Focus on understanding how to translate between Table 3.1 and Fig 3.2. Also Chap 3.4; Example 3.6; Example 3.10

Value and policy

• Want to take actions in a way that maximizes value (or return):



- This value depends on where you start and how you act
- Often assume boundedness of rewards: $r_t \in [0, R_{\text{max}}]$
 - What's the range of $\mathbb{E}\left[\sum_{t=1}^{\infty} \gamma^{t-1} r_t\right]$? $\left[0, \frac{R_{\max}}{1-\gamma}\right]$
- A (deterministic) policy $\pi: S \to A$ describes how the agent acts: at state s_t , chooses action $a_t = \pi(s_t)$.
- More generally, the agent may choose actions randomly $(\pi: S \rightarrow \Delta(A))$, or even in a way that varies across time steps ("non-stationary policies")

• Define
$$V^{\pi}(s) = \mathbb{E}\left[\sum_{t=1}^{\infty} \gamma^{t-1} r_{t} \middle| s_{1} = s, \pi\right]$$

V4 E [O, Rmex] Claim: $\forall \chi \in [0,1)$. $\sum_{t=1}^{\infty} \chi^{t-1} \chi \in [0, \frac{\text{Rusk}}{(-\chi)}]$ $\sum_{t=1}^{\infty} \sqrt{\frac{1}{t}} = \sqrt{\frac{1}{t}} = \sqrt{\frac{1}{t}}$ 2 St-1 rt = 2 St-1 Rmax. 1+8+82 = Rmax. \(\frac{26}{t=1} \) +8+8+ = Rusx, (-8. lim 5 7 - 1 = lim 1-877 T-20 +-11 (-8.) = $\sqrt{-\chi}$. S1152, -- , St. γ , γ , SI, QI, YI, SZ, QZ, YZ, SZ, QZ, YZ, (5) T(S), R(SI,OI), ~P(-|SI,QI) realization.

Bellman equation for policy evaluation

$$V^{\pi}(s) = \mathbb{E}\left[\sum_{t=1}^{\infty} \gamma^{t-1} r_{t} \mid s_{1} = s, \pi\right]$$

$$= \mathbb{E}\left[r_{1} + \sum_{t=2}^{\infty} \gamma^{t-1} r_{t} \mid s_{1} = s, \pi\right]$$

$$= R(s, \pi(s)) + \sum_{s' \in \mathcal{S}} P(s' \mid s, \pi(s)) \mathbb{E}\left[\gamma \sum_{t=2}^{\infty} \gamma^{t-2} r_{t} \mid s_{1} = s, s_{2} = s', \pi\right]$$

$$= R(s, \pi(s)) + \sum_{s' \in \mathcal{S}} P(s' \mid s, \pi(s)) \mathbb{E}\left[\gamma \sum_{t=2}^{\infty} \gamma^{t-2} r_{t} \mid s_{2} = s', \pi\right]$$

$$= R(s, \pi(s)) + \gamma \sum_{s' \in \mathcal{S}} P(s' \mid s, \pi(s)) \mathbb{E}\left[\sum_{t=1}^{\infty} \gamma^{t-1} r_{t} \mid s_{1} = s', \pi\right]$$

$$= R(s, \pi(s)) + \gamma \sum_{s' \in \mathcal{S}} P(s' \mid s, \pi(s)) V^{\pi}(s')$$

$$= R(s, \pi(s)) + \gamma \langle P(\cdot \mid s, \pi(s)), V^{\pi}(\cdot) \rangle$$

$$= R(s, \pi(s)) + \gamma \langle P(\cdot \mid s, \pi(s)), V^{\pi}(\cdot) \rangle$$

$$\begin{array}{l}
V^{T}(\underline{s}) = \$100. \quad Y = R(s, \pi(s)) = \$20. \\
Y^{T}(\underline{s}) = \$80. \\
S' \sim P(\cdot | s, \pi(s))
\end{array}$$

$$\begin{array}{l}
V^{T}(\underline{s}) = \$(s, \pi(s)) = \$20. \\
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•
$$P^{\pi}$$
 as the matrix $[P(s'|s,\pi(s))]_{s\in S,\,s'\in S}$
$$V^{\pi} = R^{\pi} + \gamma P^{\pi}V^{\pi}$$

$$(I - \gamma P^{\pi})V^{\pi} = R^{\pi}$$

$$V^{\pi} = (I - \gamma P^{\pi})^{-1}R^{\pi}$$

 $\mathbb{E}_{S'} \mathbb{P}(0|s,\pi(s)) \left[\bigvee^{\pi}(S') \right] = \mathbb{E}_{S' \in S} \mathbb{P}(S'|S,\pi(s)) \cdot \bigvee^{\pi}(S')$

Bellman equation for policy evaluation

 V^{π} as the $|S| \times 1$ vector $[V^{\pi}(s)]_{s \in S}$ R^{π} as the vector $[R(s, \pi(s))]_{s \in S}$

$$V^{\pi}(s) = R(s, \pi(s)) + \gamma \langle P(\cdot \mid s, \pi(s)), V^{\pi}(\cdot) \rangle \qquad \forall^{t}$$
m: define

<u.v> is dot product. Matrix form: define

This is always invertible (Proof?), i.e., solution

to Bellman equation is always unique

W.t.s.
$$Z-yP^{\pi}$$
 is invertible.

$$(Z-yP) \times \neq 0.$$

$$||(Z-yP) \times ||_{\infty} = || \times - \nabla P^{\pi} ||_{\infty}.$$

$$||X||_{\infty} - || yP^{\pi} ||_{\infty}.$$

$$||X||_{\infty} = ||X||_{\infty}.$$

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Some remarks about rewards

• For more general formulations of rewards (e.g., random rewards, rewards that depend on s', etc) $V^{\pi}(s) = \mathbb{E}_{r,s'|s,\pi(s)}[r + \gamma V^{\pi}(s')]$

• Can also be translated to an equivalent problem where rewards deterministically depends on (s,a):
$$R(s,a) := \mathbb{E}_{r|s,a}[r]$$

- In infinite-horizon discounted MDPs, shifting the reward function by a constant for every state-action pair does not change anything R(s,a) = R(s,a) + C.
 - If we increase the reward function by c, you are just earning an extra c units of "background" rewards however you behave
 - All value functions increase by $c/(1-\gamma)$

Interpretation of $(I - \gamma P^{\pi})^{-1}$ Each row of this matrix (indexed by s) is the unnormalized discounted state occupancy, whose (s')-th entry is $d_s^{\pi}(s')/(1-\gamma)$, where $d_{\underline{s}}^{\pi}(\underline{s'}) := \underline{(1-\gamma)} \cdot \mathbb{E} \left[\sum_{t=1}^{\infty} \gamma^{t-1} \, \underline{\mathbb{I}}[s_t = s'] \, \middle| \, s_1 = s, \pi \right]$

•
$$\mathbb{I}[\cdot]$$
 is the indicator function: =1 if (.) is true, and =0 if false.

• Each row of
$$(I - \gamma P^{\pi})^{-1}$$
 is like a distribution vector—except that the entries sum up to $1/(1-\gamma)$. Multiplying by $1-\gamma$ normalizes it

Can also be interpreted as the value function of indicator reward function: $d_s^{\pi}(s') = (1 - \gamma)V^{\pi}(s)$, where V^{π} is defined wrt the reward function that is equal to 1 at state s' and 0 elsewhere \mathcal{D}_{tienal} :

 $d_s^{\pi}(s',a') = (1-x) \cdot \mathbb{E}\left[\sum_{s=0}^{\infty} x^{t-1} \mathbb{I}[s+s], C$ Can similarly define state-action occupancy

More on State occupancy

- de disconted
- Alternative way of defining state occupancy: let $d_{s,t}^{\pi}$ be a (distribution) vector such that $d_{s,t}^{\pi}(s') = \Pr[s_t = s' | s_1 = s, \pi]$
- It's the t-th step state distribution induced by starting at state s • The discounted occupancy is $d_s^{\pi} = (1-\gamma)\sum_{t=1}^{\infty} \gamma^{t-1} d_{s,t}^{\pi}$ • The s-th row of $(I - \epsilon D^{\pi})^{-1}$
- The s-th row of $(I \gamma P^{\pi})^{-1}$ is $d_s^{\pi}/(1 \gamma)$, because:
 - Let $e_s = [0 \cdots 0 \ 1 \ 0 \cdots 0]^T$, where the 1 is at the s-th entry s-th row of $(I \gamma P^{\pi})^{-1}$ is

$$e_s^{\top} (I - \gamma P^{\pi})^{-1} = e_s^{\top} (\sum_{t=1}^{\infty} (\gamma P^{\pi})^{t-1})$$

$$= \sum_{t=1}^{\infty} \gamma^{t-1} e_s^{\top} (P^{\pi})^{t-1} = \sum_{t=1}^{\infty} \gamma^{t-1} (d_{s,t}^{\pi})^{\top}$$

Alternative formula for value function

· Some further exercise that helps understanding

•
$$V^{\pi}(s) = e_{s}^{\top} (I - \gamma P^{\pi})^{-1} R^{\pi}$$

$$= e_{s}^{\top} (\sum_{t=1}^{\infty} \gamma^{t-1} (P^{\pi})^{t-1}) R^{\pi}$$

$$= \sum_{t=1}^{\infty} \gamma^{t-1} \langle d_{s,t}^{\pi}, R^{\pi} \rangle$$

$$= \int_{s}^{\infty} V^{\pi}(s) = \int_{s}^{\infty} V^{\pi}(s) ds$$

$$= \int_{s}^{\infty} V^{\pi}(s) = \int_{s}^{\infty} V^{\pi}(s) ds$$

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$$\sqrt{T}(s) = R(s, \pi(s)) + 8 E_{sn}[s, \pi(s)] [V^{T}(s)]$$

$$\sqrt{T}(s) = E[\sum_{t=1}^{\infty} 3^{t-1} Y_{t} | s_{1} = s, \pi]$$

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$$= E[\sum_{t=1}^{\infty} 3^{t-1} Y_{t}$$

$\mathcal{T}^*: S \rightarrow A$ Optimality

- For infinite-horizon discounted MDPs, there always exists a stationary and deterministic policy that is optimal for all starting states simultaneously
 - Proof: Puterman'94, Thm 6.2.7 (reference due to Shipra Agrawal) 🗸
 - Let π^* denote this optimal policy, and $V^* := V^{\pi^*}$
 - Bellman Optimality Equation:

$$V^{\star}(s) = \max_{a \in A} \left(R(s, a) + \gamma \mathbb{E}_{s' \sim P(s, a)} \left[V^{\star}(s') \right] \right)$$

- If we know V^* , how to get π^* ?
- Easier to work with Q-values: $Q^*(s, a)$, as $\pi^*(s) = \arg\max_{s} Q^*(s, a)$

$$Q^{\star}(s,a) = R(s,a) + \gamma \mathbb{E}_{s' \sim P(s,a)} \left[\max_{a' \in A} Q^{\star}(s',a') \right]^{a}$$

• Note that $V^{\star}(s) = \max_{a \in A} Q^{\star}(s, a) = Q^{\star}(s, \pi^{\star}(s))$

$$V^* = V^{\pi^*}.$$

$$V^*(s) = R(s, \pi^*(s)) + \mathcal{E}_{s' \sim P(\cdot|s, \pi^*(s))}$$

$$\exists \pi^* : S \Rightarrow A. \quad \text{st. } \forall s. \forall \pi$$

$$V^{\pi^*}(s) \geq V^{\pi}(s).$$

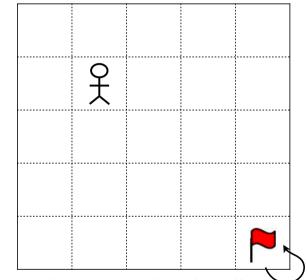
Maximize
$$E\left[\sum_{t=1}^{\infty} 3^{t-1} f_t \middle| S_1 n do, \pi\right]$$
.

 $\forall do, \forall \pi$.

 $E_{s_1 n do}\left[V^{\pi^*}(s_1)\right] \not= E_{s_1 n do}\left[V^{\pi}(s_1)\right]$.

Optimality

- Similar to the Bellman equations for policy evaluation, the Bellman optimality equations also have unique solutions V* and Q*
- But π^* may not be unique
- e.g., in the state shown in the figure, the optimal policy can take any of the following
 - Go right
 - Go down
 - Any probability distribution over right and down (stochastic policy)



 Remark: the fact that a deterministic & stationary optimal policy exists does NOT mean that all optimal policies have to be this way (they can be stochastic and/or non-stationary)

(Policy-specific) Q-functions
$$Q^{\pi}(s,a) := \mathbb{E}\left[\sum_{t=1}^{\infty} \gamma^{t-1} r_{t} \middle| s_{1} = s, a_{1} = a; \pi\right]$$

- $V^{\pi}(s) = Q^{\pi}(s, \pi(s))$
 - When π is stochastic, RHS becomes $E_{a \sim \pi(\cdot \mid s)}[Q^{\pi}(s, a)]$
 - We will often abbreviate $Q^{\pi}(s, \pi(s))$ as $Q^{\pi}(s, \pi)$
- Also satisfies a similar Bellman equation $Q^{\pi}(s, a) = R(s, a) + \gamma \mathbb{E}_{s' \sim P(\cdot | s, a)} \left[Q^{\pi}(s', \pi) \right]$
- Compare to the optimality equation

$$Q^{\star}(s, a) = R(s, a) + \gamma \mathbb{E}_{s' \sim P(\cdot \mid s, a)} \left[\max_{a' \in A} Q^{\star}(s', a') \right]$$

 The only difference is in the action-selection operator at the next-state s': if you choose a' greedily (max operator), you get Q*; if you choose a' according to π, you get Q^π

Clarification on definition of value functions

- $V^{\pi}(s)$, $Q^{\pi}(s, a)$, $V^{*}(s)$, $Q^{*}(s, a)$
- they are the expected return when starting from of $s_1=s$ and following the behaviors below:
 - $V^{\pi}(s)$: $a_1 \sim \pi(s_1)$, $a_2 \sim \pi(s_2)$, $a_3 \sim \pi(s_3)$, ...
 - $Q^{\pi}(s, a)$: $a_1 = a, a_2 \sim \pi(s_2), a_3 \sim \pi(s_3), ...$
 - $V^*(s) = V^{\pi^*}(s)$: $a_1 \sim \pi^*(s_1)$, $a_2 \sim \pi^*(s_2)$, $a_3 \sim \pi^*(s_3)$, ...
 - $Q^*(s, a) = Q^{\pi^*}(s, a)$: $a_1 = a, a_2 \sim \pi^*(s_2), a_3 \sim \pi^*(s_3), \dots$
- The policy (or *) on the superscript denotes the long-term behavior
- For Q values, the second argument of the function specifies the first action; all future actions are according to the policy on the superscript

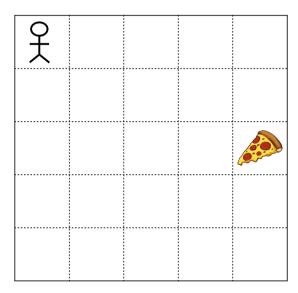
Some Subtleties in Formulating

Problems as MDPs



Defining the state (in toy problems)

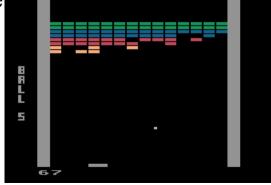




- The agent can move around just as in the previous example
- Reward: +1 when reaching food for the first time, and 0 otherwise
 - i.e., food is consumable
- How to define state?
 - The status of the food (consumed or not) also needs to be part of the state representation
- In general, make sure that you can fully determine reward and (the distribution of) next-state using (s, a) alone without other info
- The tricky part of this example is that dynamics are Markovian in the coordinates, but reward function is not

Defining state beyond toy problems

- In toy problems, we can give any information about the system to the agent, so that the agent always has a (Markov) state
- In reality, agent receives limited sensory inputs every time step
- i.e., a trajectory looks like o_1 , a_1 , r_1 , o_2 , a_2 , r_2 , o_3 ...
- We say that the problem is Markov (in o), if the future observations and rewards are independent of the past conditioned on the current observation (and o is state)
- But this is generally not true...
- Need to construct an (approximate) state from history
- Will come back to this when we discuss POMDPs later in this course



Alternative notions of horizons

- It is often more natural to model the problem as indefinite-horizon undiscounted MDPs
 - Some states are considered terminal
 - Trajectory does not go on forever—it stops at terminal states
 - The length of a trajectory is not fixed—it's random and/or may depend on the policy
 - e.g., navigation task: goal state is terminal, -1 per step before you terminate
 - Natural to model episodic tasks in this way
- Bellman equations remain the same for non-terminal states
- For terminal states, V(s) = 0 (regardless of V^{π} or V^{*})

Fixed-horizon MDPs

- Specified by (*S*, *A*, *R*, *P*, *H*)
- All trajectories end in precisely H steps
- No terminal states; termination is enforced "externally"
- Optimal policy may additionally depend on the time step
 - When selling goods, may price things differently near the end of the season, even if we assume the demand doesn't change
 - In the navigation example, when you are too far away from goal to reach it within the remaining steps, any action is optimal (there is nothing you can do)
- So do (policy-specific/optimal) value functions: $V_{H+1}^{\pi}(s) \equiv 0$ $V_h^{\pi}(s) = R(s, \pi(s)) + \mathbb{E}_{s' \sim P(s,a)}[V_{h+1}^{\pi}(s')]$
- Similar to the discounted setting, shifting rewards by constant doesn't change the relative preference over policies (all value functions increase by cH)

Translating between indefinite-horizon and fixed horizon MDPs

- "=>": If trajectory length has an upper bound, set H to be this upper bound and add a dummy absorbing state; if a trajectory terminates early, loop in the dummy state for the remaining steps
- "<=": Augment state space: include time step as part of the state representation, and define all states at time H+1 as terminal, i.e., If P is the dynamics of the fixed horizon MDP, then define a new transition function

$$P'((s',h') | (s,h), a) = \mathbb{I}[h' = h+1] \cdot P(s' | s, a)$$

 State augmentation is a common trick when we convert between different formulations in RL (e.g., non-Markov problems become Markov if we view history as state)

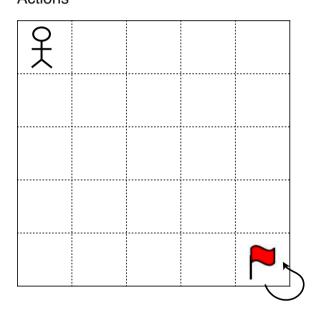
Translating between different formulations

- For discounted & fixed horizon, shifting rewards don't matter
- What about indefinite-horizon?
 - Think about what happens with the navigation example
 - Shift -1 to 1: you are rewarded if you don't reach the goal!
- Why is that?
 - For indefinite-horizon problems, since trajectory length is a variable, the positivity of reward actually carries a meaning: "+" means "live longer", and "-" means "finish faster"
 - For the other two formulations, such meaning doesn't exist
 - In-class exercise: formulate the navigation problem as a fixed horizon problem, then shift the reward. Explain why shifting rewards is fine in this case.

The navigation example

- Original formulation: indef-horizon
 - -1 reward per step everywhere
 - Goal is terminal
 - Cannot shift reward
- Translate into fixed-horizon
 - Make goal state absorbing
 - 0 reward in goal and -1 everywhere else
 - Terminate in H steps
- Shift reward?
 - Have to shift everywhere, including the goal





- e.g., if shift by 1, then +1 in goal and 0 everywhere else
- No penalty, but being rewarded when looping in goal