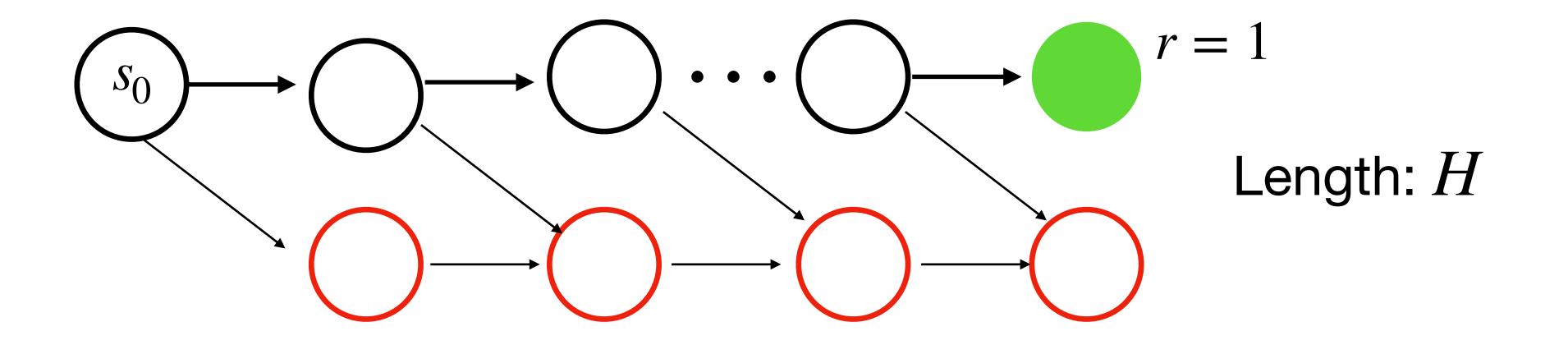
# **Multi-armed Bandits**

# Sham Kakade and Wen Sun 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)

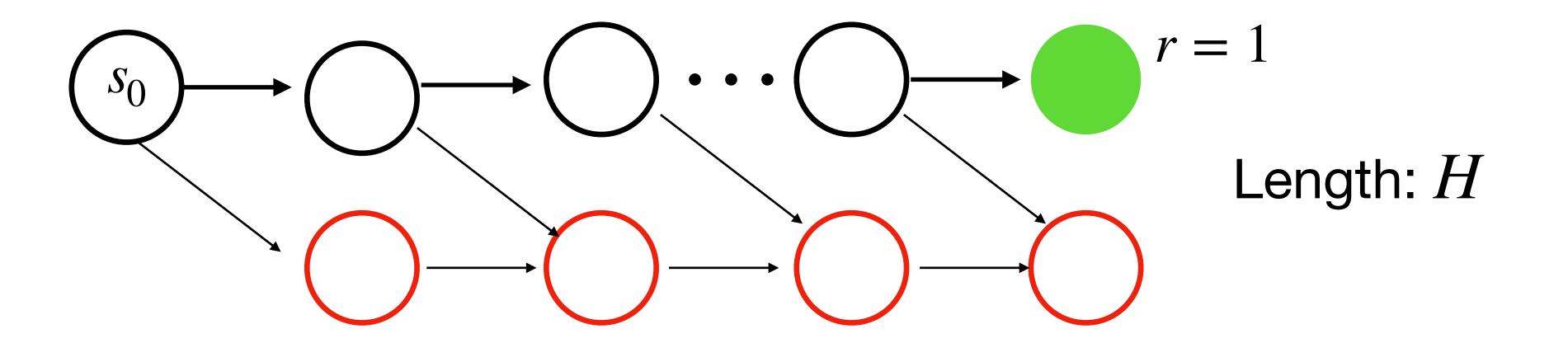




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What is the probability of a random policy generating a trajectory that hits the goal?





# **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:

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

i.e., MDP with one state, one-step transition, and K actions This is also called Multi-armed Bandits

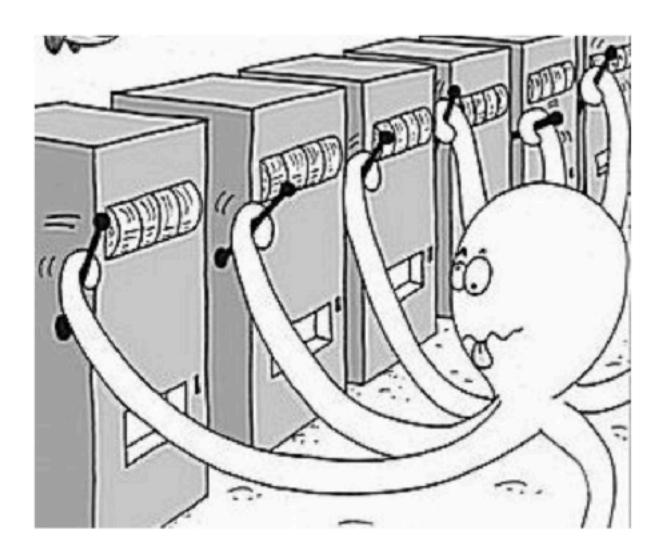
# Plan for today:

- 2. Attempt 1: Greedy Algorithm (a bad algorithm)
  - 3. Attempt 2: Explore and Commit
- 4. Attempt 3: Upper Confidence Bound (UCB) Algorithm

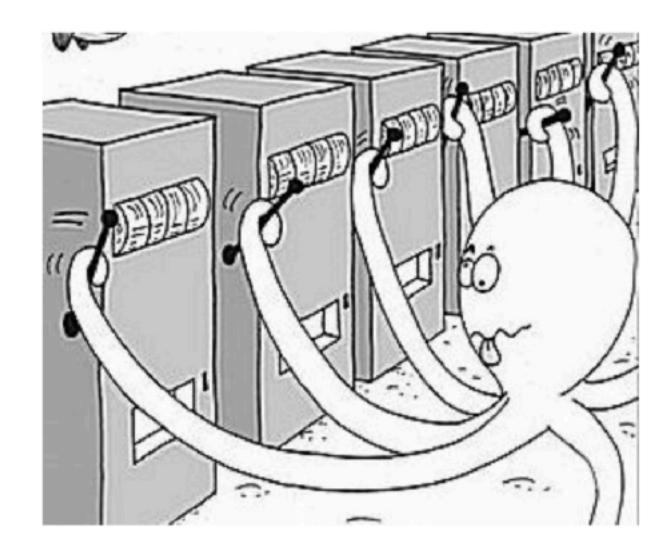
1. Introduction of MAB

### **Setting:**

We have K many arms:  $a_1, \ldots, a_K$ 

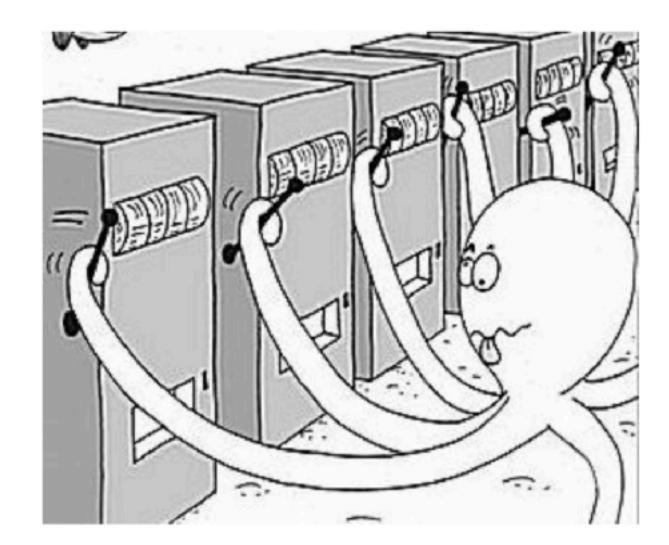


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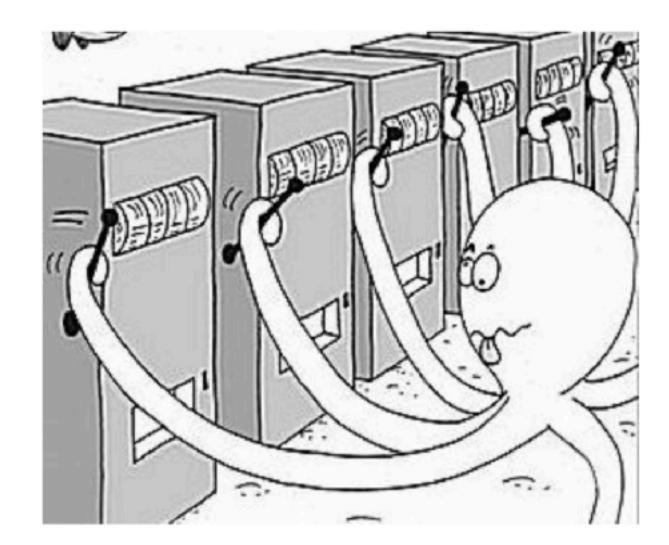
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- **Example:**  $a_i$  has a Bernoulli distribution  $\nu_i$  w/ mean  $\mu_i := p$ : Every time we pull arm  $a_i$ , we observe an i.i.d reward  $r = \begin{cases} 1 & \text{w/ prop } p \\ 0 & \text{w/ prob } 1 - p \end{cases}$





### 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:

- 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

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

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

1. Learner pulls arm  $I_t \in \{1, \ldots, K\}$ 

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

# Intro to MAB

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2. Learner observes an i.i.d reward  $r_t \sim \nu_{I_t}$  of arm  $I_t$ 



 $\operatorname{Regret}_{T} =$ 

## Intro to MAB

$$= T\mu^{\star} - \sum_{t=0}^{T-1} \mu_{I_t}$$

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

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Total expected reward if we pulled best arm over T rounds

## Intro to MAB

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# Intro to MAB

t=0

Total expected reward of the arms we pulled over T rounds

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



 $\operatorname{Regret}_{T} = T\mu^{\star} - \sum_{I_{t}}^{T} \mu_{I_{t}}$ 

Total expected reward if we pulled best arm over T rounds

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

# Intro to MAB

<u>T-1</u>

t=0

Total expected reward of the arms we pulled over T rounds

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



### Why the problem is hard?

### **Exploration and Exploitation Tradeoff:**

# Intro to MAB

### **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)?

# Intro to MAB

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# Plan for today:



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Alg: try each arm once, and then commit to the one that has the **highest observed** reward

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)

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

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  - - Clearly  $a_1$  is a better arm!
- 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



# Plan for today:



3. Attempt 2: Explore and Commit

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

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

# 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





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

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

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

Pull arm-k N times, observe  $\{r_i\}_{i=1}^N \sim \nu_k$ 

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Pull arm-k N times, ob

Calculate arm k's emp

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Given a distribution  $\mu \in \Delta([0,1])$ , and N i.i.d samples  $\{r_i\}_{i=1}^N \sim \mu, \text{ w/ probability at least } 1 - \delta, \text{ we have:}$  $\left| \sum_{i=1}^N r_i/N - \mu \right| \le O\left(\sqrt{\frac{\ln(1/\delta)}{N}}\right)$ 

$$\leq O\left(\sqrt{\frac{\ln(1/\delta)}{N}}\right)$$

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 $\hat{\mu} - \sqrt{\ln(1/\delta)/N}$ 

#### Statistical Tools: Combine Hoeffding and Union Bound, we have:

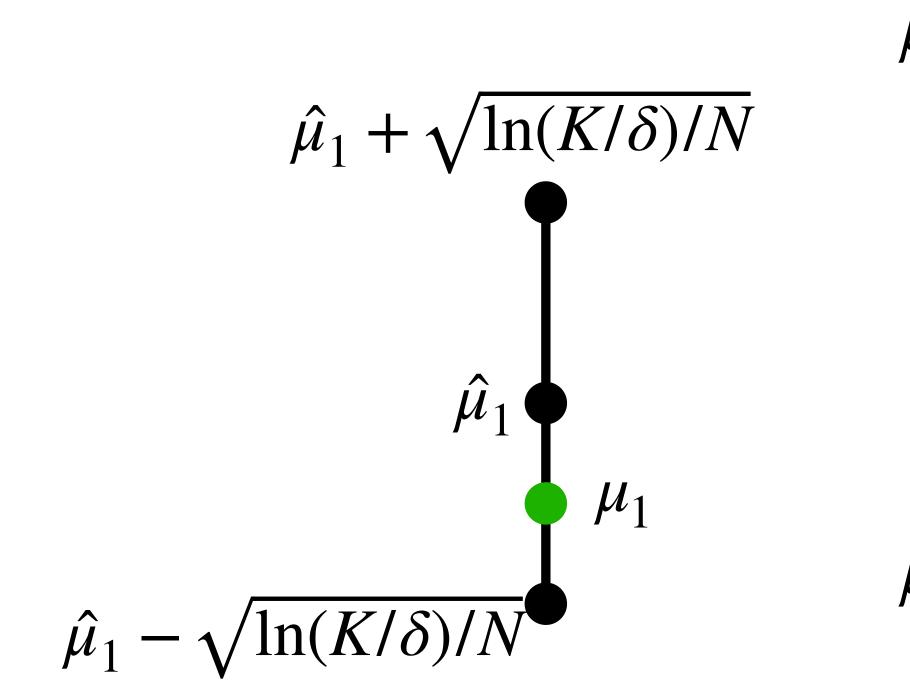
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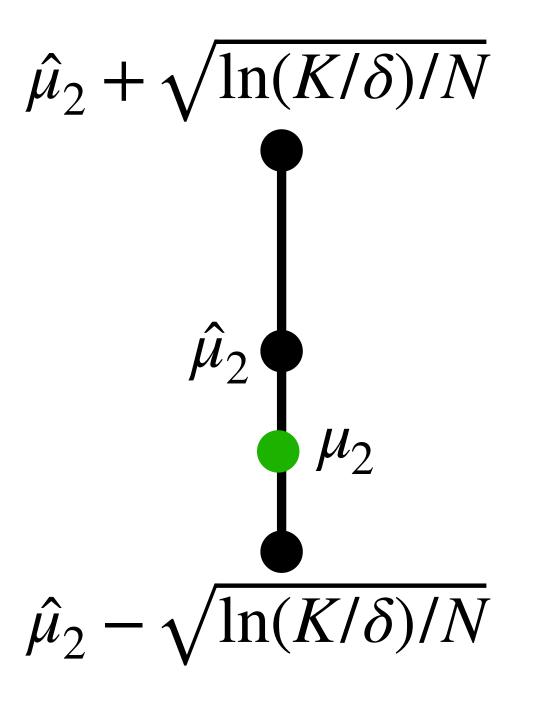
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 $\hat{\mu}_3 + \sqrt{\ln(K/\delta)/N}$  $\mu_3$  $\hat{\mu}_3 - \sqrt{\ln(K/\delta)/N}$ 

# 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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 $i \in [K]$ 

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Let's now bound Regret<sub>exploit</sub>



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- $i \in [K]$
- What's the regret in the exploitation phase:
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$$\mu_{I^\star} - \mu_{\hat{I}} \leq \left[\hat{\mu}_{I^\star} + \sqrt{\ln(K/\delta)/N}\right] - \left[\hat{\mu}_{\hat{I}} - \sqrt{\ln(K/\delta)/N}\right]$$

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

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Q: why?  $\leq 2\sqrt{\ln(K/\delta)/N}$ 

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





#### Finally, combine two regret together:

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

 $\mathsf{Regret}_{exploit} \leq (T - NK) \left( \mu_{I^{\star}} - \mu_{\hat{I}} \right) \leq T \sqrt{\frac{\ln(K/\delta)}{N}}$ 

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

#### Finally, combine two regret together:

 $\operatorname{Regret}_{exploit} \leq (T - N)$ 

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

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Minimize the upper bound via optimizing N:



#### Finally, combine two regret together:

Regret<sub>explore</sub>

 $\operatorname{Regret}_{exploit} \leq (T - N)$ 

 $\operatorname{Regret}_{T} = \operatorname{Regret}_{explore} + F$ 

$$\leq N(K-1) \leq NK$$

$$K)(\mu_{I^{\star}} - \mu_{\hat{I}}) \leq T\sqrt{\frac{\ln(K/\delta)}{N}}$$

$$\operatorname{Regret}_{exploit} \le NK + 2T\sqrt{\frac{\ln(K/\delta)}{N}}$$

Minimize the upper bound via optimizing N:

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

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



#### To conclude on Explore then Commit:

[Theorem] Fix  $\delta \in (0,1)$ , se

 $\operatorname{Regret}_{T} \leq O(T')$ 

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

et 
$$N = \left(\frac{T\sqrt{\ln(K/\delta)}}{2K}\right)^{2/3}$$
, with

probability at least  $1 - \delta$ , **Explore and Commit** has the following regret:

$$2^{/3}K^{1/3} \cdot \ln^{1/3}(K/\delta)$$

#### Plan for today:



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



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

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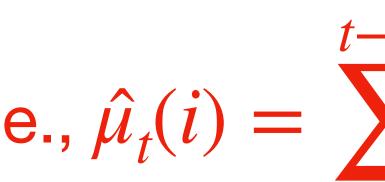
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i.e.,  $\hat{\mu}_t(i) = \sum_{\tau=1}^{t-1} \mathbf{1}\{I_{\tau} = i\}r_{\tau}/N_t(i)$  $\tau = 0$ 

#### 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  $1 - \delta$ ,  $|\hat{\mu}_k(i) - \mu_k| \le \sqrt{\frac{\ln(KT/\delta)}{N_t(k)}}$ 



### Recall the Tool for Building Confidence Interval:

Thus, we can show that for all iteration t, we have the for all  $k \in [K]$ , w/ prob  $1 - \delta$ ,  $|\hat{\mu}_k(i) - \mu_k| \le \sqrt{\frac{\ln(KT/\delta)}{N_t(k)}}$ 

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)



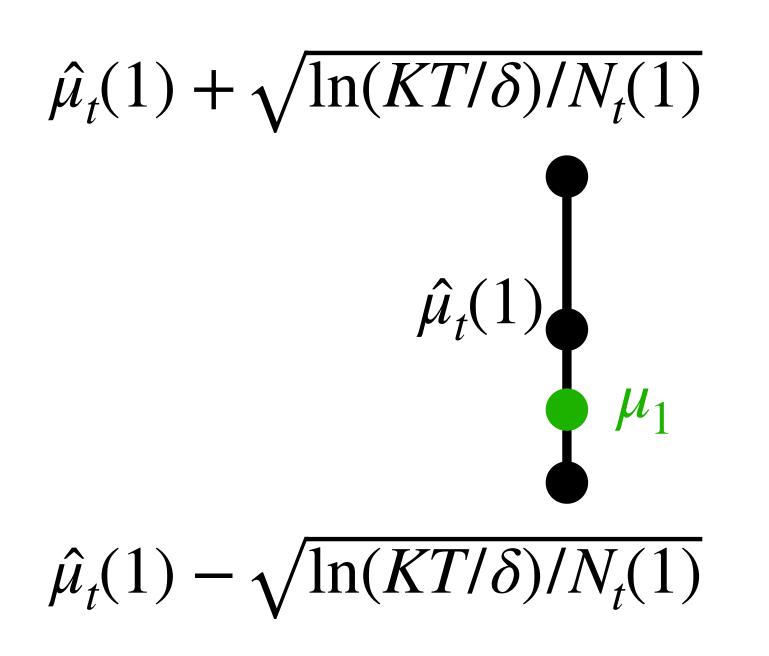
### UCB: Optimism in the face of Uncertainty

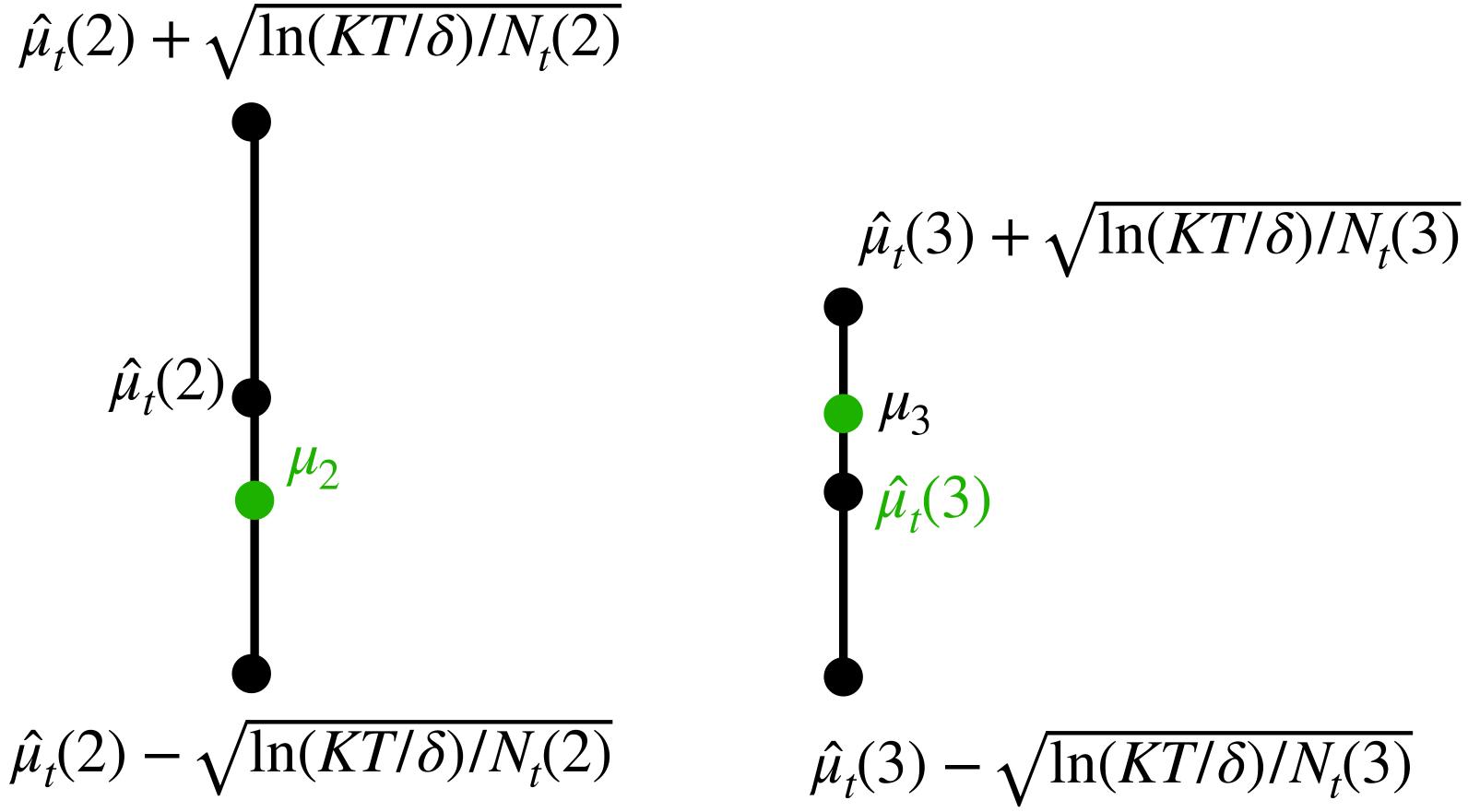
Given the confidence interval, we pick arm that has the highest Upper-Conf-Bound:



## UCB: Optimism in the face of Uncertainty

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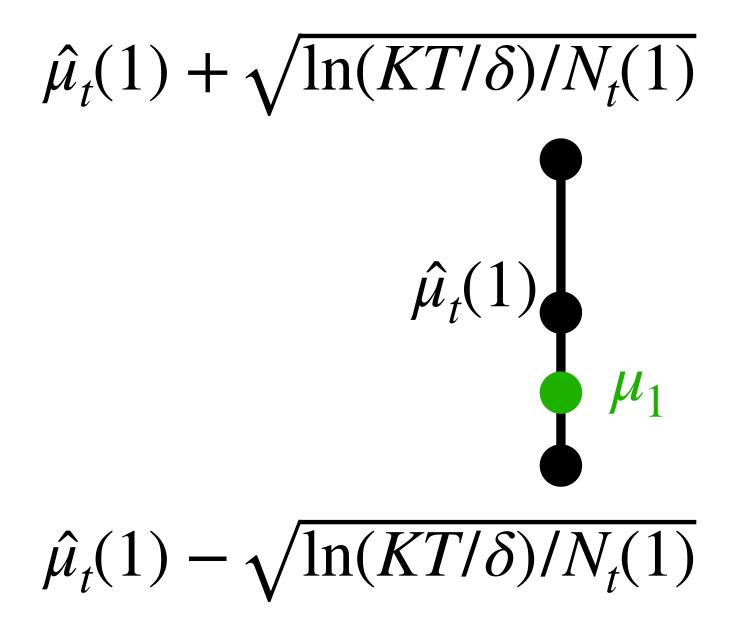






## UCB: Optimism in the face of Uncertainty

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



 $\hat{\mu}_t(2) + \sqrt{\ln(KT/\delta)/N_t(2)}$ Set  $I_t = 2$  $\hat{\mu}_t(3) + \sqrt{\ln(KT/\delta)}/N_t(3)$  $\hat{\mu}_t(2)$  $\mu_3$  $\hat{\mu}_t(3)$  $\hat{\mu}_t(2) - \sqrt{\ln(KT/\delta)}/N_t(2)$  $\hat{\mu}_t(3) - \sqrt{\ln(KT/\delta)/N_t(3)}$ 





#### Put things together: UCB Algorithm:

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

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

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

#### Put things together: UCB Algorithm:

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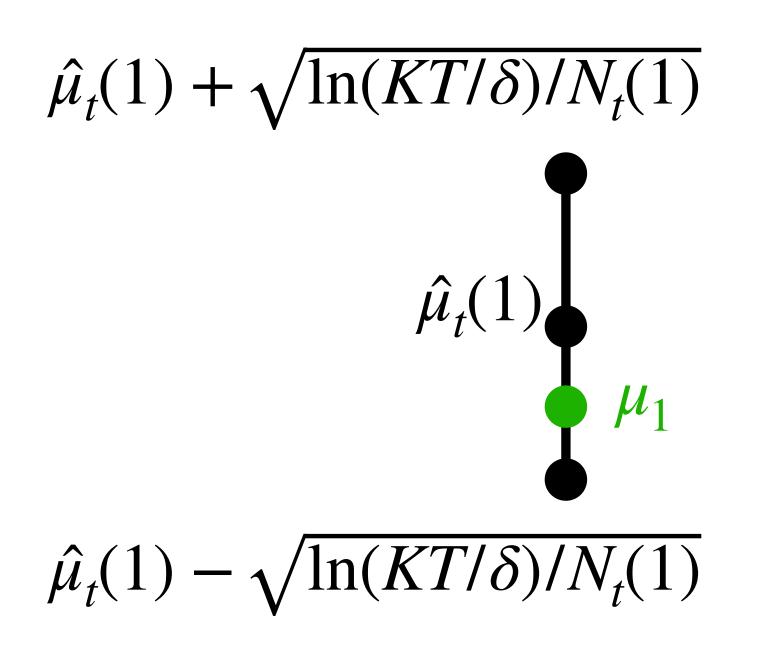
(# Upper-conf-bound of arm i)



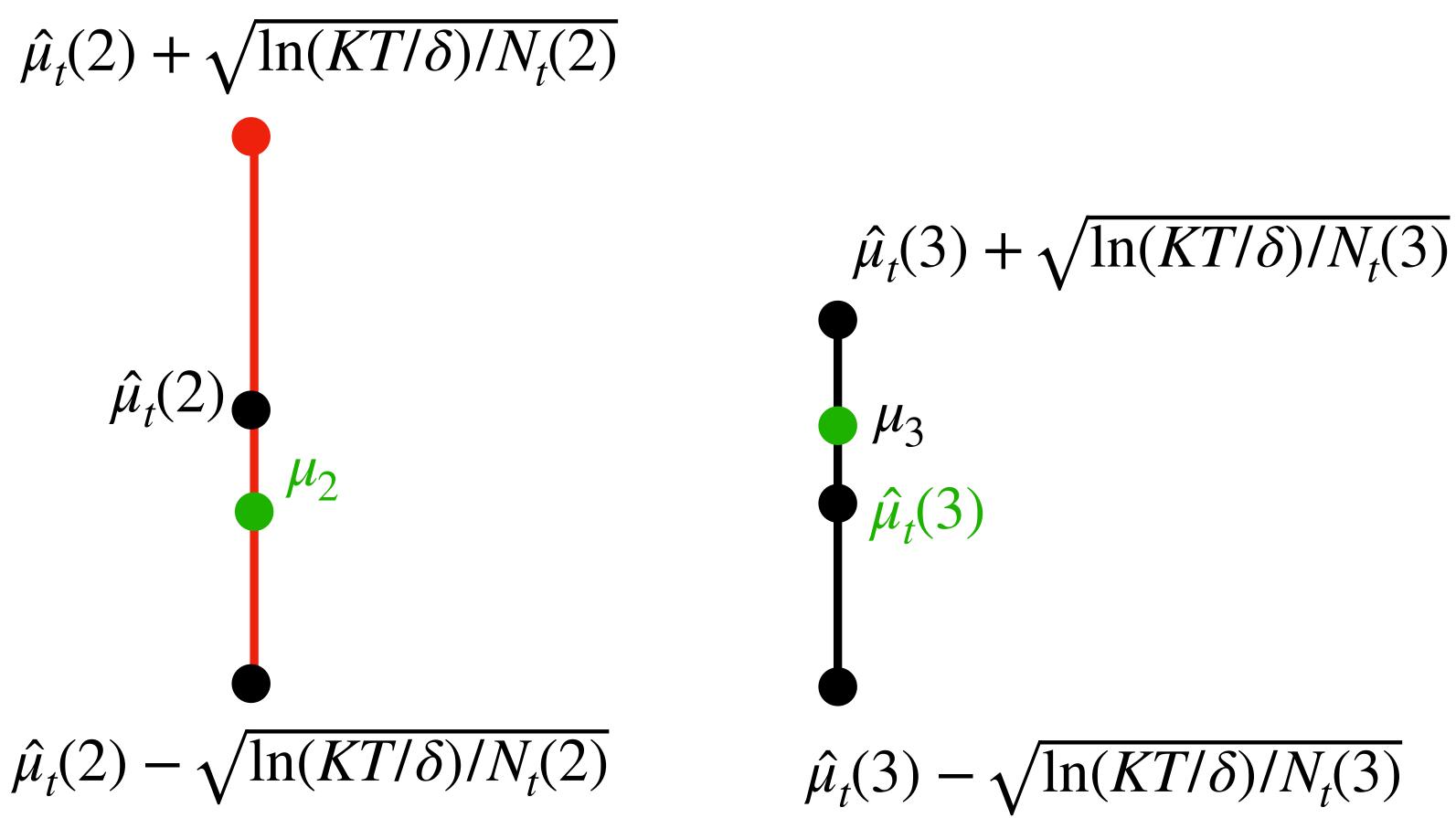
#### UCB Regret:

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

 $\operatorname{Regret}_{T} = \widetilde{O}\left(\sqrt{KT}\right)$ 



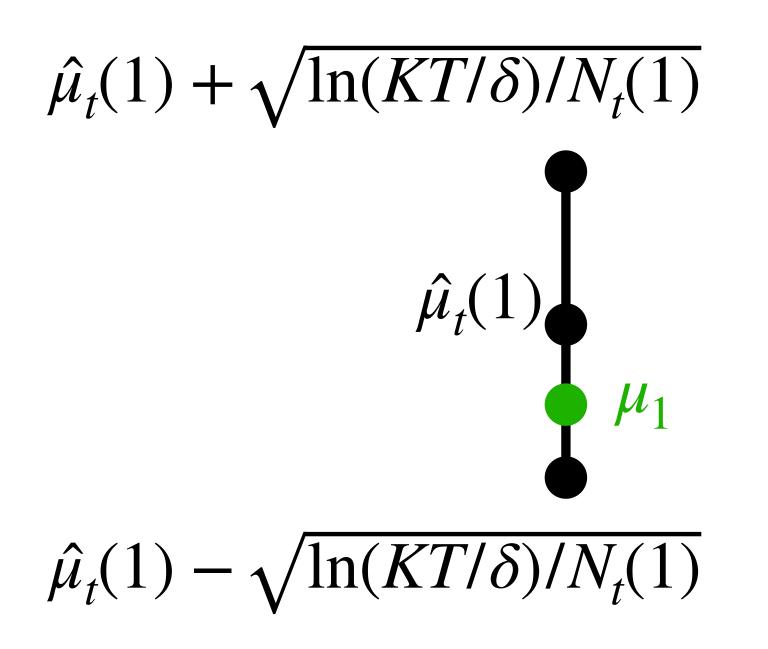
 $\hat{\mu}_t(2)$ 



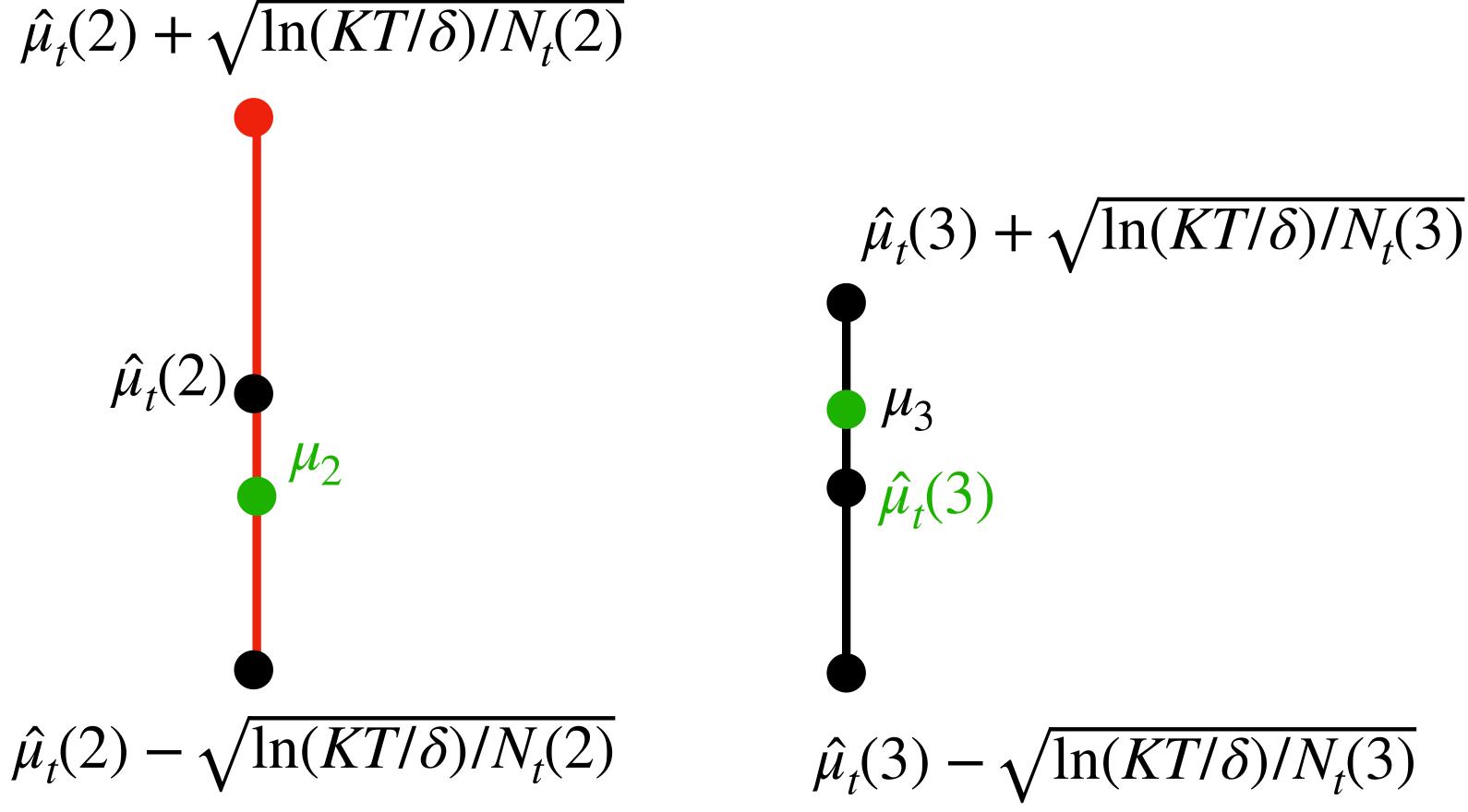




Case 1: it has large conf-interval, which means that it has not been tried many times yet (high uncertainty)



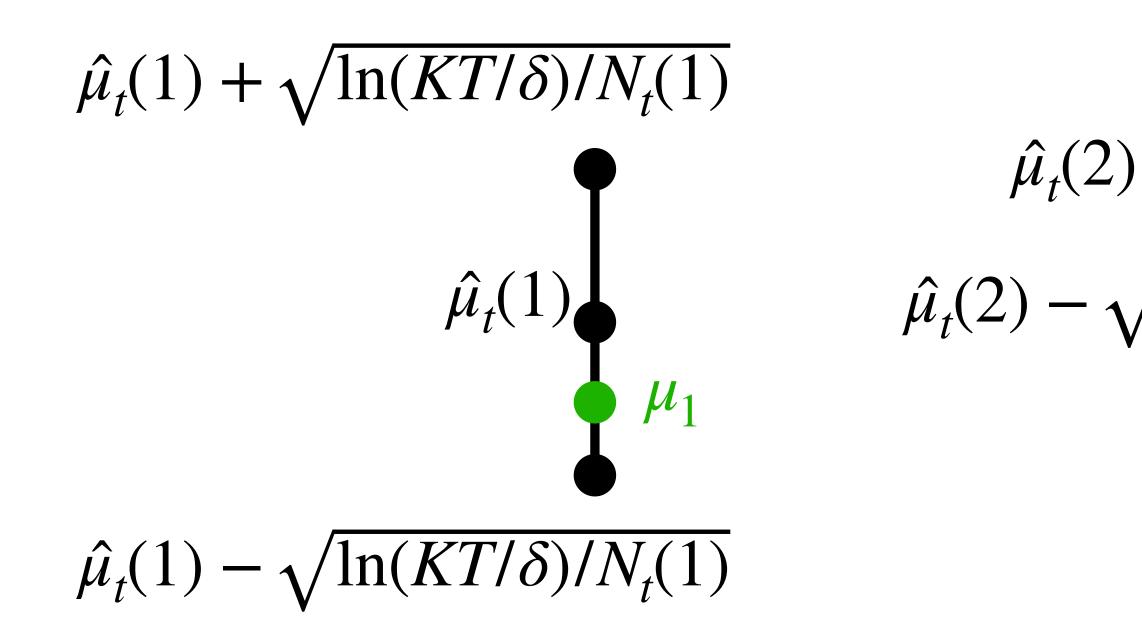
 $\hat{\mu}_t(2)$ 







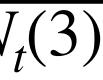
 $\hat{\mu}_t(2) + \sqrt{\ln(KT/\delta)/N_t(2)}$ 





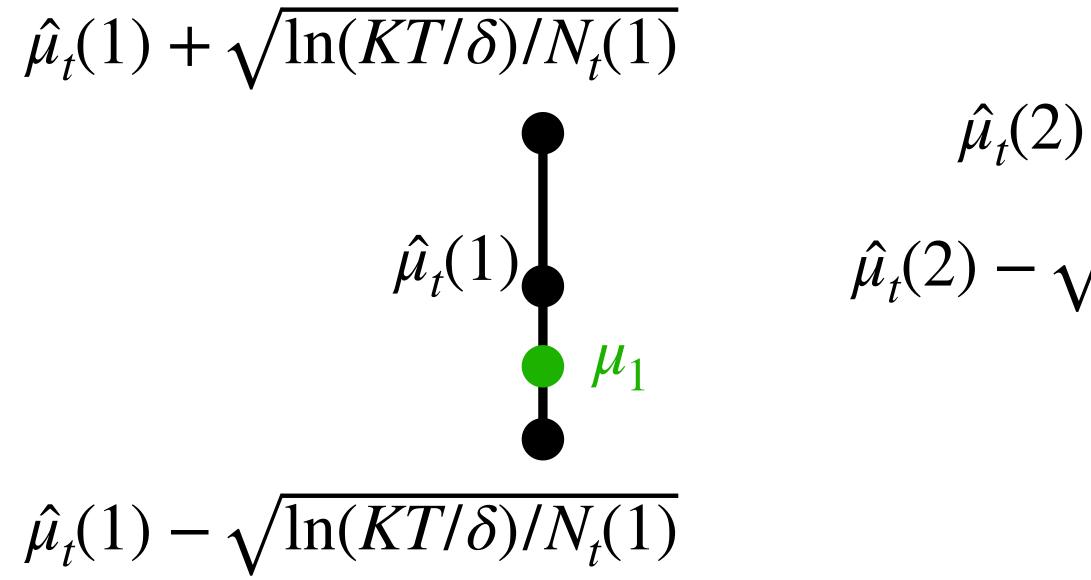
 $\ln(KT/\delta)/N_t(2)$ 

 $\hat{\mu}_t(3) + \sqrt{\ln(KT/\delta)/N_t(3)}$  $\mu_3$  $\hat{\mu}_t(3)$  $\hat{\mu}_t(3) - \sqrt{\ln(KT/\delta)/N_t(3)}$ 





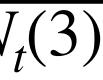
Case 2: it has low uncertainty, then it is simply a good arm, i.e., it's true mean is high!



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



 $\hat{\mu}_t(3) + \sqrt{\ln(KT/\delta)/I}$  $\mu_3$  $\hat{\mu}_t(3) - \sqrt{\ln(KT/\delta)/N_t(3)}$ 



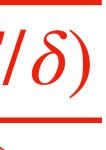


#### **Explore and Exploration Tradeoff**

- **Case 1**:  $I_{f}$  has large conf-interval, which means that it has not been tried many times yet (high uncertainty)
  - Thus, we do exploration in this case!

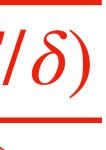
#### Explore and Exploration Tradeoff

- 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!



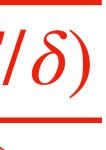


Regret-at-t =  $\mu^{\star} - \mu_{I_t}$ 



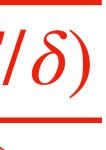


Regret-at-t = 
$$\mu^{\star} - \mu_{I_t}$$
  
 $\leq \hat{\mu}_t(I_t) + \sqrt{\frac{\ln(TK/\delta)}{N_t(I_t)}} - \mu_{I_t}$ 



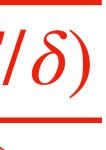


Regret-at-t = 
$$\mu^{\star} - \mu_{I_t}$$
  
Q: why?  
 $\leq \hat{\mu}_t(I_t) + \sqrt{\frac{\ln(TK/\delta)}{N_t(I_t)}} - \mu_{I_t}$ 





Regret-at-t =  $\mu^{\star} - \mu_{L}$ Q: why?  $\leq \hat{\mu}_t(I_t) + \sqrt{\frac{\ln(TK/\delta)}{N_t(I_t)}} - \mu_{I_t}$  $\leq 2_1 / \frac{\ln(TK/\delta)}{1}$  $N_t(I_t)$ 



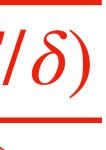


Denote the optimal arm  $I^{\star} = \arg \max_{i \in [K]} \mu_i$ ; recall  $I_t = \arg \max_{i \in [K]} \hat{\mu}_t(i) + \sqrt{\frac{\ln(KT/\delta)}{N_t(i)}}$ 

Regret-at-t =  $\mu^{\star} - \mu_{I_t}$ Q: why?  $\leq \hat{\mu}_t(I_t) + \sqrt{\frac{\ln(TK/\delta)}{N_t(I_t)}} - \mu_{I_t}$  $\leq 21/\frac{\ln(TK/\delta)}{1}$  $N_t(I_t)$ 

#### **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!



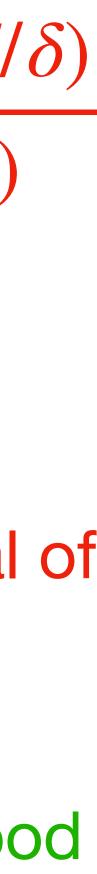


$$\begin{aligned} \text{Regret-at-t} &= \mu^{\star} - \mu_{I_t} \\ &\leq \widehat{\mu}_t(I_t) + \sqrt{\frac{\ln(TK/\delta)}{N_t(I_t)}} - \mu_{I_t} \\ &\leq 2\sqrt{\frac{\ln(TK/\delta)}{N_t(I_t)}} \end{aligned}$$

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

#### **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  $\mu^{\star}$  &  $\mu_{I_t}$  is small)!

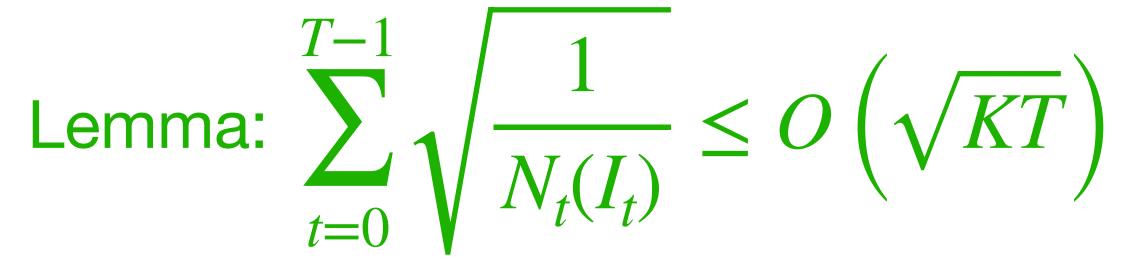


Finally, let's add all per-iter regret together:

$$\begin{aligned} \operatorname{Regret}_{T} &= \sum_{t=0}^{T-1} \left( \mu^{\star} - \mu_{I_{t}} \right) \\ &\leq \sum_{t=0}^{T-1} 2 \sqrt{\frac{\ln(TK/\delta)}{N_{t}(I_{t})}} \\ &\leq 2 \sqrt{\ln(TK/\delta)} \cdot \sum_{t=0}^{T-1} \sqrt{\frac{1}{N_{t}(I_{t})}} \end{aligned}$$

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

$$\operatorname{Regret}_{T} = \sum_{t=0}^{T-1} \left( \mu^{\star} - \mu_{I_{t}} \right)$$
$$\leq \sum_{t=0}^{T-1} 2 \sqrt{\frac{\ln(TK/\delta)}{N_{t}(I_{t})}}$$
$$\leq 2 \sqrt{\ln(TK/\delta)} \cdot \sum_{t=0}^{T-1} \sqrt{\frac{1}{N_{t}(I_{t})}}$$



3. The Principle of Optimism in the face of Uncertainty

#### Summary

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

2. Need to carefully balance exploration and exploitation