Multi-armed Bandits

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CS 6789: Foundations of Reinforcement Learning
The need for Exploration in RL:

The Combination Lock Example (i.e., the sparse reward problem)

(1) We have reward zero everywhere except at the goal (the right end);
(2) Every black node, one of the two actions will lead the agent to the dead state (red)
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What is the probability of a random policy generating a trajectory that hits the goal?
Exploration!

We need to perform systematic exploration, i.e., remember where we visited, and purposely try to visit unexplored regions.
What we will do today:

Study Exploration in a very simple MDP:

\[ \mathcal{M} = \{ s_0, \{ a_1, \ldots, a_K \}, H = 1, R \} \]

i.e., MDP with one state, one-step transition, and K actions

This is also called Multi-armed Bandits
Plan for today:

1. Introduction of MAB

2. Attempt 1: Greedy Algorithm (a bad algorithm)

3. Attempt 2: Explore and Commit

4. Attempt 3: Upper Confidence Bound (UCB) Algorithm
Intro to MAB

Setting:

We have $K$ many arms: $a_1, \ldots, a_K$
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**Example:** \( a_i \) has a Bernoulli distribution \( \nu_i \) w/ mean \( \mu_i := p \):
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Example: \( a_i \) has a Bernoulli distribution \( \nu_i \) w/ mean \( \mu_i := p \):

Every time we pull arm \( a_i \), we observe an i.i.d reward \( r = \begin{cases} 1 & \text{w/ prob } p \\ 0 & \text{w/ prob } 1 - p \end{cases} \)
Intro to MAB

Applications on online advertisement:

Arms correspond to Ads

Each arm has **click-through-rate** (CTR): probability of getting clicked (unknown)
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A learning system aims to maximize CTR in a long run:

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2. **Observe** if it is clicked (see a zero-one reward)

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1. **Try** an Ad (pull an arm)
2. **Observe** if it is clicked (see a zero-one reward)
3. **Update**: Decide what ad to recommend for next round
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(# based on historical information)
Intro to MAB

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*Note:* each iteration, we do not observe rewards of arms that we did not try
Intro to MAB

More formally, we have the following learning objective:

\[
\text{Regret}_T = T\mu^* - \sum_{t=0}^{T-1} \mu_{I_t}
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\mu^* = \max_{i \in [K]} \mu_i
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Total expected reward if we pulled best arm over T rounds
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- Total expected reward if we pulled best arm over T rounds
- Total expected reward of the arms we pulled over T rounds

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Goal: no-regret, i.e., \( \text{Regret}_T / T \to 0 \), as \( T \to \infty \)
Intro to MAB

Why the problem is hard?

Exploration and Exploitation Tradeoff:
Intro to MAB

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Exploration and Exploitation Tradeoff:

Every round, we need to ask ourselves:

Should we pull arms that are less frequently tried in the past (i.e., explore),
Or should we commit to the current best arm (i.e., exploit)?
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Attempt 1: Greedy Algorithm

Alg: try each arm once, and then commit to the one that has the highest observed reward
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Q: what could be wrong?
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Q: what could be wrong?

A bad arm (i.e., low $\mu_i$) may generate a high reward by chance!
(recall we have $r \sim \nu$, i.i.d)
Attempt 1: Greedy Algorithm

More concretely, let’s say we have two arms $a_1, a_2$:

Reward dist for $a_1$: w/ prob 60%, $r = 1$; else $r = 0$

Reward dist for $a_2$: w/ prob 40%, $r = 1$; else $r = 0$
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But try $a_1, a_2$ once, with probability 16%, we will observe reward pair $(0,1)$

The greedy alg will pick $a_2$—loosing expected reward 0.2 every time in the future
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What lessons we learned from the Greedy Alg:

Due to randomness in the reward distribution, trying each arm once is not enough, i.e., observed single reward may be far away from the mean.
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Due to randomness in the reward distribution, trying each arm once is not enough, i.e., observed single reward may be far away from the mean.

Q: what’s the fix here?

Yes, let’s (1) try each arm multiple times, (2) compute the empirical mean of each arm, (3) commit to the one that has the highest empirical mean.
Alg: Explore and Commit:

Algorithm hyper parameter $N < T/K$ (we assume $T >> K$)

For $k = 1 \rightarrow K$: (# Exploration phase)
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Pull arm-$k$ $N$ times, observe $\{r_i\}_{i=1}^N \sim \nu_k$
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Calculate arm $k$’s empirical mean: $\hat{\mu}_k = \sum_{i=1}^N r_i/N$

(*# Exploration phase*)
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For $t = NK \rightarrow T - 1$: (# Exploitation phase)
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Pull arm-\( k \) \( N \) times, observe \( \{r_i\}_{i=1}^{N} \sim \nu_k \)

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Q: how to set \( N \)?
Statistical Tools:

1. Hoeffding inequality (optional, no need to remember or understand it)
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Given a distribution $\mu \in \Delta([0,1])$, and $N$ i.i.d samples $\{r_i\}_{i=1}^N \sim \mu$, with probability at least $1 - \delta$, we have:

$$\left| \sum_{i=1}^{N} \frac{r_i}{N} - \mu \right| \leq O\left( \sqrt{\frac{\ln(1/\delta)}{N}} \right)$$
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i.e., this gives us a confidence interval:
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i.e., this gives us a confidence interval:

$$\hat{\mu} - \sqrt{\ln(1/\delta)/N} \leq \mu \leq \hat{\mu} + \sqrt{\ln(1/\delta)/N}$$
Statistical Tools:
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Combine Hoeffding and Union Bound, we have:
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After the Exploration phase, with probability at least $1-\delta$, for all arm $k \in [K]$, we have:

$$\left| \hat{\mu}_k - \mu_k \right| \leq O \left( \sqrt{\frac{\ln(K/\delta)}{N}} \right)$$
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After the Exploration phase, with probability at least 1-\(\delta\), for all arm \(k \in [K]\), we have:

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Calculate the final regret:

Denote empirical best arm $\hat{I} = \arg \max_{i \in [K]} \hat{\mu}_i$, and THE best arm $I^* = \arg \max_{i \in [K]} \mu_i$. 
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Let’s now bound $\text{Regret}_{\text{exploit}}$
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$$\text{Regret}_{\text{exploit}} \leq (T - NK)(\mu_{I^*} - \mu_{\hat{I}})$$

$$\mu_{I^*} - \mu_{\hat{I}} \leq \left[ \hat{\mu}_{I^*} + \sqrt{\ln(K/\delta)/N} \right] - \left[ \hat{\mu}_{\hat{I}} - \sqrt{\ln(K/\delta)/N} \right]$$

$$\geq \mu_{I^*} \leq \mu_{I^*}$$
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$$= \hat{\mu}_{I^*} - \hat{\mu}_{\hat{I}} + 2\sqrt{\ln(K/\delta)/N}$$

Q: why?

$$\leq 2\sqrt{\ln(K/\delta)/N}$$

$$\text{Regret}_{\text{exploit}} \leq (T - NK) \left( \mu_{I^*} - \mu_{\hat{I}} \right) \leq 2T \sqrt{\frac{\ln(K/\delta)}{N}}$$
Finally, combine two regret together:

\[
\text{Regret}_{\text{explore}} \leq N(K - 1) \leq NK
\]

\[
\text{Regret}_{\text{exploit}} \leq (T - NK)(\mu_{1^*} - \mu_i) \leq T \sqrt{\frac{\ln(K/\delta)}{N}}
\]

\[
\text{Regret}_T = \text{Regret}_{\text{explore}} + \text{Regret}_{\text{exploit}} \leq NK + 2T \sqrt{\frac{\ln(K/\delta)}{N}}
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Minimize the upper bound via optimizing N:
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Minimize the upper bound via optimizing N:

Set \( N \) = \( \left( \frac{T\sqrt{\ln(K/\delta)}}{2K} \right)^{2/3} \), we have:

\[
\text{Regret}_T \leq \mathcal{O}(T^{2/3} K^{1/3} \ln^{1/3}(K/\delta))
\]
To conclude on Explore then Commit:

[Theorem] Fix $\delta \in (0,1)$, set $N = \left( \frac{T \sqrt{\ln(K/\delta)}}{2K} \right)^{2/3}$, with probability at least $1 - \delta$, Explore and Commit has the following regret:

$$\text{Regret}_T \leq O \left( T^{2/3} K^{1/3} \cdot \ln^{1/3}(K/\delta) \right)$$

Q: can we do better, particularly, can we get $\sqrt{T}$ regret bound?
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We maintain the following statistics during the learning process:

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\[ N_t(i) = \sum_{\tau=0}^{i-1} 1\{I_{\tau} = i\} \]

i.e., $N_t(i)$ = \# of Times we tried $i$.
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i.e., $N_t(i)$

and its empirical mean $\hat{\mu}_t(i)$ so far;
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and its empirical mean $\hat{\mu}_t(i)$ so far;

\[
i.e., \ \hat{\mu}_t(i) = \sum_{\tau=0}^{t-1} 1\{I_\tau = i\} r_\tau / N_t(i)
\]
Recall the Tool for Building Confidence Interval:
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Thus, we can show that for all iteration $t$, we have the for all $k \in [K]$, w/ prob $1 - \delta$, 

$$|\hat{\mu}_k(i) - \mu_k| \leq \sqrt{\frac{\ln(KT/\delta)}{N_t(k)}}$$
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Proving this result actually requires reasoning Martinalges, as samples are not i.i.d, i.e., whether or not you pull arm $k$ in this round depends on previous random outcomes (See Ch 6 for more details)
UCB: Optimism in the face of Uncertainty

Given the confidence interval, we pick arm that has the highest Upper-Conf-Bound:
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Given the confidence interval, we pick arm that has the highest Upper-Conf-Bound:

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\hat{\mu}_t(1) + \sqrt{\frac{\ln(KT/\delta)}{N_t(1)}}
\]

\[
\hat{\mu}_t(1) - \sqrt{\frac{\ln(KT/\delta)}{N_t(1)}}
\]

\[
\hat{\mu}_t(2) + \sqrt{\frac{\ln(KT/\delta)}{N_t(2)}}
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\[
\hat{\mu}_t(2) - \sqrt{\frac{\ln(KT/\delta)}{N_t(2)}}
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\hat{\mu}_t(3) + \sqrt{\frac{\ln(KT/\delta)}{N_t(3)}}
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Given the confidence interval, we pick arm that has the highest Upper-Conf-Bound:

\[
\hat{\mu}_t(2) + \sqrt{\frac{\ln(KT/\delta)}{N_t(2)}}
\]

Set \( I_t = 2 \)

\[
\hat{\mu}_t(1) + \sqrt{\frac{\ln(KT/\delta)}{N_t(1)}}
\]

\[
\hat{\mu}_t(1) - \sqrt{\frac{\ln(KT/\delta)}{N_t(1)}}
\]

\[
\hat{\mu}_t(2) - \sqrt{\frac{\ln(KT/\delta)}{N_t(2)}}
\]

\[
\hat{\mu}_t(3) + \sqrt{\frac{\ln(KT/\delta)}{N_t(3)}}
\]

\[
\hat{\mu}_t(3) - \sqrt{\frac{\ln(KT/\delta)}{N_t(3)}}
\]
Put things together: UCB Algorithm:

For $t = 0 \rightarrow T - 1$:

$$I_t = \arg \max_{i \in [K]} \left( \hat{\mu}_t(i) + \sqrt{\frac{\ln(KT/\delta)}{N_t(i)}} \right)$$

Receive $r \sim \mathcal{N}_{1_t}$

$$N_{t+1}(I_t) = N_t(I_t) + 1$$
Put things together: UCB Algorithm:

For $t = 0 \rightarrow T - 1$:

$$I_t = \arg \max_{i \in [K]} \left( \hat{\mu}_t(i) + \sqrt{\frac{\ln(KT/\delta)}{N_t(i)}} \right)$$

(# Upper-conf-bound of arm $i$)
Put things together: UCB Algorithm:

For $t = 0 \rightarrow T - 1$:

$$I_t = \arg \max_{i \in [K]} \left( \hat{\mu}_t(i) + \sqrt{\frac{\ln(KT/\delta)}{N_t(i)}} \right)$$

(# Upper-conf-bound of arm $i$)

“Reward Bonus”: $\sqrt{\frac{\ln(KT/\delta)}{N_t(i)}}$
UCB Regret:

[Theorem (informal)] With high probability, UCB has the following regret:

$$\text{Regret}_T = \tilde{O}\left(\sqrt{KT}\right)$$
Intuitive Explanation of UCB
Intuitive Explanation of UCB

\[
\hat{\mu}_t(1) + \sqrt{\ln(KT/\delta)/N_t(1)}
\]

\[
\hat{\mu}_t(1) - \sqrt{\ln(KT/\delta)/N_t(1)}
\]

\[
\hat{\mu}_t(2) + \sqrt{\ln(KT/\delta)/N_t(2)}
\]

\[
\hat{\mu}_t(2) - \sqrt{\ln(KT/\delta)/N_t(2)}
\]

\[
\hat{\mu}_t(3) + \sqrt{\ln(KT/\delta)/N_t(3)}
\]

\[
\hat{\mu}_t(3) - \sqrt{\ln(KT/\delta)/N_t(3)}
\]
Intuitive Explanation of UCB

Case 1: it has large conf-interval, which means that it has not been tried many times yet (high uncertainty)

\[ \hat{\mu}_t(1) + \sqrt{\ln(KT/\delta)/N_t(1)} \]

\[ \hat{\mu}_t(1) - \sqrt{\ln(KT/\delta)/N_t(1)} \]

\[ \hat{\mu}_t(2) + \sqrt{\ln(KT/\delta)/N_t(2)} \]

\[ \hat{\mu}_t(2) - \sqrt{\ln(KT/\delta)/N_t(2)} \]

\[ \hat{\mu}_t(3) + \sqrt{\ln(KT/\delta)/N_t(3)} \]

\[ \hat{\mu}_t(3) - \sqrt{\ln(KT/\delta)/N_t(3)} \]
Intuitive Explanation of UCB
Intuitive Explanation of UCB

\[ \hat{\mu}_t(1) + \frac{\sqrt{\ln(K\Delta)/N_t(1)}}{\sqrt{\Delta}} \]

\[ \hat{\mu}_t(1) - \frac{\sqrt{\ln(K\Delta)/N_t(1)}}{\sqrt{\Delta}} \]

\[ \hat{\mu}_t(2) + \frac{\ln(K\Delta)/N_t(2)}{\sqrt{\Delta}} \]

\[ \hat{\mu}_t(2) - \frac{\ln(K\Delta)/N_t(2)}{\sqrt{\Delta}} \]

\[ \hat{\mu}_t(3) + \frac{\ln(K\Delta)/N_t(3)}{\sqrt{\Delta}} \]

\[ \hat{\mu}_t(3) - \frac{\ln(K\Delta)/N_t(3)}{\sqrt{\Delta}} \]
Intuitive Explanation of UCB

Case 2: it has low uncertainty, then it is simply a good arm, i.e., it’s true mean is high!
Explore and Exploration Tradeoff

**Case 1:** $I_t$ has large conf-interval, which means that it has not been tried many times yet (high uncertainty)

Thus, we do exploration in this case!
Explore and Exploration Tradeoff

**Case 1:** $I_t$ has large conf-interval, which means that it has not been tried many times yet (high uncertainty)

Thus, we do exploration in this case!

**Case 2:** $I_t$ has small conf-interval, then it is simply a good arm, i.e., it’s true mean is pretty high!

Thus, we do exploitation in this case!
Let’s formalize the intuition

Denote the optimal arm $I^* = \arg \max_{i \in [K]} \mu_i$; recall $I_t = \arg \max_{i \in [K]} \hat{\mu}_t(i) + \sqrt{\frac{\ln(KT/\delta)}{N_t(i)}}$.
Let’s formalize the intuition

Denote the optimal arm $I^* = \arg \max_{i \in [K]} \mu_i$; recall $I_t = \arg \max_{i \in [K]} \hat{\mu}_t(i) + \sqrt{\frac{\ln(KT/\delta)}{N_t(i)}}$

Regret-at-$t = \mu^* - \mu_{I_t}$
Let’s formalize the intuition

Denote the optimal arm $I^* = \arg \max \mu_i$; recall $I_t = \arg \max \hat{\mu}_t(i) + \sqrt{\frac{\ln(KT/\delta)}{N_t(i)}}$

Regret-at-$t = \mu^* - \mu_{I_t}$

$\leq \hat{\mu}_t(I_t) + \sqrt{\frac{\ln(TK/\delta)}{N_t(I_t)}} - \mu_{I_t}$

$\cup \mathcal{B}(I_t) \geq \cup \mathcal{B}(I^*)$

$\geq \mu(I^*)$
Let’s formalize the intuition

Denote the optimal arm $I^* = \arg \max_{i \in [K]} \mu_i$; recall $I_t = \arg \max_{i \in [K]} \hat{\mu}_t(i) + \sqrt{\frac{\ln(KT/\delta)}{N_t(i)}}$

Regret-at-$t = \mu^* - \mu_{I_t}$

Q: why?

$\leq \hat{\mu}_t(I_t) + \sqrt{\frac{\ln(TK/\delta)}{N_t(I_t)}} - \mu_{I_t}$
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Denote the optimal arm \( I^* = \arg\max_{i \in [K]} \mu_i \); recall \( I_t = \arg\max_{i \in [K]} \hat{\mu}_t(i) + \sqrt{\frac{\ln(KT/\delta)}{N_t(i)}} \)

Regret-at-t = \( \mu^* - \mu_{I_t} \)

Q: why?

\[
\leq \hat{\mu}_t(I_t) + \sqrt{\frac{\ln(TK/\delta)}{N_t(I_t)}} - \mu_{I_t}
\]

\[
\leq 2\sqrt{\frac{\ln(TK/\delta)}{N_t(I_t)}}
\]
Let’s formalize the intuition

Denote the optimal arm $I^* = \arg \max \mu_i$; recall $I_t = \arg \max \hat{\mu}_t(i) + \sqrt{\frac{\ln(KT/\delta)}{N_t(i)}}$

Regret-at-$t = \mu^* - \mu_{I_t}$

Q: why?

\[
\leq \hat{\mu}_t(I_t) + \sqrt{\frac{\ln(TK/\delta)}{N_t(I_t)}} - \mu_{I_t} \\
\leq 2\sqrt{\frac{\ln(TK/\delta)}{N_t(I_t)}}
\]

Case 1: $N_t(I_t)$ is small (i.e., uncertainty about $I_t$ is large);

We pay regret, BUT we **explore** here, as we just tried $I_t$ at iter $t$!
Let’s formalize the intuition

Denote the optimal arm \( I^* = \arg\max_{i \in [K]} \mu_i \); recall \( I_t = \arg\max_{i \in [K]} \hat{\mu}_t(i) + \sqrt{\frac{\ln(KT/\delta)}{N_t(i)}} \)

\[
\text{Regret-at-}t = \mu^* - \mu_{I_t} \\
\leq \hat{\mu}_t(I_t) + \sqrt{\frac{\ln(TK/\delta)}{N_t(I_t)}} - \mu_{I_t} \\
\leq 2 \sqrt{\frac{\ln(TK/\delta)}{N_t(I_t)}}
\]

**Case 2:** \( N_t(I_t) \) is large, i.e., conf-interval of \( I_t \) is small,

Then we **exploit** here, as \( I_t \) is pretty good (the gap between \( \mu^* \) & \( \mu_{I_t} \) is small)!
Let’s formalize the intuition

Finally, let’s add all per-iter regret together:

\[
\text{Regret}_T = \sum_{t=0}^{T-1} \left( \mu^* - \mu_{I_t} \right)
\]

\[
\leq \sum_{t=0}^{T-1} 2\sqrt{\frac{\ln(TK/\delta)}{N_t(I_t)}}
\]

\[
\leq 2\sqrt{\ln(TK/\delta)} \cdot \sum_{t=0}^{T-1} \sqrt{\frac{1}{N_t(I_t)}}
\]
Let’s formalize the intuition

Finally, let’s add all per-iter regret together:

\[
\text{Regret}_T = \sum_{t=0}^{T-1} (\mu^* - \mu_{I_t})
\]

\[
\leq \sum_{t=0}^{T-1} 2 \sqrt{\frac{\ln(TK/\delta)}{N_t(I_t)}}
\]

\[
\leq 2\sqrt{\ln(TK/\delta)} \cdot \sum_{t=0}^{T-1} \sqrt{\frac{1}{N_t(I_t)}}
\]

Lemma:

\[
\sum_{t=0}^{T-1} \sqrt{\frac{1}{N_t(I_t)}} \leq O\left(\sqrt{KT}\right)
\]

\[
= \sum_{k=1}^{K} \sum_{t=0}^{t_k-1} \frac{1}{N_t(I_t)} \leq \sqrt{K} \cdot \sum_{k=1}^{K} \sqrt{N_t(k)} \leq \sqrt{K} \cdot \sum_{k=1}^{K} \sqrt{N_t(k)}
\]
Summary

1. Setting of Multi-armed Bandit: MDP with one state, and K actions, $H = 1$

2. Need to carefully balance exploration and exploitation

3. The Principle of Optimism in the face of Uncertainty