Algorithmic and Theoretical Foundations of RL

Online Planning

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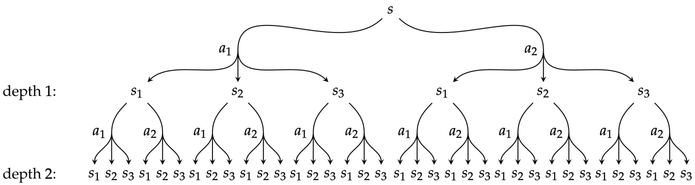
Problem Description

The methods discussed so far focus on solving RL problem **globally in an offline way** via (approximate) dynamic programming or optimization. That is, we would like to find a good action for every state. In contrast, **online planning** methods attempt to find a good action for a single state based on reasoning about states that are reachable from that state. The reachable state space is often orders of magnitude smaller than the full state space, which can significantly reduce storage and computational requirements compared to offline methods.

A typical scheme for online planning is known as **receding horizon planning**, which plans from the current state to a maximum fixed horizon or depth d, then executes the action from current state, transitions to the next state, and replans.

Materials from "Algorithms for decision making" by Kochenderfer et al., 2022

Forward Search



- Forward search builds a search tree with current state as root by expanding all possible transitions up to certain depth via a MDP model, and determines the best action at initial state by for example dynamic programming.
- If it requires planning beyond depth that can be computed online, one can use estimated values obtained using offline RL methods as leaf values.
- In contrast, MCTS is simulation-based search which attempts to reduce computational complexity of forward search by building a tree incrementally based on the balance between exploration and exploitation.

Figure from "Algorithms for decision making" by Kochenderfer et al., 2022

Remark

In order to conduct search, it requires a model of environment so that sampling and evaluation can be done repeatedly (even in online setting). While in some applications the model is clear, there are also applications in which model needs to be estimated and stored.

Indeed, there are RL algorithms which combines model free methods with a model estimated from data (for example Dyna-Q). The estimated model (though not accurate) allows us to apply RL algorithms (model based or model free) repeatedly which can improve the efficiency of data usage.

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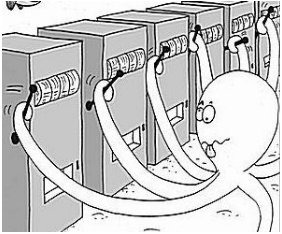
MAB

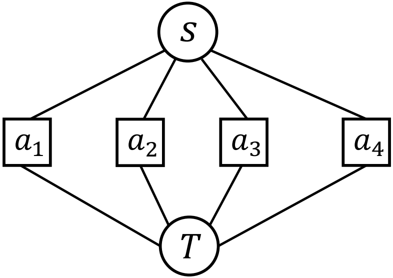


- K actions (arms): $\mathcal{A} = \{1, \cdots, K\}$.
- $r \in [0, 1] \sim \mathcal{D}_a$, unknown probability distribution over rewards for action a.
- At time t, agent selects an action a_t, receives a reward $r_t(a_t) \sim \mathcal{D}_{a_t}$.
- Goal: Maximize cumulative reward $\sum_{t=1}^{T} \mathbb{E}[r_t(a_t)]$.

- There are different settings of bandits, and we only discuss the simplest stochastic setting where rewards of each action at all time steps are i.i.d.
- A fundamental dilemma in online planning is exploration and exploitation tradeoff when facing uncertainty. On one hand, we want to make good decision given current information; on the other hand, uncertainty may mislead and thus requires to explore more decisions before making good decision with high confidence. Overall, a good strategy should count the uncertainty in or we should learn/use the data distribution.

MAB as RL

MAB is special RL with single state, multiple actions, and random rewards.



SARSA/Q-Learning for MAB

Algorithm 1: SARSA/Q-Learning

Initialization: K arms, $Q^0(a) = 0, \ \forall a \in \mathcal{A}$

for $t = 0, 1, 2, \ldots$ **do**

  Take $a_t \sim \epsilon_t$-greedy$(Q^t(\cdot))$

  Observe reward r_t

  Update $Q^{t+1}(a) = \begin{cases} Q^t(a) + \alpha_t(a) \cdot (r_t - Q^t(a)) & \text{if } a = a_t \\ Q^t(a) & \text{otherwise} \end{cases}$

end

- Classic RL algorithms do not focus on the efficient action sampling at each time step. As can be seen later, there exist more efficient algorithms for MAB.

How to Evaluate an Algorithm? Regret

- μ_a is mean reward of action a: $\mu_a = \mathbb{E}_{r \sim \mathcal{D}_a}[r]$.
- $\mu_* = \mu_{a_*} = \max_a \mu_a$, where $a_* = \operatorname{argmax}_a \mu_a$ is maximum mean reward.

Given a sequential of actions a_t up to time T, the total **regret** (or regret for simplicity) is defined as the total loss:

$$R_T = \sum_{t=1}^{T} (\mu_* - \mu_{a_t}).$$

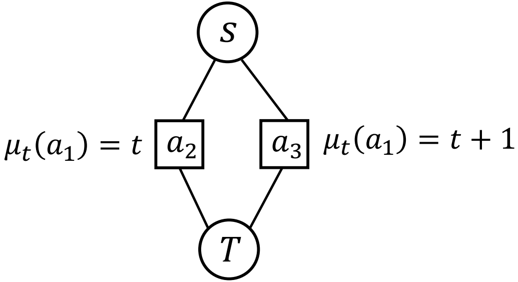
R_T is a random variable, whose randomness comes from the selections of a_t.

Remark about Regret

- Regret characterizes the difference between online performance and offline performance. In the offline setting, we want to choose an action a such that $\sum_{t=1}^{T} \mathbb{E}\left[r_t(a)\right]$ is maximized. It is clear the solution is a_*, and the regret is the difference between offline and online cumulative rewards.
- Asymptotically, most algorithms can find action that is close to the best in terms cumulative reward. Then how to compare the performance of different algorithms? Regret provides a micro-level measure based on the loss in the process of applying algorithms, reflecting the speed converging to optimum.

Regret Identifies Higher Order Performance Difference

For intuitive explanation, consider a non-stationary two-armed bandit problem:



No matter which action is selected in each step, leading order of $\sum_{t=1}^{T} \mu_{a_t}$ is T^2.
However, regret is T if a_1 is always selected while it is 0 if a_2 is always selected.

Probability Tools Needed for Regret Analysis

Hoeffding Inequality

Definition 1 (Sub-Gaussian distribution)
A random variable X with mean μ is sub-Gaussian if there exists a $\nu > 0$ such that

$$\mathbb{E}\left[e^{\lambda(X-\mu)}\right] \leq e^{\frac{\lambda^2\nu^2}{2}}, \quad \forall \lambda \in \mathbb{R}.$$

- Gaussian random variables and bounded random variables are sub-Gaussian.

Theorem 1 (Hoeffding inequality)
Let $\{X_k\}_{k=1}^n$ ($\mathbb{E}[X_k] = \mu$) be i.i.d sub-Gaussian with parameter ν. Then one has,

$$P\left(\left|\frac{1}{n}\sum_{k=1}^{n}(X_k - \mu)\right| \geq t\right) \leq 2\exp\left(-\frac{nt^2}{2\nu^2}\right).$$

Overview of Algorithms

- **Explore-First**: Try each arm N rounds first, then pull the empirically best arm.
- **Epsilon-Greedy**: In each round, with an probability ϵ_t, pull all the arms uniformly at random; otherwise pull the best arm so far.
- **UCB:** Be optimism in face of uncertainty. In each round, pull the most promising arm, and this can be done by constructing confidence intervals.

Explore-First

Algorithm

There are two phases in Explore-First:

- **Exploration:** Pulls all the arms N rounds;
- **Exploitation:** Pulls the arm with highest empirical mean in remaining rounds.

Algorithm 2: Explore-First

Initialization: Parameter N.

for $a = 1, 2, .., K$ **do**

  Pull arm a for N rounds and collect rewards $\{r_{a,t}\}_{t=1}^{N}$

  Calculate empirical mean reward $\bar{\mu}_a := \frac{1}{N}\sum_{t=1}^{N} r_{a,t}$

end

Select the arm $\hat{a} = \underset{a \in [K]}{\operatorname{argmax}} \ \bar{\mu}_a$ (break ties arbitraily)

Pull arm $\hat{a}$ in all remaining $T - NK$ rounds

Explore-First

Regret Analysis

The regret of Explore-First consists of two parts,

$$\mathbb{E}[R_T] = \underbrace{\sum_{\mathrm{a} \neq \mathrm{a}^*} N\left(\mu_* - \mu_a\right)}_{\text{Regret on Exploration Phase}} + \underbrace{(T - NK) \quad (\mathbb{E}[\mu_* - \mu_{\hat{a}}])}_{\text{Regret on Exploitation Phase}}.$$

The choice of N reflects tradeoff between exploration and exploitation. As N increases, regret on exploration increases but regret on exploitation phases decreases with high probability since both $T - NK$ and $P(\hat{a} \neq a^*)$ decreases.

Theorem 2 (Regret Bound of Explore-First)

Explore-First achieves the following bound when $N = (T/K)^{\frac{2}{3}} \cdot O\left(\log T\right)^{\frac{1}{3}}$,

$$\mathbb{E}\left[R_T\right] \leq T^{\frac{2}{3}} \cdot O\left(K \log T\right)^{\frac{1}{3}}.$$

Epsilon-Greedy

Algorithm

Algorithm 3: Epsilon-Greedy

Initialization: sequence $\{\varepsilon_t\}_{t=1}^{T}$.

for $t = 1, 2, .., T$ **do**

  Denote $\bar{\mu}_t(a) := \frac{\sum_{i=1}^{t-1} r_i \cdot \mathbf{1}\{a_i = a\}}{\sum_{i=1}^{t-1} \mathbf{1}\{a_i = a\}}$

  Toss a coin with success probability ϵ_t;

  if *success* **then**

    Explore: $a_t \sim U([K])$

  else

    Exploit: $a_t = \arg\max_{a \in [K]} \bar{\mu}_t(a)$

  end

end

- Epsilon-Greedy is the same as SARSA/Q-Learning for MAB.

Regret Analysis

In Epsilon-Greedy, ϵ_t controls balance between exploration and exploitation. It's natural to let ϵ_t decrease with t since mean reward of each arm will be estimated more accurately with t increasing.

Theorem 3 (Regret Bound of Epsilon-Greedy)

Epsilon-Greedy achieves the following regret for every t when $\epsilon_t = t^{-\frac{1}{3}} \cdot (K \log t)^{\frac{1}{3}}$,

$$\mathbb{E}[R_t] \leq t^{\frac{2}{3}} \cdot O(K \log t)^{\frac{1}{3}} .$$

Optimism in Face of Uncertainty

The key idea of *optimism in face of uncertainty* is to select the most promising action or the action that might have a high reward in an uncertain environment. A random reward might be high if the mean is large or there is more uncertainty in the reward distribution. Thus, a measure should include both information of reward (mean) and uncertainty (more distribution information, e.g., variance).

Two outcomes of this scheme:

- Get high reward if the arm really has a high mean reward;
- For arm really having a lower mean reward, pulling it can reduce average reward and mitigate uncertainty.

Upper Confidence Bound

Overall Idea

UCB selects arms with highest upper confidence bound: At time step t, for each arm a, construct the confidence interval (for a fixed confidence) of μ_a with radius $r_t(a)$ based on the empirical mean $\bar{\mu}_t(a)$. Then UCB selects

$$a_t = \operatorname*{argmax}_{a \in [K]} \mathrm{UCB}_t(a) := \bar{\mu}_t(a) + r_t(a).$$

An arm can have a large $\mathrm{UCB}_t(a)$ for two reasons (or combination thereof):

- $\bar{\mu}_t(a)$ is large: this arm is likely to have a high mean reward;
- $r_t(a)$ is large: this arm has not been explored much.

Either suggests the arm is worth selecting. Thus, $\bar{\mu}_t(a)$ and $r_t(a)$ represent exploitation and exploration. Moreover, UCB counts in effect of finite samples.

Construction of Upper Confidence Bound

Lemma 1

Let $n_t(a)$ be the number of pulling arm a at time step t. For any $0 < \delta < 1$, the following equality holds with probability $1 - \delta$:

$$|\bar{\mu}_t(a) - \mu(a)| \le \sqrt{\frac{1}{2n_t(a)} \log \frac{2}{\delta}}.$$

- By this lemma, the UCB of arm a at time step t can be constructed as

$$\mathrm{UCB}_t(a) = \bar{\mu}_t(a) + \sqrt{\frac{1}{2n_t(a)} \log \frac{2}{\delta}}.$$

Upper Confidence Bound

Algorithm

Algorithm 4: UCB

Initialization: parameter δ

for $a = 1, ..., K$ **do**

  Pull arm a and collect reward r_a

end

for $t = 1, 2, .., T - K$ **do**

  $n_t(a) \leftarrow 1 + \sum_{i=1}^{t-1} \mathbf{1}\{a_i = a\}$

  $\bar{\mu}_t(a) = \frac{1}{n_t(a)} \left(r_a + \sum_{i=1}^{t-1} r_t \cdot 1\{a_i = a\} \right)$

  $\mathrm{UCB}_t(a) \leftarrow \bar{\mu}_t(a) + \sqrt{\frac{1}{2n_t(a)} \log \frac{2}{\delta}}$

  Select $a_t = \underset{a \in [K]}{\operatorname{argmax}}\ \mathrm{UCB}_t(a)$

end

- Typical empirical choice for δ is $\delta = n_t^{\beta}$, where n_t is total number of simulations, leading to the UCB bound $\mathrm{UCB}_t(a) \leftarrow \bar{\mu}_t(a) + C\sqrt{\frac{\log n_t}{2n_t(a)}}$.

Upper Confidence Bound

Regret Analysis

Theorem 4 (Regret Bound of UCB)
UCB achieves the following regret for each round $t \leq T$ when $\delta = \frac{2}{T^4}$,

$$\mathbb{E}\left[R_t\right] \leq O\left(\sqrt{Kt \log T}\right).$$

Regret bound for other choice of δ is also available. Moreover, the lower regret bound for stochastic bandits is $\Omega(\sqrt{KT})$. See "Introduction to Multi-Armed Bandits" by Slivkins 2022 for more details.

Bayesian Bandits: Probability Matching

Bayesian bandits assume $\{\mu_a\}_{a=1}^K$ obey a prior distribution $Q(\mu_1, \cdots, \mu_K)$. Given history $H_{t-1} = \{(a_1, r_1, \cdots, a_{t-1}, r_{t-1})\}$, the idea of **probability matching** is:

- Compute posterior distribution $P(\mu_1, \cdots, \mu_K | H_{t-1})$ by Bayes law;
- Compute $p_a = P(\operatorname{argmax}_{a \in [K]} \mu_a = a | H_{t-1})$ and select a with largest p_a.

Compute p_a from posterior P is difficult. Thompson sampling implements this by sampling: Sample $(\mu_1, \cdots, \mu_K) \sim P(\cdot | H_{t-1})$ and choose the arm with largest μ_a.

Bayesian Bandits: Thompson Sampling

In the independent setting, $P(\mu_1, \cdots, \mu_K | H_{t-1})$ is decomposable and we can compute the posterior of each arm independently.

Algorithm 5: Thompson Sampling

Initialization:

for $t = 1, 2, .., $ **do**

- Observe the history $H_{t-1} = \{(a_1, r_1), ..., (a_{t-1}, r_{t-1})\}$.
- Compute posterior for each arm $P(\mu_a | H_{t-1})$
- Sample $\bar{\mu}_t(a) \sim P(\mu_a | H_{t-1})$
- Choose the best arm $\hat{a}_t = \underset{a}{\mathrm{argmax}}\, \bar{\mu}_t(a)$ and collect reward r_t

end

- Thompson sampling achieves nearly optimal Bayesian regret $O(\sqrt{KT \log T})$.

See "Introduction to Multi-Armed Bandits" by Slivkins 2022 for more details.

Bayesian Bandits: A Special Case

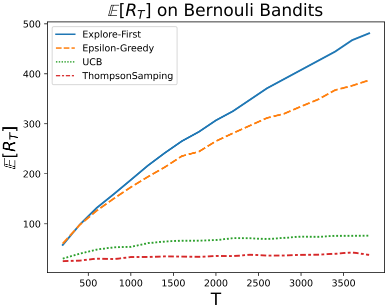
Consider Bernoulli reward case $r|\mu_a \sim \text{Bernouli}\,(\mu_a)$, where μ_a indicates the probability $r = 1$ (also mean of r). Assume uniform prior distribution for μ_a, i.e., $\mu_a \sim U([0, 1])$. Given independent random rewards $r_1, \cdots, r_n$ sampled for arm a, by Bayes law, pdf for posterior distribution $P(\mu_a|r_1, \cdots, r_n)$ is

$$\begin{aligned} p(\mu_a|r_1, \cdots, r_n) &\propto p(r_1, \cdots, r_n|\mu_a)p(\mu_a) \\ &= \prod_{k=1}^{n} \mu_a^{r_k}(1-\mu_a)^{1-r_k} = \mu_a^{\sum_{k=1}^{n} r_k}(1-\mu_a)^{\sum_{k=1}^{n}(1-r_k)}. \end{aligned}$$

It follows that $P(\mu_a|r_1, \cdots, r_n) = \textbf{Beta}(1 + m_1, 1 + m_2)$, where m_1 is the number of rewards that $r_k = 1$ and m_2 is the number of rewards that $r_k = 0$.

- Note $\mathbb{E}\left[\textbf{Beta}(\alpha, \beta)\right] = \frac{\alpha}{\alpha+\beta}$ and $U[0, 1] = \textbf{Beta}(1, 1)$. Thus, prior and posterior distributions are in the same distribution family, known as **conjugate prior**.

Illustrative Example



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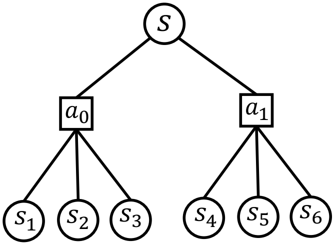
One-Step Policy Improvement as Stochastic MAB



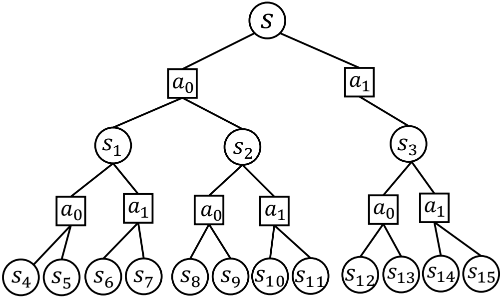
Consider the one-step policy improvement problem for state s,

$$\underset{a}{\operatorname{argmax}} \mathbb{E}_{s' \sim P(\cdot|s,a)} \left[r(s,a,s') + \gamma V(s') \right],$$

where we assume state values $V(s')$ at s' are available.

- If model P is known, we can compute expectation and then choose largest a.
- If P is not known, sample a and receive random reward $r(s,a,s') + \gamma v(s')$. Equivalent to stochastic MAB problem. UCB provides a way of efficient search.

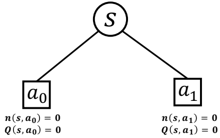
What about Multi-Step Policy Improvement?



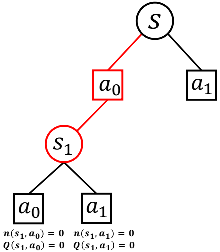
What about $\operatorname{argmax}_a \mathbb{E}_{s_{t+1} \sim P(\cdot|s_t,a_t)} \left[\sum_{t=0}^{H-1} \gamma^t r(s_t, a_t, s_{t+1}) + \gamma^H V(s_H) | s_0 = s, a_0 = a \right]$?

- MCTS builds a search tree incrementally, conducts UCB search in each depth and propagates optimal action values from bottom to top.

Illustration of MCTS



- **Expand** root state s and initialize n and Q



- **Select** action via UCB $Q(s,a) + C\sqrt{\frac{\log n(s)}{n(s,a)}}$.
  Assume a_0 selected, transition to s_1 (leaf).
  Use $V(s_1)$ to update node a_0 (**Propagate**):

$$n(s, a_0) = n(s, a_0) + 1,$$

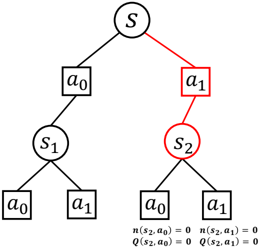
$$r = r(s, a_0, s_1) + \gamma V(s_1)$$

$$Q(s, a_0) = \frac{n(s, a_0) - 1}{n(s, a_0)} Q(s, a_0) + \frac{r}{n(s, a_0)}$$

- Expand s_1, initialize, restart search from s.

There are different versions of MCTS up to different tasks, and we only illustrate one for multi-step policy improvement.

Illustration of MCTS



- Now a_1 should be selected since it has large UCB, and transition to s_2 (leaf). Use $V(s_2)$ to update note a_1:

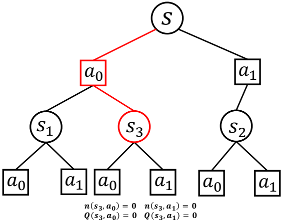
$$n(s, a_1) = n(s, a_1) + 1,$$

$$r = r(s, a_1, s_2) + \gamma V(s_2)$$

$$Q(s, a_1) = \frac{n(s, a_1) - 1}{n(s, a_1)} Q(s, a_1) + \frac{r}{n(s, a_1)}$$

- Expand s_2, initialize, restart search from s.

Illustration of MCTS



- Assume a_0 is again selected and transition to s_3 (leaf). Use $V(s_3)$ to update note a_0:

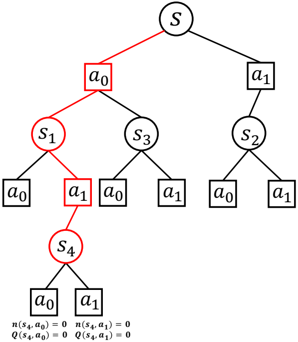
$$n(s, a_0) = n(s, a_0) + 1,$$

$$r = r(s, a_0, s_3) + \gamma V(s_3)$$

$$Q(s, a_0) = \frac{n(s, a_0) - 1}{n(s, a_0)} Q(s, a_0) + \frac{r}{n(s, a_0)}$$

- Expand s_3, initialize, restart search from s.

Illustration of MCTS



- Assume a_0 is again selected and transition to s_1 (**not** leaf). Assume from s_1, a_1 is selected, transition to s_4 (leaf). Use $V(s_4)$ to update actions a_1 and a_0 on the path.
- Update a_1:

$$n(s_1, a_1) = n(s_1, a_1) + 1,$$
$$r = r(s_1, a_1, s_4) + \gamma V(s_4)$$
$$Q(s_1, a_1) = \frac{n(s_1, a_1) - 1}{n(s_1, a_1)} Q(s_1, a_1) + \frac{r}{n(s_1, a_1)}$$

- Update a_0:

$$n(s, a_0) = n(s, a_0) + 1,$$
$$r = r(s, a_0, s_1) + \gamma r(s_1, a_1, s_4) + \gamma^2 V(s_4)$$
$$Q(s, a_0) = \frac{n(s, a_0) - 1}{n(s, a_0)} Q(s, a_0) + \frac{r}{n(s, a_0)}$$

- Expand s_4, initialize, restart search from s.

Remark

- MCTS repeats this process until some termination conditions are met. Note that we have mentioned "select", "expand", "propagate" in this process. There is another operation "simulate" in MCTS when state values are not given.
- Using UCB to select the action, optimal actions tend to be selected more and more asymptotically from bottom to top. Thus, MCTS is a trajectory-search way for finding the optimal action at current state by smart sampling.

Questions?