

Multi-armed Bandits

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CS 2824: Foundations of Reinforcement Learning

Announcements

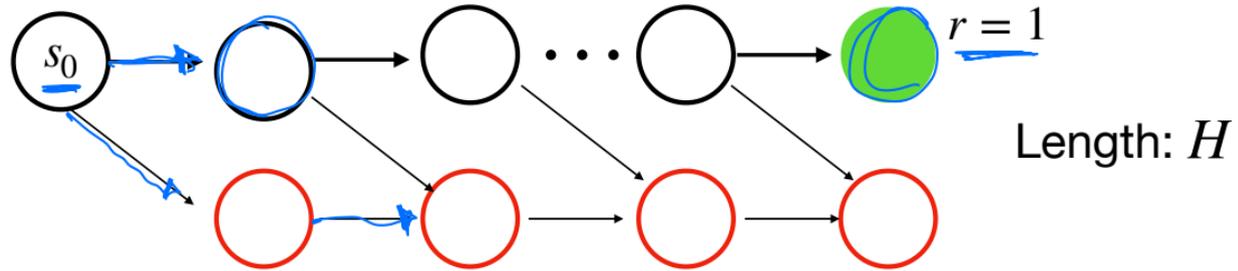
Course Projects

- Check the course website for the project deadline dates
- Three important dates:
 - Proposal due after spring break
 - Midterm report due before project presentations
 - Final report due after reading period
- Groups
 - Group sizes are at ~~max 3~~ min 3
 - Group presentations will be in the last three lectures; we know this overlaps with ICLR, and we'll poll for presentation slots before ICLR.

The need for Exploration in RL:

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

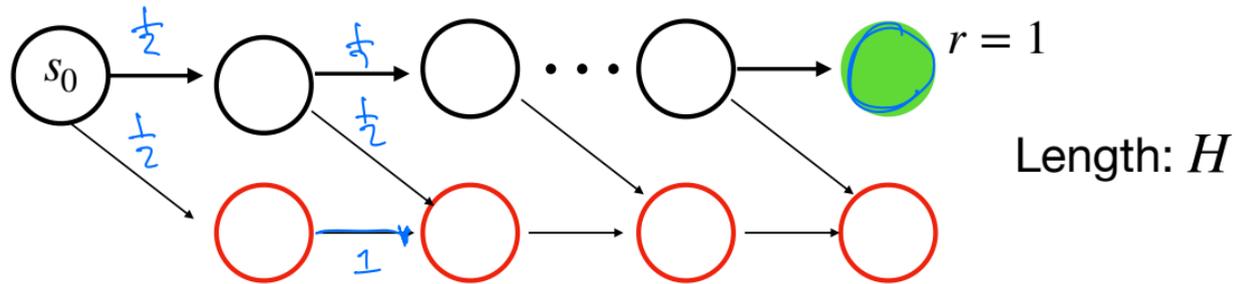
- (1) We have reward zero everywhere except at the goal (the right end);
- (2) Every black node, one of the two actions will lead the agent to the dead state (red)



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)



What is the probability of a random policy generating a trajectory that hits the goal?

$$\left(\frac{1}{2}\right)^H = 2^{-H}$$

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:

$$\mathcal{M} = \{s_0, \{a_1, \dots, a_K\}, H = 1, R\}$$

Δ a₁ ... a_K

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

This is also called Multi-armed Bandits

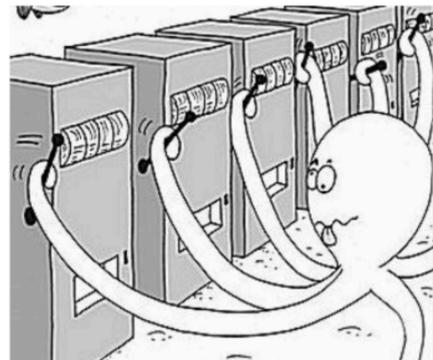
Plan for today:

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 , ..., a_K



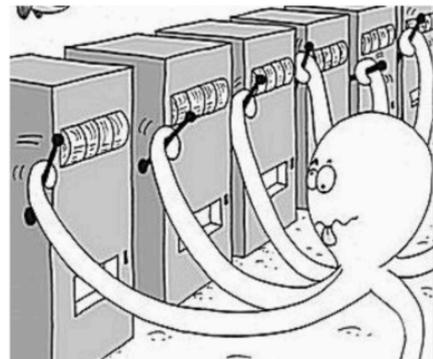
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w/ mean $\mu_i = \mathbb{E}_{r \sim \nu_i}[r]$



Intro to MAB

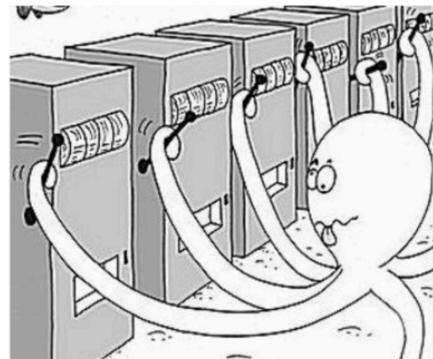
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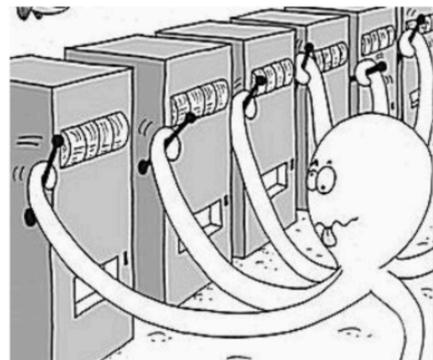
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Example: a_i has a Bernoulli distribution ν_i w/ mean $\mu_i := p$:

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**
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maximize CTR in a long run:

Intro to MAB

Applications on online advertisement:



Arms correspond to Ads

Each arm has **click-through-rate** (CTR): probability of getting clicked (unknown)

A learning system aims to maximize CTR in a long run:

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

Intro to MAB

More formally, we have the following interactive learning process:

For $t = 0 \rightarrow T - 1$

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Note: each iteration, we do not observe rewards of arms that we did not try

Intro to MAB

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$$\text{Regret}_T = T\mu^* - \sum_{t=0}^{T-1} \mu_{I_t}$$

$$\mu^* = \max_{i \in [K]} \mu_i$$

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Best arm we see *non best arm we see* *best arm we see*

$$\mu^* = \max_{i \in [K]} \mu_i$$

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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Total expected reward if we pulled best arm over T rounds

Total expected reward of the arms we pulled over T rounds

Goal: no-regret, i.e., $\text{Regret}_T/T \rightarrow 0$, as $T \rightarrow \infty$

Intro to MAB

Why the problem is hard?

Exploration and Exploitation Tradeoff:

Intro to MAB

Why the problem is hard?

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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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?

A bad arm (i.e., low μ_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 $r = 0$ $\mu_1 = .6$

Reward dist for a_2 : w/ prob 40%, $r = 1$; else $r = 0$ $\mu_2 = .4$

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Clearly a_1 is a better arm!

$$.4 \times .4 = 16\%$$

But try a_1, a_2 once, with probability 16%, we will observe reward pair (0,1)

$$\begin{aligned} & (\mu^* - \mu_2) (T-2) \\ & (6 - .4) (T-2) \\ R_T &= .2(T-2) \end{aligned}$$

$$\frac{R_T}{T} = \frac{.2(T-2)}{T}$$

$T \rightarrow \infty$

$$R_T \rightarrow .2$$

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The greedy alg will pick a_2 —**loosing expected reward 0.2 every time in the future**

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1. Introduction of MAB



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

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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,
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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

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

Q: How many times is enough?

Alg: Explore and Commit:

times that we visit each arm K

Algorithm hyper parameter $\underline{N} < T/K$ (we assume $\underline{T} \gg K$)

For $k = 1 \rightarrow K$: (# Exploration phase)

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Calculate arm k 's empirical mean: $\hat{\mu}_k = \sum_{i=1}^N r_i / N$

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$$N = \frac{T}{K}$$
$$NK = \frac{T}{K} \cdot K = T$$

For $t = NK \rightarrow T - 1$: (# Exploitation phase)

Pull the best empirical arm, i.e., $I_t = \arg \max_{i \in [K]} \hat{\mu}_i$

Q: how to set N ?

Statistical Tools:

1. Hoeffding inequality (optional, no need to remember or understand it)

$$v \in [0, 1] \quad v_1, \dots, v_r \sim v.$$

$$|\hat{\mu} - \mu| \leq \sqrt{\frac{r}{n}}$$

Statistical Tools:

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Given a distribution $\nu \in \Delta([0,1])$, and N i.i.d samples

$\{r_i\}_{i=1}^N \sim \nu$, w/ probability at least $1 - \delta$, we have:

$$\left| \sum_{i=1}^N r_i / N - \mu \right| \leq O \left(\sqrt{\frac{\ln(1/\delta)}{N}} \right) \approx O\left(\frac{6.6}{N}\right)$$

empirical mean ground truth $\log_2(1.00) \approx 6.6$

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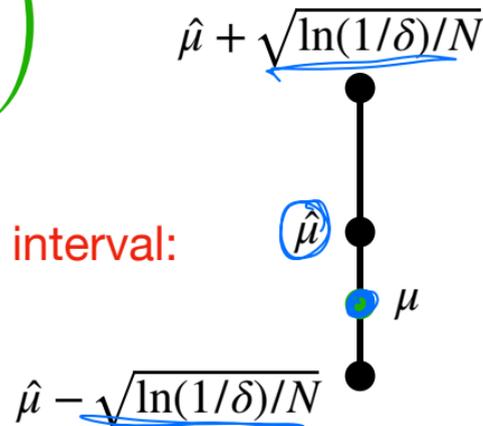
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$$P(A \text{ or } B) \leq P(A) + P(B)$$

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After the Exploration phase, with probability at least $1-\delta$,

for all arm $k \in [K]$, we have:

$$\underline{|\hat{\mu}_k - \mu_k|} \leq O\left(\sqrt{\frac{\ln(K/\delta)}{N}}\right)$$

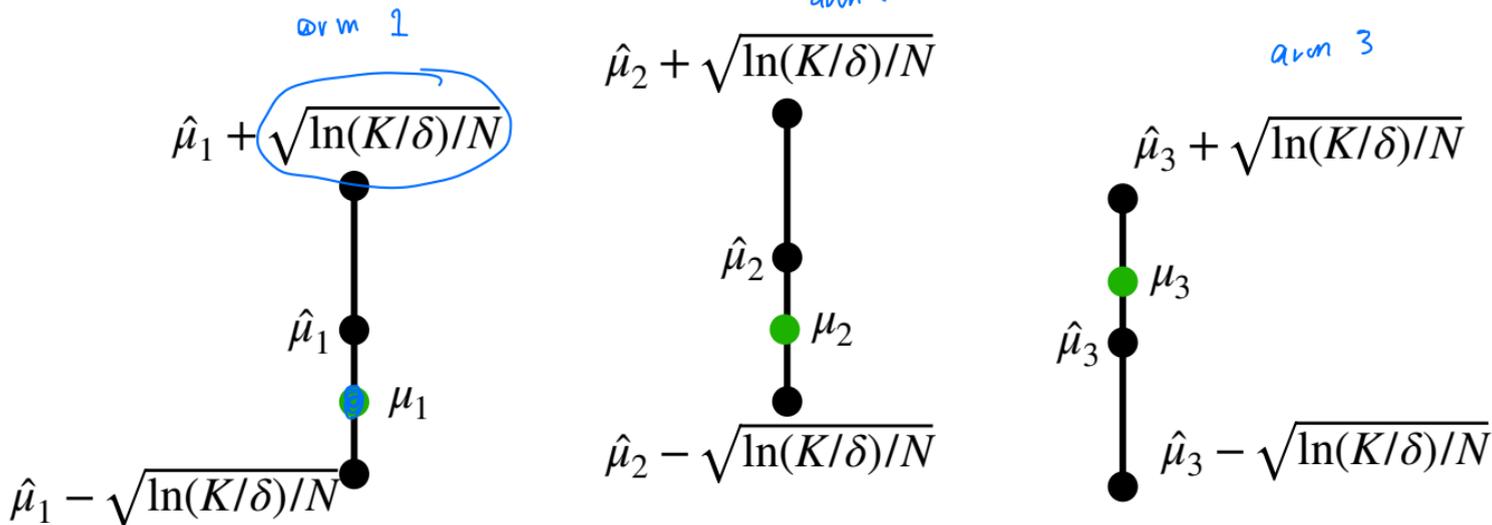
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Denote **empirical best arm** $\hat{I} = \arg \max_{i \in [K]} \hat{\mu}_i$ and **THE best arm** $I^* = \arg \max_{i \in [K]} \mu_i$

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$$\text{Regret}_{\text{explore}} \leq N(K - 1) \leq \underline{NK}$$

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Total regret

Regret explore +

Regret exploit

2. What's the regret in the exploitation phase:

$$\text{Regret}_{\text{exploit}} \leq (T - NK)(\mu_{I^*} - \mu_{\hat{I}})$$

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Let's now bound $\text{Regret}_{\text{exploit}}$

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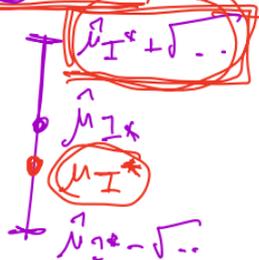
What's the regret in the exploitation phase:

$$\hat{\mu}_{I^*} \in \left[\hat{\mu}_{I^*} - \sqrt{\frac{\ln(K/\delta)}{n}}, \hat{\mu}_{I^*} + \sqrt{\frac{\ln(K/\delta)}{n}} \right]$$

$$\text{Regret}_{\text{exploit}} \leq (T - NK) (\mu_{I^*} - \mu_{\hat{I}})$$

$$\hat{\mu}_{\hat{I}} \in \left[\hat{\mu}_{\hat{I}} - \sqrt{\dots}, \hat{\mu}_{\hat{I}} + \sqrt{\dots} \right]$$

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



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upper bound *lower bound*

$$\begin{aligned} \mu_{I^*} - \mu_{\hat{I}} &\leq \left[\hat{\mu}_{I^*} + \sqrt{\ln(K/\delta)/N} \right] - \left[\hat{\mu}_{\hat{I}} - \sqrt{\ln(K/\delta)/N} \right] \\ &= \hat{\mu}_{I^*} - \hat{\mu}_{\hat{I}} + \underline{\underline{2\sqrt{\ln(K/\delta)/N}}} \end{aligned}$$

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Calculate the regret in the exploitation phase

Denote empirical best arm $\hat{I} = \arg \max_{i \in [K]} \hat{\mu}_i$, and THE best arm $I^* = \arg \max_{i \in [K]} \mu_i$

$$\hat{\mu}_{\hat{I}} \geq \hat{\mu}_{I^*} \Rightarrow 0 \geq \hat{\mu}_{\hat{I}} - \hat{\mu}_{I^*}$$

What's the regret in the exploitation phase:

$$\text{Regret}_{\text{exploit}} \leq (T - NK)(\mu_{I^*} - \mu_{\hat{I}})$$

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

$$= \underbrace{\hat{\mu}_{I^*} - \hat{\mu}_{\hat{I}}}_{\geq 0} + 2\sqrt{\ln(K/\delta)/N}$$

Q: why?

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

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

Q: why?

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

$$\text{Regret}_{\text{exploit}} \leq \underbrace{(T - NK)}_{+} (\mu_{I^*} - \mu_{\hat{I}}) \leq 2T \sqrt{\frac{\ln(K/\delta)}{N}}$$

Finally, combine two regret together:

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

$$\text{Regret}_{\text{exploit}} \leq (T - NK)(\mu_{I^*} - \mu_{\hat{I}}) \leq 2T \sqrt{\frac{\ln(K/\delta)}{N}}$$

$$\text{Regret}_T = \text{Regret}_{\text{explore}} + \text{Regret}_{\text{exploit}} \leq NK + 2T \sqrt{\frac{\ln(K/\delta)}{N}}$$

f(n) =

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Minimize the upper bound via optimizing N:

$$R_T = T^{2/3} \cdot K^{1/3}$$

$$\frac{R_T}{T} = \frac{T^{2/3} \cdot K^{1/3}}{T} = T^{-1/3} \cdot K^{1/3}$$

$R_T \rightarrow 0$

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

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

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:

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

Q: can we do better, particularly, can we get \sqrt{T} regret bound?

Plan for today:



1. Introduction of MAB



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



3. Attempt 2: Explore and Commit

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

Statistics that we maintain during learning:

We maintain the following statistics during the learning process:

At the beginning of iteration t , for all $i \in [K]$, # of times we have tried arm i ,

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$$\text{i.e., } \hat{\mu}_t(i) = \frac{\sum_{\tau=0}^{t-1} \mathbf{1}\{I_\tau = i\} r_\tau}{N_t(i)}$$

Recall the Tool for Building Confidence Interval:

We can show that for all iterations t , we have the for all $k \in [K]$, w/ prob $1 - \delta$,

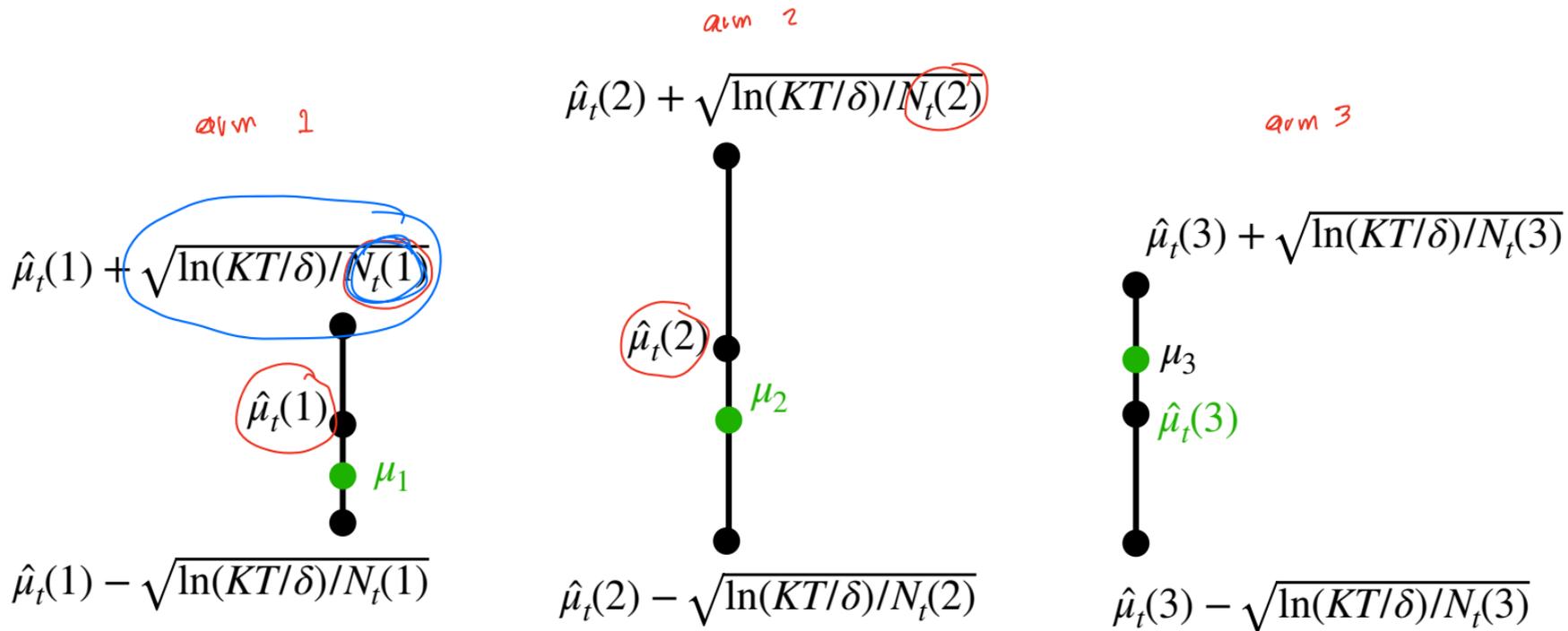
$$\underbrace{|\hat{\mu}_k(i) - \mu_k|}_{\substack{\text{computed} \\ \text{mean}}} \leq \sqrt{\frac{\ln(KT/\delta)}{\underbrace{N_t(k)}_N}} \quad \mathbb{N}$$

UCB: Optimism in the face of Uncertainty

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

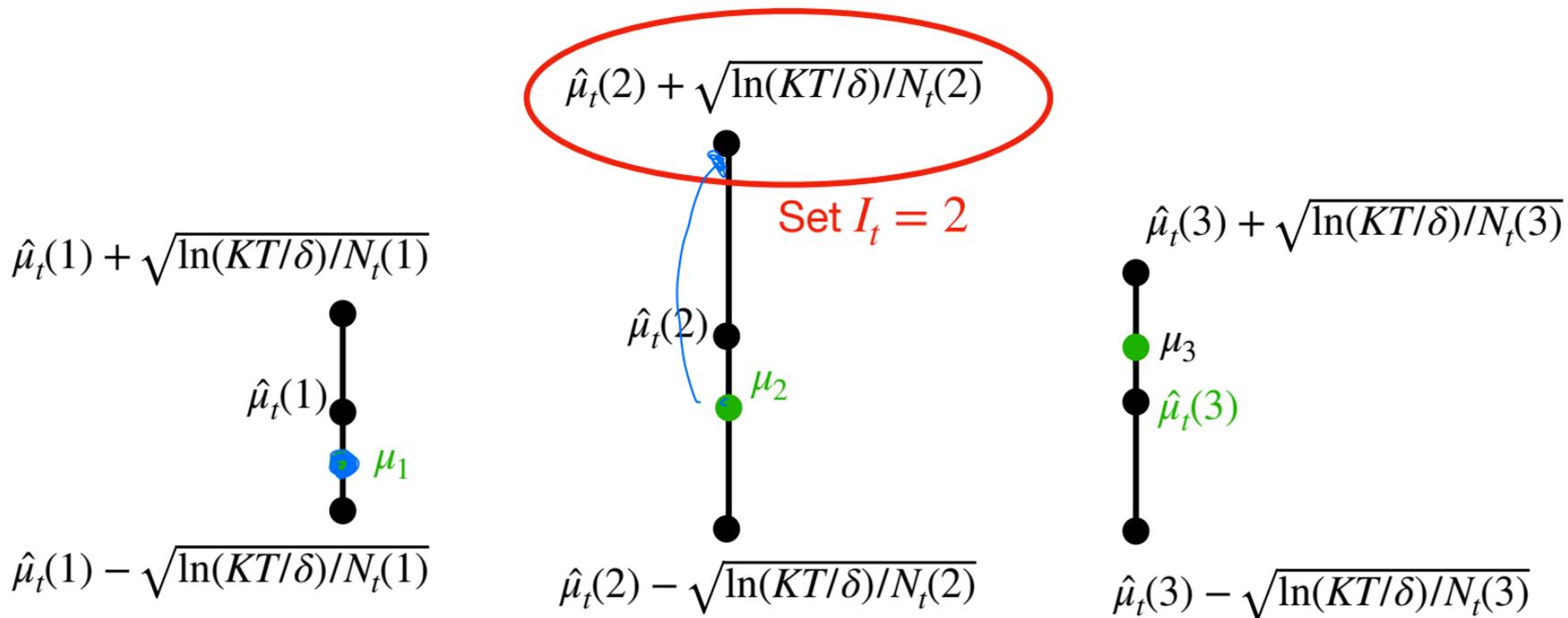
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Put things together: UCB Algorithm:

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

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

Handwritten annotations:

- A blue arrow labeled "CI" points to the square root term.
- A blue arrow labeled "empirical mean" points to $\hat{\mu}_t(i)$.
- A blue bracket is drawn above the entire expression inside the parentheses.

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(# Upper-conf-bound of arm i)

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

$N_t(i) \downarrow$ Bonus \uparrow

$N_t(i) \uparrow$ Bonus \downarrow

UCB Regret:

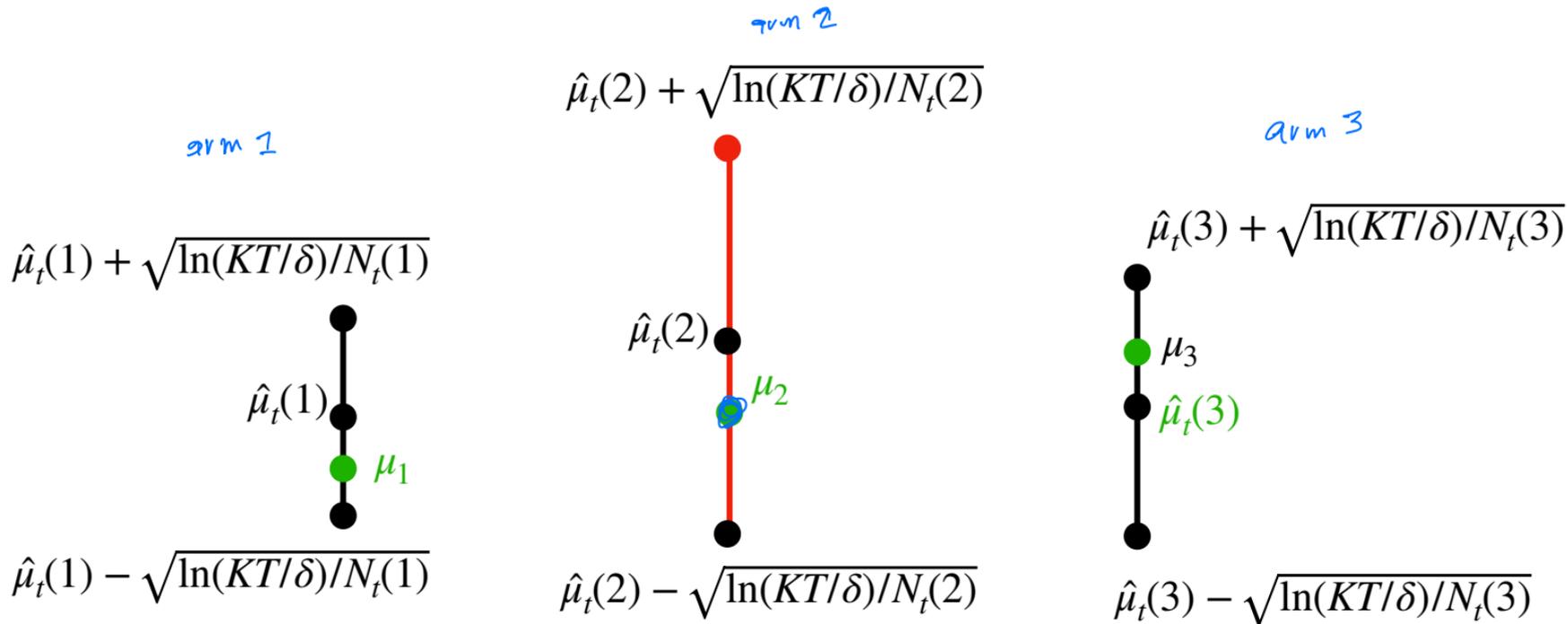
[Theorem (informal)] With high probability, UCB has the following regret:

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

Intuitive Explanation of UCB

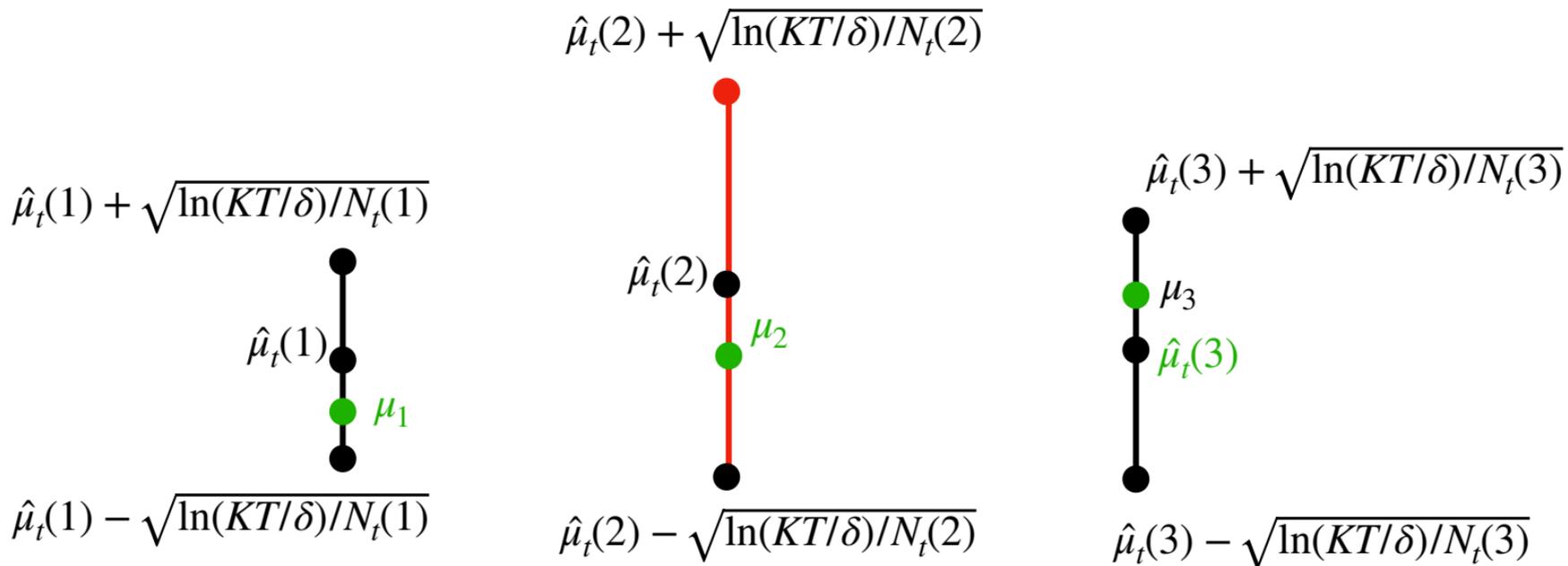
Intuitive Explanation of UCB

Q: why upper confidence is high for arm 2?



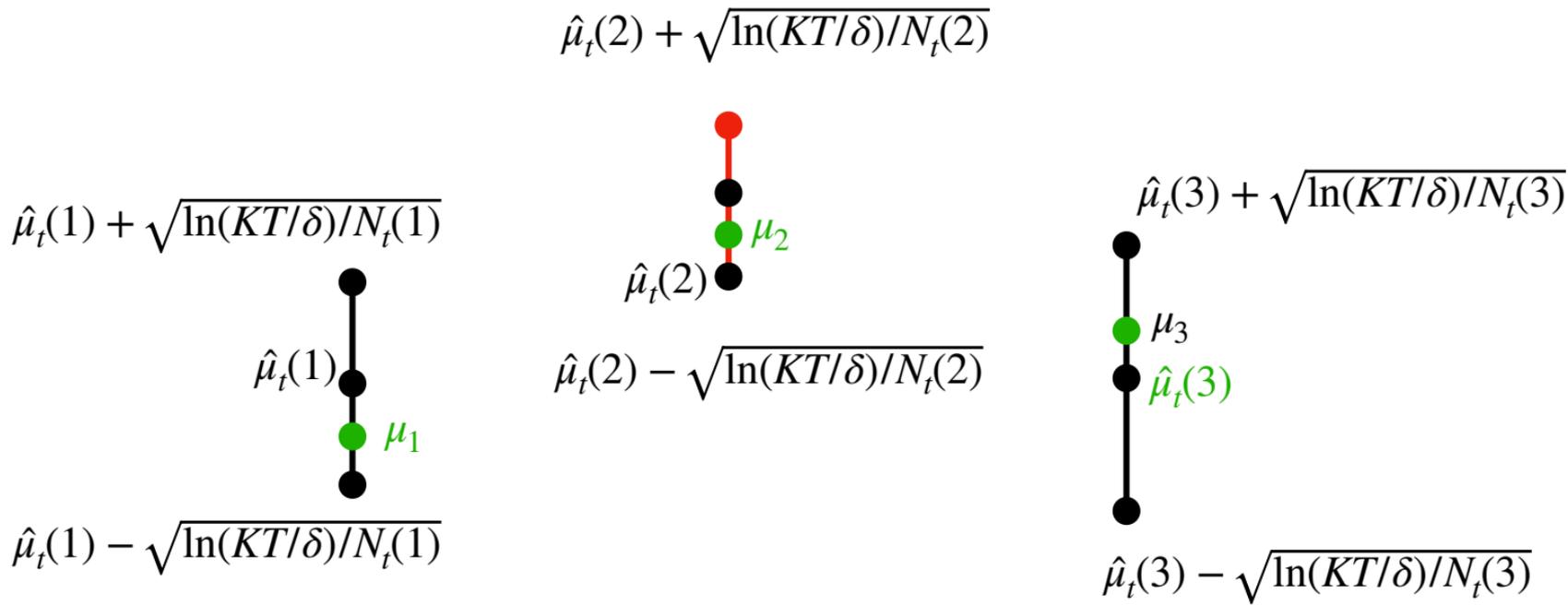
Intuitive Explanation of UCB

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



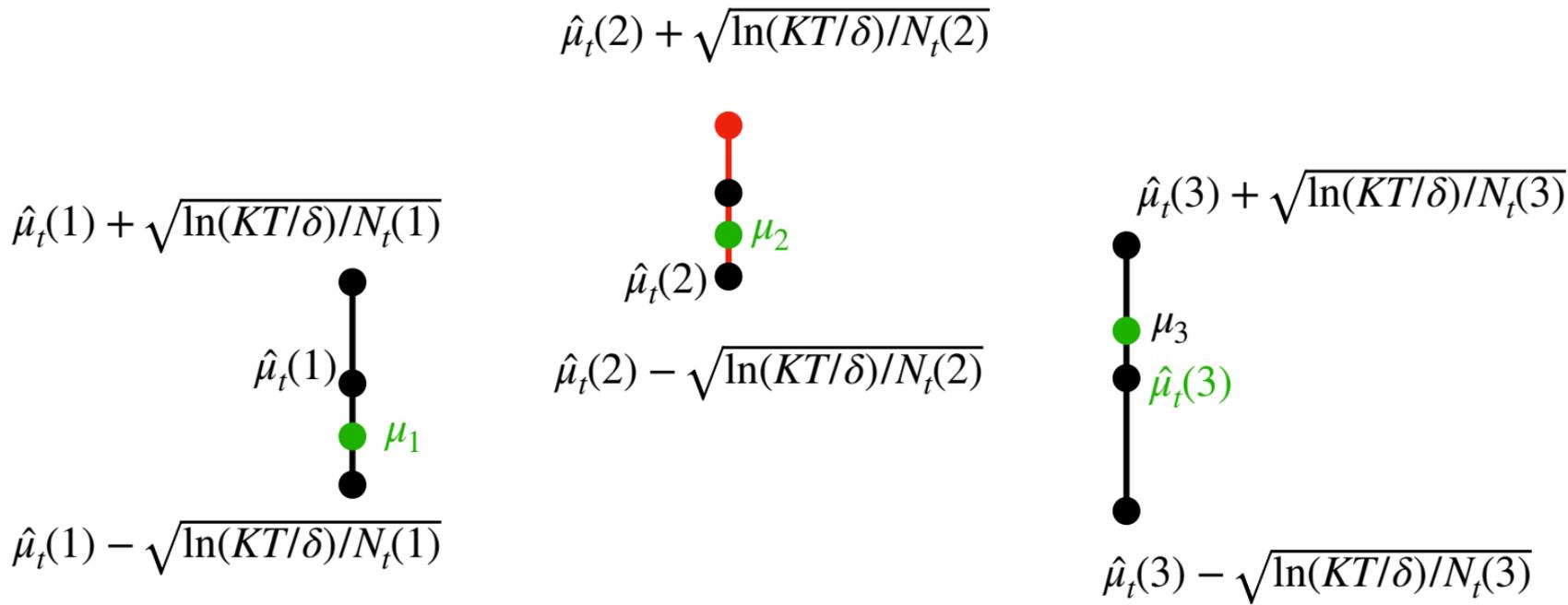
Intuitive Explanation of UCB

Q: why upper confidence is high for arm 2?



Intuitive Explanation of UCB

Case 2: it has low uncertainty, then it is simply a good arm, i.e., its 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 $I_t = \arg \max_{i \in [K]} \hat{\mu}_t(i) + \sqrt{\frac{\ln(KT/\delta)}{N_t(i)}}$

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