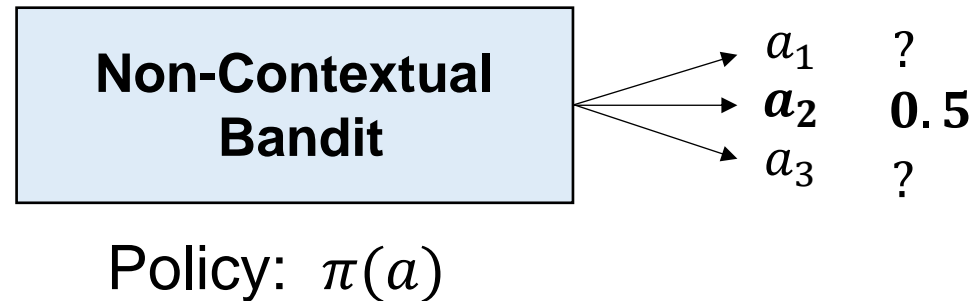
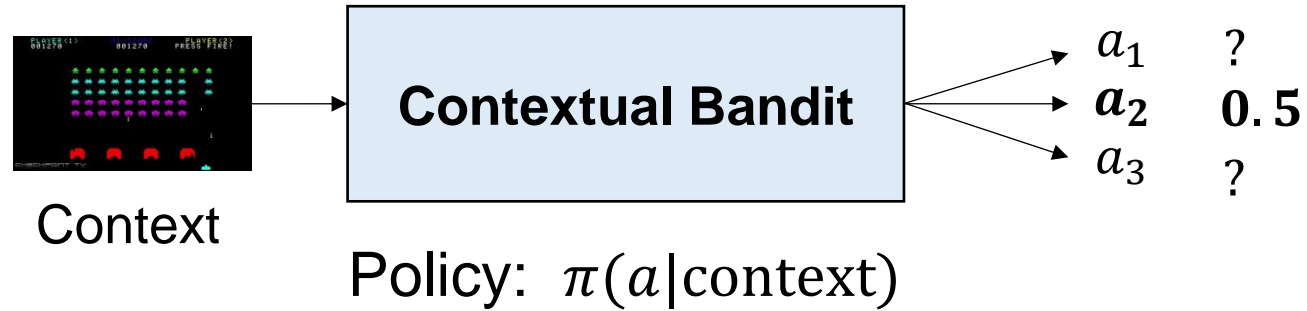


Bandits 1

Chen-Yu Wei

Contextual Bandits and Non-Contextual Bandits



Multi-Armed Bandits

Multi-Armed Bandits



A slot machine
One-armed bandit



A row of slot machines
Multi-armed bandit

Multi-Armed Bandits

Given: arm set $\mathcal{A} = \{1, \dots, A\}$

For time $t = 1, 2, \dots, T$:

Learner chooses an arm $a_t \in \mathcal{A}$

Learner observes $r_t = R(a_t) + w_t$

Arm = Action

Assumption: $R(a)$ is the (hidden) ground-truth reward function

w_t is a zero-mean noise

Goal: maximize the total reward $\sum_{t=1}^T R(a_t)$ (or $\sum_{t=1}^T r_t$)

How to Evaluate an Algorithm's Performance?

- “My algorithm obtains $0.3T$ total reward within T rounds”
– Is my algorithm good or bad?
- Benchmarking the problem

$$\Rightarrow \max_a R(a) - \frac{1}{T} \sum_{t=1}^T R(a_t) \leq \frac{1}{\sqrt{T}}$$

$$\text{Regret} := \underbrace{\max_{\pi} \sum_{t=1}^T R(\pi)}_{\text{The total reward of the best policy}} - \sum_{t=1}^T R(a_t) = \max_a \underbrace{TR(a)}_{\substack{\uparrow \\ \text{In MAB}}} - \sum_{t=1}^T R(a_t) \leq \sqrt{T}$$

- “My algorithm ensures $\text{Regret} \leq 5T^{\frac{3}{4}}$ ”
- $\text{Regret} = o(T) \Rightarrow$ the algorithm is as good as the optimal policy asymptotically

Multi-Armed Bandits

- Key challenge: Exploration
- The other three challenges we will discuss for RL
 - Generalization (there is no input in MAB)
 - Temporal credit assignments (there is no delayed feedback)
 - Distribution mismatch (there is no pre-collected data)
- We will discuss about two categories of exploration strategies
 - Based on mean estimation
 - Based on mean and uncertainty estimation

Multi-Armed Bandits

Based on mean estimation

The Exploration and Exploitation Trade-off in MAB

- To perform as well as the best policy (i.e., best arm) asymptotically, the learner has to pull the best arm most of the time
⇒ need to **exploit**
- To identify the best arm, the learner has to try every arm sufficiently many times
⇒ need to **explore**

A Simple Strategy: Explore-then-Exploit

Explore-then-exploit (Parameter: T_0)

In the first T_0 rounds, sample each arm T_0/A times. **(Explore)**

Compute the **empirical mean** $\hat{R}(a)$ for each arm a

In the remaining $T - T_0$ rounds, draw $\hat{a} = \operatorname{argmax}_a \hat{R}(a)$ **(Exploit)**

What is the *right* amount of exploration (T_0)?

Another Simple Strategy: ϵ -Greedy

Mixing exploration and exploitation in time

ϵ -Greedy (Parameter: ϵ)

In the first A rounds, draw each arm once.

In the remaining rounds $t > A$,

Take action

$$a_t = \begin{cases} \text{uniform}(\mathcal{A}) & \text{with prob. } \epsilon & \textbf{(Explore)} \\ \operatorname{argmax}_a \hat{R}_t(a) & \text{with prob. } 1 - \epsilon & \textbf{(Exploit)} \end{cases}$$

where $\hat{R}_t(a) = \frac{\sum_{s=1}^{t-1} \mathbb{I}\{a_s=a\} r_s}{\sum_{s=1}^{t-1} \mathbb{I}\{a_s=a\}}$ is the empirical mean of arm a using samples up to time $t - 1$.

Comparison

- ϵ -Greedy is more **robust to non-stationarity** than Explore-then-Exploit
- ϵ -Greedy has a better performance in the early phase of the learning process

Quantifying the Estimation Error

In the exploration phase, we obtain $N = T_0/A$ i.i.d. samples of each arm.

Key Question:

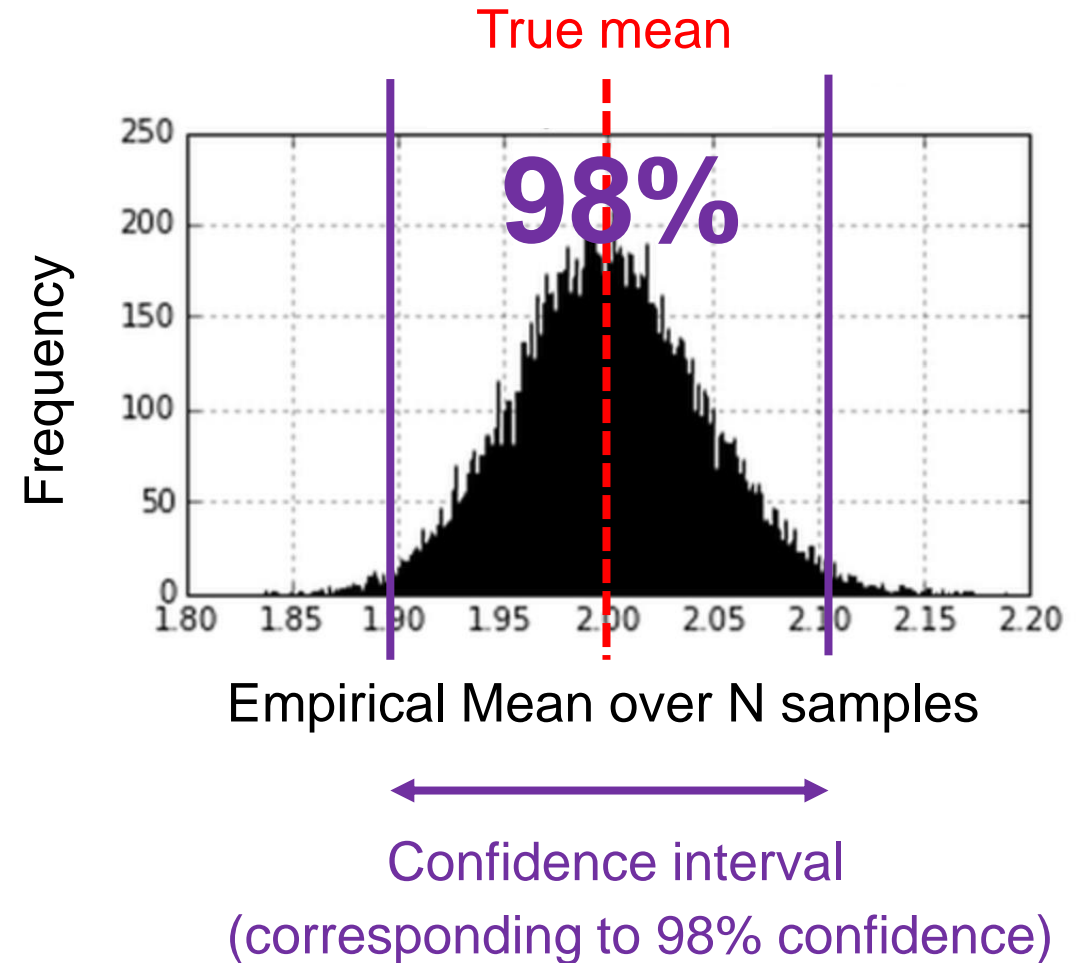
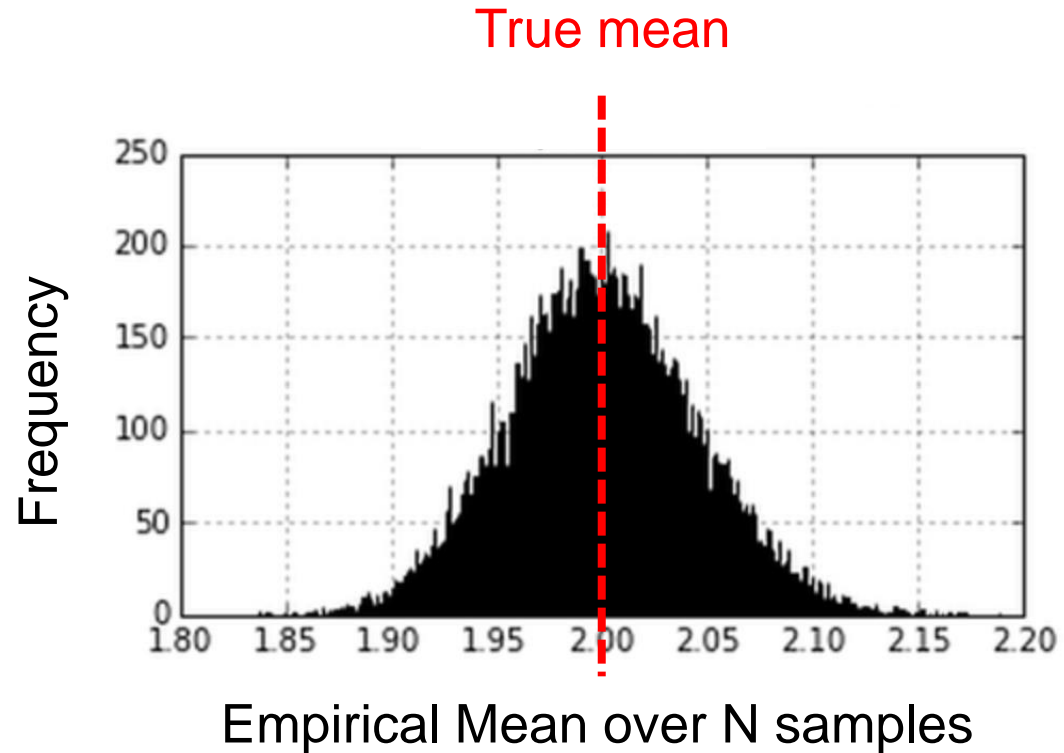
$$\left| \hat{R}(a) - R(a) \right| \leq ? \quad f(N)$$

some decreasing function of N

Empirical mean
of N i.i.d. samples

True mean

Quantifying the Estimation Error



Quantifying the Estimation Error

In the exploration phase, we obtain $N = T_0/A$ i.i.d. samples of each arm.

Key Question:

$$\left| \hat{R}(a) - R(a) \right| \leq ? \quad f(N)$$

some decreasing function of N

Empirical mean
of N i.i.d. samples

True mean

Quantifying the Estimation Error

In the exploration phase, we obtain $N = T_0/A$ i.i.d. samples of each arm.

Key Question:

With probability at least $1 - \delta$, $\delta = 0.02$
 ≈ 0.98

$$\left| \hat{R}(a) - R(a) \right| \leq ? \quad f(N, \delta)$$

some decreasing function of N

Empirical mean
of N i.i.d. samples

True mean

Quantifying the Error: Concentration Inequality

Theorem. Hoeffding's Inequality

Let X_1, \dots, X_N be independent σ -**sub-Gaussian** random variables.

Then with probability at least $1 - \delta$,

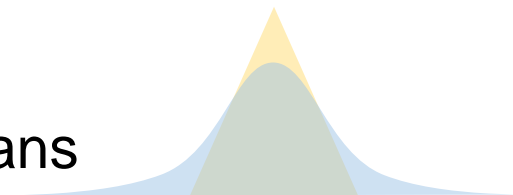
$$\left| \frac{1}{N} \sum_{i=1}^N X_i - \frac{1}{N} \sum_{i=1}^N \mathbb{E}[X_i] \right| \leq \sigma \sqrt{\frac{2 \log(2/\delta)}{N}} .$$

A random variable is called σ -sub-Gaussian if $\mathbb{E}[e^{\lambda(X - \mathbb{E}[X])}] \leq e^{\lambda^2 \sigma^2 / 2} \quad \forall \lambda \in \mathbb{R}$.

Fact 1. $\mathcal{N}(\mu, \sigma^2)$ is σ -sub-Gaussian.

Fact 2. A random variable $\in [a, b]$ is $(b - a)$ -sub-Gaussian.

Intuition: tail probability $\Pr\{|X - \mathbb{E}[X]| \geq z\}$ bounded by that of Gaussians



Quantifying the Estimation Error

With probability at least $1 - \delta$, $\left| \hat{R}(a) - R(a) \right| = O \left(\sqrt{\frac{\log(1/\delta)}{N}} \right)$

↑ Omit constants

With high probability, $\left| \hat{R}(a) - R(a) \right| = \tilde{O} \left(\sqrt{\frac{1}{N}} \right)$

$\left| \hat{R}(a) - R(a) \right| \lesssim \sqrt{\frac{1}{N}}$ ↙

↑ Omit constants and $\log(1/\delta)$ factors

Explore-then-Exploit Regret Bound Analysis

In the first T_0 rounds, sample each arm T_0/A times.

Compute the **empirical mean** $\hat{R}(a)$ for each arm a

In the remaining $T - T_0$ rounds, draw $\hat{a} = \operatorname{argmax}_a \hat{R}(a)$

$$a^* = \operatorname{argmax}_a R(a) \text{ (True best arm)}$$

After the exploration phase, we have $|\hat{R}(a) - R(a)| \lesssim \sqrt{\frac{1}{N}} = \sqrt{\frac{A}{T_0}}$

In the exploitation phase,

At any time $t \in$ exploitation phase, $R(a^*) - R(\hat{a})$

$$= \underbrace{\hat{R}(a^*) - \hat{R}(\hat{a})}_{\leq 0} + \underbrace{[R(a^*) - \hat{R}(a^*)]}_{\lesssim \sqrt{\frac{A}{T_0}}} + \underbrace{[\hat{R}(\hat{a}) - R(\hat{a})]}_{\sqrt{\frac{A}{T_0}}}$$

$$\text{Regret} \lesssim \text{cost of exploration} + \sum_{t \in \text{second phase}} (R(a^*) - R(\hat{a})) \lesssim T_0 + (T - T_0) \cdot 2\sqrt{\frac{A}{T_0}}$$

Regret Bound of Explore-then-Exploit and ϵ -Greedy

Theorem. Regret Bound of Explore-then-Exploit

Suppose that $R(a) \in [0,1]$ and w_t is 1-sub-Gaussian.
Then Explore-then-Exploit ensures with high probability,

$$\text{Regret} \lesssim T_0 + T \sqrt{\frac{A}{T_0}} \approx A^{1/3} T^{2/3} \text{ (choosing } T_0 = A^{1/3} T^{2/3} \text{)}$$

Theorem. Regret Bound of ϵ -Greedy (Your Exercise)

Suppose that $R(a) \in [0,1]$ and w_t is 1-sub-Gaussian.
Then ϵ -Greedy ensures with high probability,

$$\text{Regret} \lesssim \epsilon T + \sqrt{\frac{AT}{\epsilon}} \approx A^{1/3} T^{2/3} \text{ (choosing } \epsilon = \left(\frac{A}{T}\right)^{1/3} \text{)}$$

$$\xi_t \approx \left(\frac{A}{t}\right)^{1/3}$$

Can We Do Better?

In explore-then-exploit and ϵ -greedy, the probability to choose arms do not depend on the estimated mean (except for the empirically best arm).

... Maybe, the probability of choosing arms can be adaptive to the estimated mean?

Solution: Refine the amount of exploration for each arm **based on the current mean estimation.**

(Has to do this carefully to avoid **under-exploration**)

Refined Exploration

$$1 \leq \gamma'_t \leq A$$

$$\gamma'_t = A \Rightarrow \pi_t(a) \leq \frac{1}{A}$$

$$\gamma'_t = 1 \Rightarrow \pi_t(b) = 1$$

where $b = \underset{\downarrow}{\operatorname{argmax}} \hat{R}_t(b)$

Boltzmann Exploration (Parameter: λ)

In each round, sample a_t according to

$$\pi_t(a) \propto \exp(\lambda \hat{R}_t(a))$$

$\propto \frac{e^{\lambda \hat{R}_t(a)}}{\left(\sum_b e^{\lambda \hat{R}_t(b)} \right)}$

$$\begin{cases} \gamma'_t = A \Rightarrow \sum_a \pi_t(a) \leq 1 \\ \gamma'_t = 1 \Rightarrow \sum_a \pi_t(a) \geq 1 \end{cases}$$

$$\pi_t(a) = \frac{1}{A + \lambda \operatorname{Gap}_t(a)} \leq \frac{1}{A}$$

where $\hat{R}_t(a)$ is the empirical mean of arm a using samples up to time $t - 1$.

Inverse Gap Weighting (Parameter: λ)

γ_t is a **normalization factor**
that makes $\sum_a \pi_t(a) = 1$

$$\pi_t(a) = \frac{1}{\gamma_t - \lambda \hat{R}_t(a)} = \frac{1}{\gamma'_t + \lambda \operatorname{Gap}_t(a)}$$

where $\operatorname{Gap}_t(a) = \max_b \hat{R}_t(b) - \hat{R}_t(a) \geq 0$

$$\gamma_t = \gamma'_t + \max_b \hat{R}_t(b)$$

Refined Exploration

Variant of Inverse Gap Weighting Easier for Implementation (Parameter: λ)

$$\pi_t(a) = \begin{cases} \frac{1}{A + \lambda \text{Gap}_t(a)} & \text{if } a \neq \operatorname{argmax} \hat{R}_t(a) \\ 1 - \sum_{a' \neq a} \pi_t(a') & \text{if } a = \operatorname{argmax} \hat{R}_t(a) \end{cases}$$

where $\text{Gap}_t(a) = \max_b \hat{R}_t(b) - \hat{R}_t(a)$

Refined Exploration

- Boltzmann Exploration

- A quite commonly used exploration strategy (like ϵ -greedy)
- However, it's theoretically less desirable. For fixed parameter $\lambda \geq 2\log t$, there is always a problem instance making BE suffer $\Theta(T)$ regret
- There is no known regret bound for it yet (?)

Cesa-Bianchi, Gentile, Lugosi, Neu. Boltzmann Exploration Done Right, 2017.

Bian and Jun. Maillard Sampling: Boltzmann Exploration Done Optimally. 2021.

- Inverse Gap Weighting

- Less well-known
- We can show a near-optimal regret bound \sqrt{AT} for it, improving the $A^{1/3}T^{2/3}$ by ϵ -greedy

$$\sqrt{AT} \leq A^{1/3} T^{2/3}$$

\uparrow
where $A \leq T$

Foster and Rakhlin. Beyond UCB: Optimal and Efficient Contextual Bandits with Regression Oracles. 2020.

Guarantee of Inverse Gap Weighting

Inverse Gap Weighting ensures with high probability,

$$\text{Regret} \lesssim \frac{A}{\lambda} + \lambda \log T \approx \sqrt{AT \log T} \text{ (choosing } \lambda = \sqrt{\frac{T}{A \log T}})$$

D. Foster and A. Rakhlin. Beyond UCB: Optimal and Efficient Contextual Bandits with Regression Oracles. 2020.

See supplementary materials for a formal proof.

Summary: MAB Based on Mean Estimation

For $t = 1, 2, \dots, T$,

Design a distribution $\pi_t(\cdot)$ based on the current mean estimation $\hat{R}_t(\cdot)$

EG $\pi_t(a) = (1 - \epsilon)\mathbb{I}\{a = \operatorname{argmax} \hat{R}_t(\cdot)\} + \frac{\epsilon}{A}$ $A^{1/3}T^{2/3}$

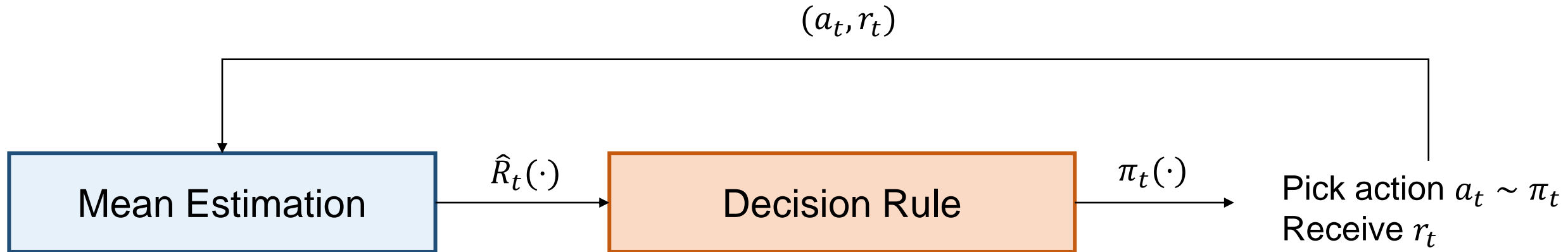
BE $\pi_t(a) \propto \exp(\lambda \hat{R}_t(a))$ $\leftarrow \lambda_t \text{ increasing over } t \text{ XXX}$

IGW $\pi_t(a) = \frac{1}{\gamma_t - \lambda \hat{R}_t(a)}$ $\swarrow \sqrt{AT \log T}$

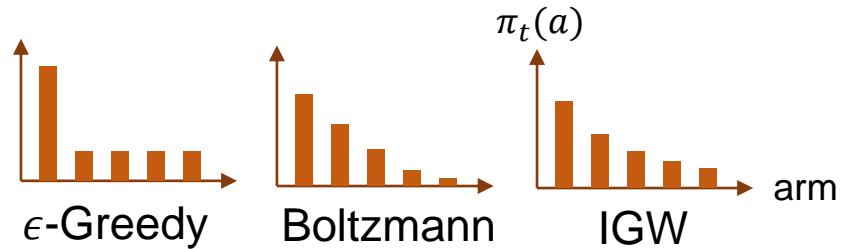
Sample an arm $a_t \sim \pi_t$ and receive the corresponding reward r_t .

Refine the mean estimation $\hat{R}_{t+1}(\cdot)$ with the new sample (a_t, r_t) .

Summary: MAB Based on Mean Estimation



$$\hat{R}_t(a) = \frac{\sum_{s=1}^{t-1} \mathbb{I}\{a_s = a\} r_s}{\sum_{s=1}^{t-1} \mathbb{I}\{a_s = a\}}$$



$$\pi_t(a) = (1 - \epsilon) \mathbb{I}\{a = \operatorname{argmax} \hat{R}_t(\cdot)\} + \frac{\epsilon}{A}$$

$$\pi_t(a) \propto \exp(\lambda \hat{R}_t(a))$$

$$\pi_t(a) = \frac{1}{\gamma_t - \lambda \hat{R}_t(a)}$$

Summary: MAB Based on Mean Estimation

- All 3 methods are based on the same **mean estimation**
 - ϵ -Greedy, Boltzmann exploration, Inverse gap weighting
- The key difference is in the **decision rule**, i.e., the mapping from estimated means \hat{R}_t to a distribution π_t .
 - The **shape** of the mapping makes differences
- There is a **scalar hyperparameter** that allows for a tradeoff between exploration and exploitation (ϵ in EG, λ in BE or IGW)

Some Experiments

$T = 10000$ rounds

$A = 2$ arms

Reward mean $R = [0.5, 0.5 - \Delta]$

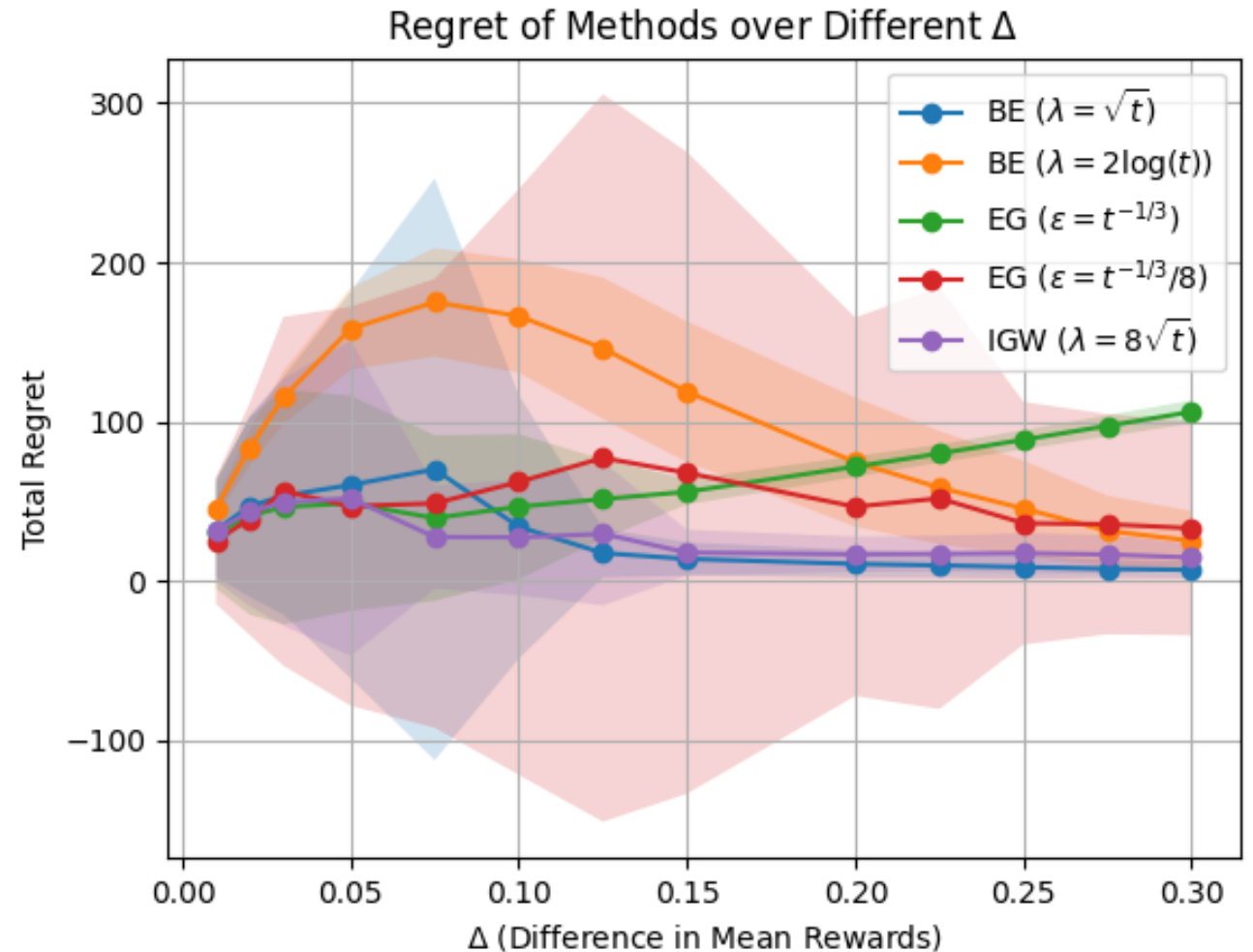
Bernoulli distribution

Time-dependent parameters

30 random seeds

Observations:

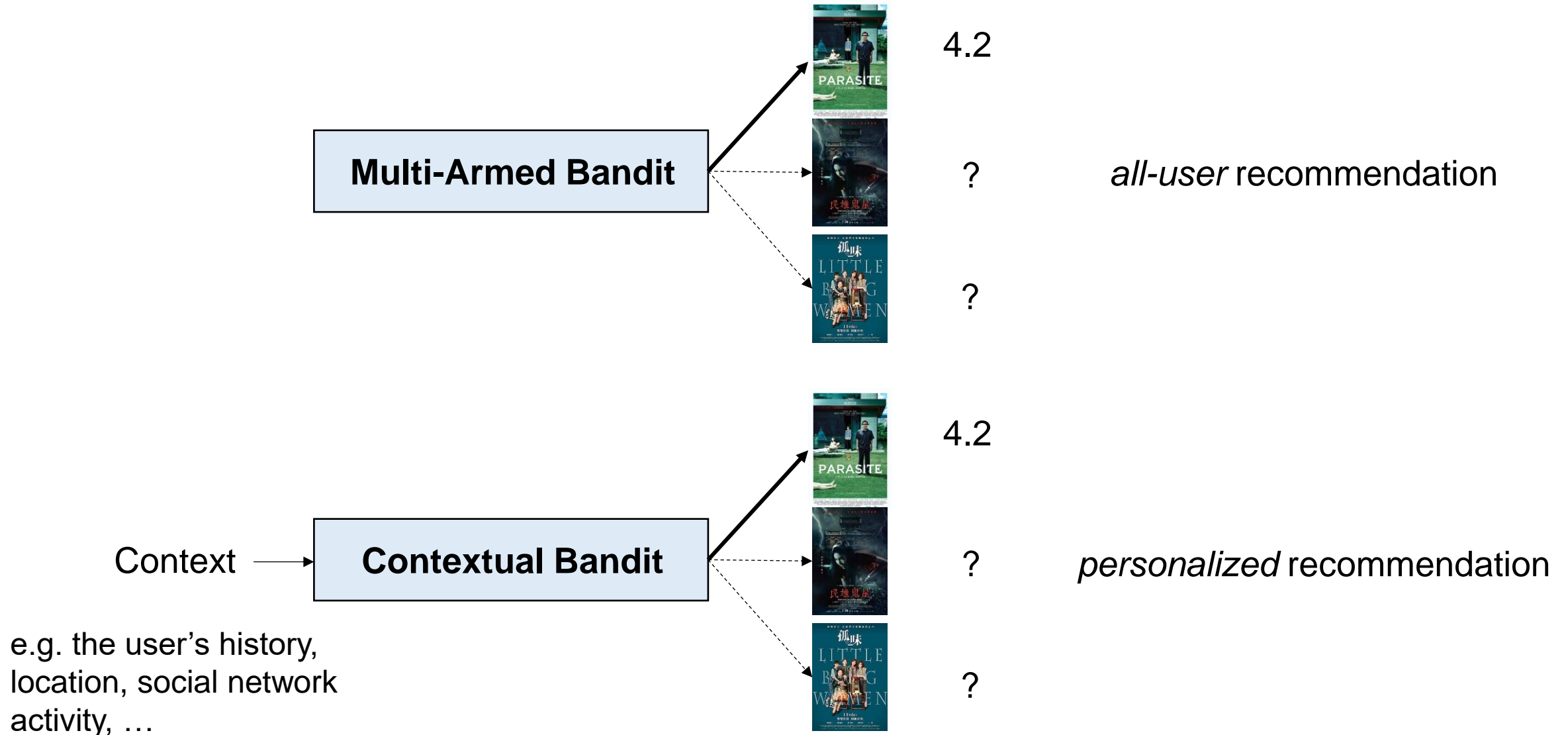
- Bound from theory could be loose
-- theory captures **worst-case** guarantee
- Most algorithms seem to have its worst regret at some intermediate Δ value
-- will be studied in Homework 1



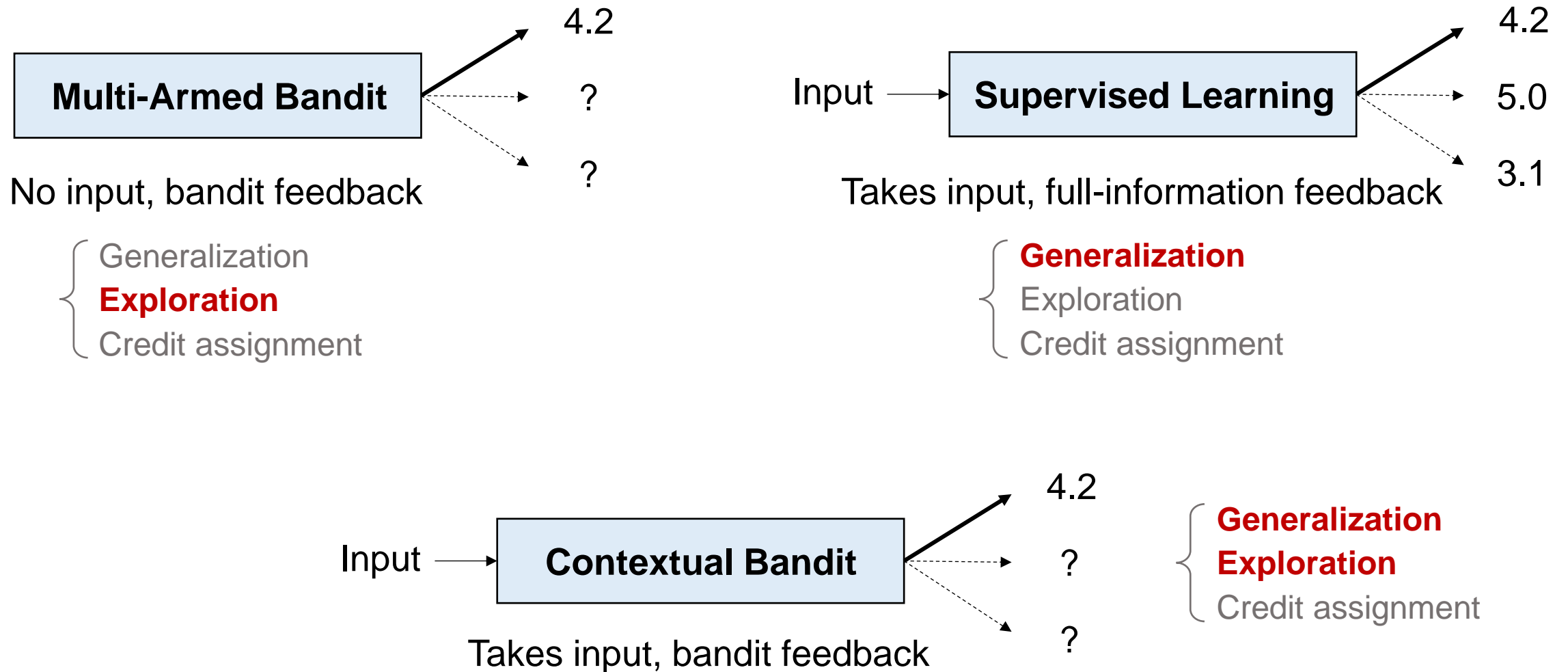
Contextual Bandits

Based on reward function estimation

Multi-Armed Bandits vs. Contextual Bandits



Contextual Bandits Generalizes MAB and SL



Contextual Bandits

For time $t = 1, 2, \dots, T$:

Environment generates a context $x_t \in \mathcal{X}$

Learner chooses an action $a_t \in \mathcal{A}$

Learner observes $r_t = R(x_t, a_t) + w_t$ *noise*

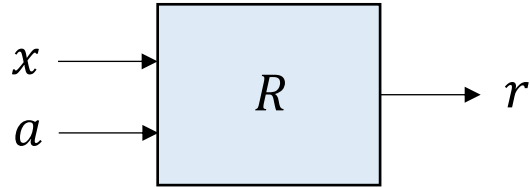
$$\frac{|R(x, a)| \leq 1}{|w_t| \leq 1}$$

Discussion

- Contextual bandits is a minimal simultaneous generalization of supervised learning (SL) and multi-armed bandits (MAB)
- We learned a lot about SL in machine learning courses
- We just learned some simple MAB algorithms
 - 3 strategies based on mean estimation
- **Question:** Can you design a contextual bandits algorithm based on the techniques you know for SL and MAB?

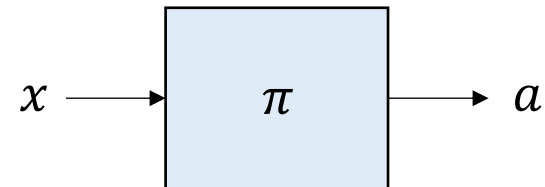
Two ways to leverage SL techniques in CB

x : context, a : action, r : reward



Learn a mapping from
(context, action) to reward

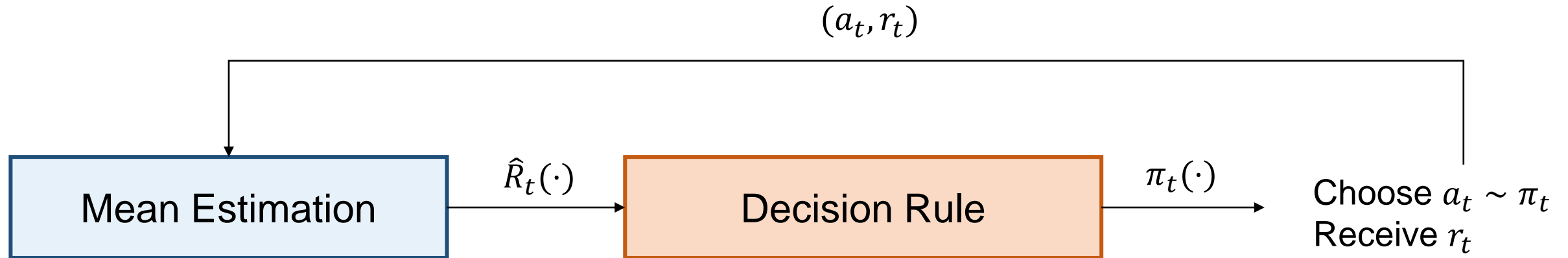
CB with **regression oracle**
Value-based approach
(discussed next)



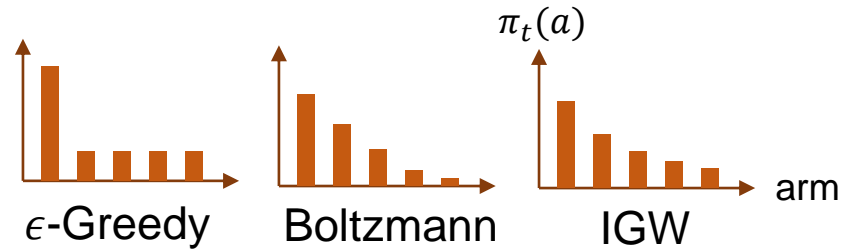
Learn a mapping from
context to action (or action distribution)

CB with **classification oracle**
Policy-based approach
(slightly later in the course)

Recall: MAB Based on Mean Estimation



$$\hat{R}_t(a) = \frac{\sum_{s=1}^{t-1} \mathbb{I}\{a_s = a\} r_s}{\sum_{s=1}^{t-1} \mathbb{I}\{a_s = a\}}$$



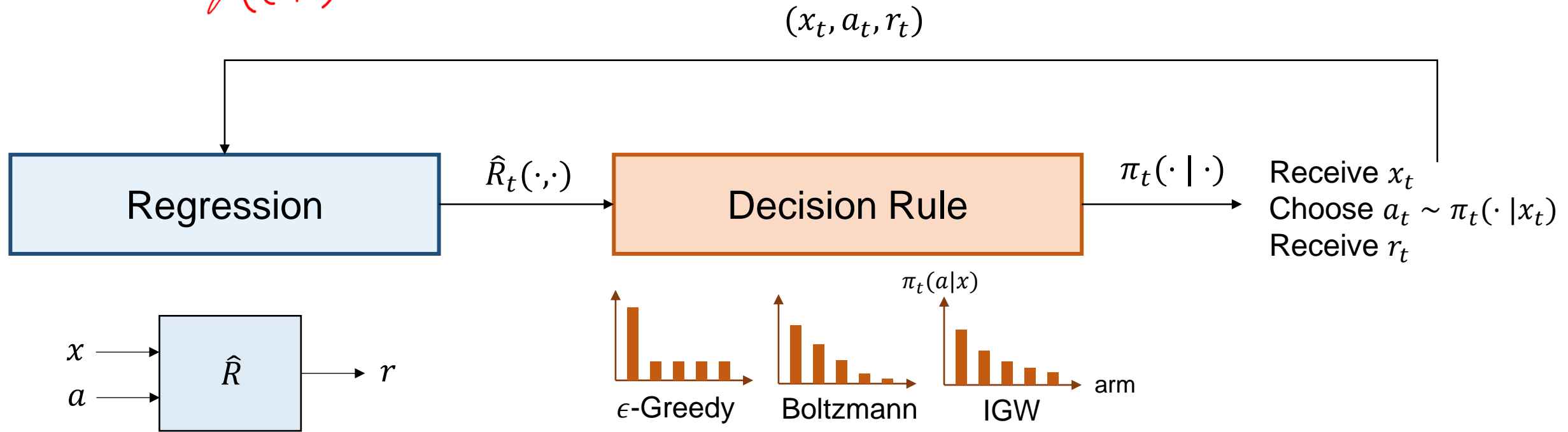
$$\pi_t(a) = (1 - \epsilon) \mathbb{I}\{a = \operatorname{argmax} \hat{R}_t(\cdot)\} + \frac{\epsilon}{A}$$

$$\pi_t(a) \propto \exp(\lambda \hat{R}_t(a))$$

$$\pi_t(a) = \frac{1}{\gamma_t - \lambda \hat{R}_t(a)}$$

CB Based on Reward Function Estimation (Regression)

$\mathcal{R}(x, a)$



Train a \hat{R} such that $r_i \approx \hat{R}(x_i, a_i)$

$$\pi_t(a|x) = (1 - \epsilon) \mathbb{I}\{a = \operatorname{argmax} \hat{R}_t(x, \cdot)\} + \frac{\epsilon}{A}$$

$$\pi_t(a|x) \propto \exp(\lambda \hat{R}_t(x, a))$$

$$\pi_t(a|x) = \frac{1}{\gamma_t - \lambda \hat{R}_t(x, a)}$$

CB Based on Reward Function Estimation

Instantiate a regression procedure \hat{R}_1

For $t = 1, 2, \dots, T$,

Receive context x_t

Design a distribution $\pi_t(\cdot|x_t)$ based on the estimated reward $\hat{R}_t(x_t, \cdot)$

$$\mathbf{EG} \quad \pi_t(a|x_t) = (1 - \epsilon)\mathbb{I}\{a = \operatorname{argmax} \hat{R}_t(x_t, \cdot)\} + \frac{\epsilon}{A}$$

$$\mathbf{BE} \quad \pi_t(a|x_t) \propto \exp(\lambda \hat{R}_t(x_t, a))$$

$$\mathbf{IGW} \quad \pi_t(a|x_t) = \frac{1}{\gamma_t - \lambda \hat{R}_t(x_t, a)}$$

Sample an action $a_t \sim \pi_t(\cdot | x_t)$ and receive the corresponding reward r_t .

Refine the reward estimator $\hat{R}_{t+1}(\cdot, \cdot)$ with the new sample (x_t, a_t, r_t) .

Regret in Contextual Bandits

For time $t = 1, 2, \dots, T$:

Environment generates a context $x_t \in \mathcal{X}$

Learner chooses an action $a_t \in \mathcal{A}$

Learner observes $r_t = R(x_t, a_t) + w_t$

$$\begin{aligned} \text{Regret} &= \sum_{t=1}^T R(x_t, \pi^*(x_t)) - \sum_{t=1}^T R(x_t, a_t) & \text{Benchmark policy: } \pi^*(x) &= \operatorname{argmax}_{a \in \mathcal{A}} R(x, a) \\ &= \sum_{t=1}^T \max_{a \in \mathcal{A}} R(x_t, a) - \sum_{t=1}^T R(x_t, a_t) \end{aligned}$$

Regret in Contextual Bandits

Regret Bound of ϵ -Greedy

ϵ -Greedy ensures

$$\text{Regret} \lesssim \epsilon T + \sqrt{\frac{AT \cdot \text{Err}}{\epsilon}}$$

Regression error

$$\text{Err} = \sum_{t=1}^T \left(\hat{R}_t(x_t, a_t) - R(x_t, a_t) \right)^2$$

Regret Bound of Inverse Gap Weighting

IGW ensures

$$\text{Regret} \lesssim \frac{AT}{\lambda} + \lambda \cdot \text{Err}$$

Will be proven in HW1

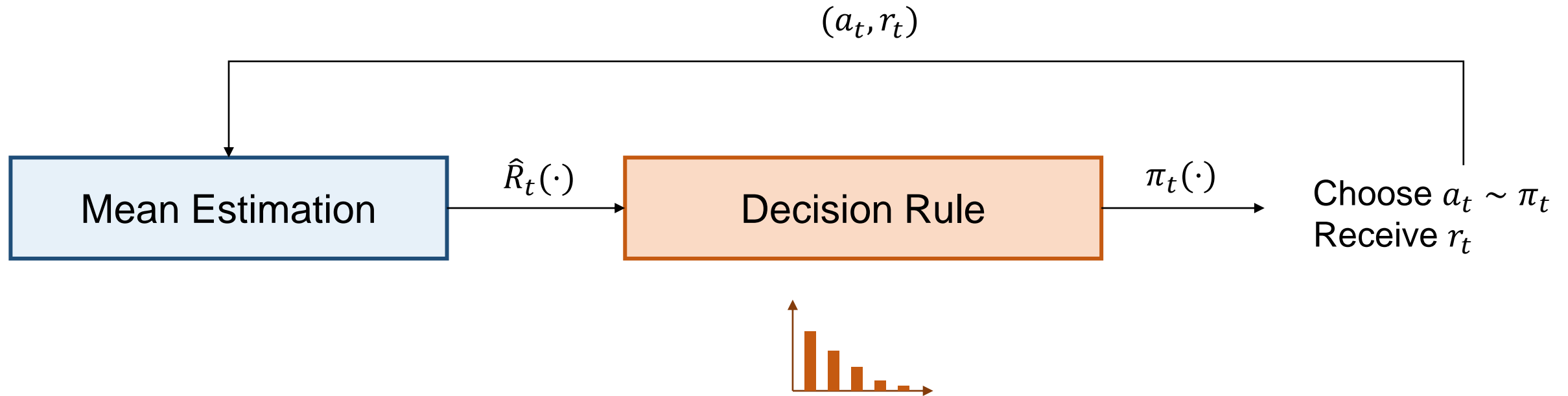
Summary

- Contextual bandits (CB) simultaneously generalizes supervised learning (SL) and multi-armed bandits (MAB). It captures the challenges of **generalization** and **exploration** in online RL.
- Any MAB algorithm based on “**mean estimation**” can be lifted as a CB algorithm with “**reward function estimation**” by leveraging a regression oracle.
 - This gives a general framework for value-based CB

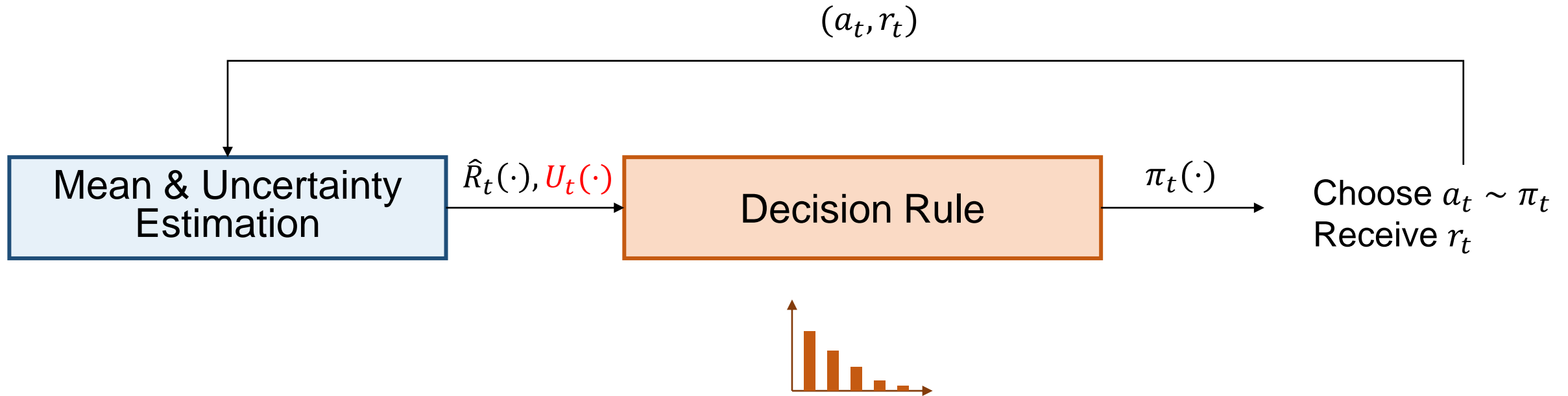
Multi-Armed Bandits

Based on mean and uncertainty estimation

Recall: MAB Based on Mean Estimation



MAB Based on Mean and Uncertainty Estimation



$U_t(a)$: measures the uncertainty of $\hat{R}_t(a)$

$$|\hat{R}_t(a) - R(a)| \leq \sqrt{\frac{2\log(2/\delta)}{N_t(a)}} \triangleq U_t(a)$$

This inequality is used in the **math analysis** of ϵ -Greedy and IGW, but not in their **algorithm**.

Useful Idea: “Optimism in the Face of Uncertainty”

In words:

Act according to the **best plausible world**.

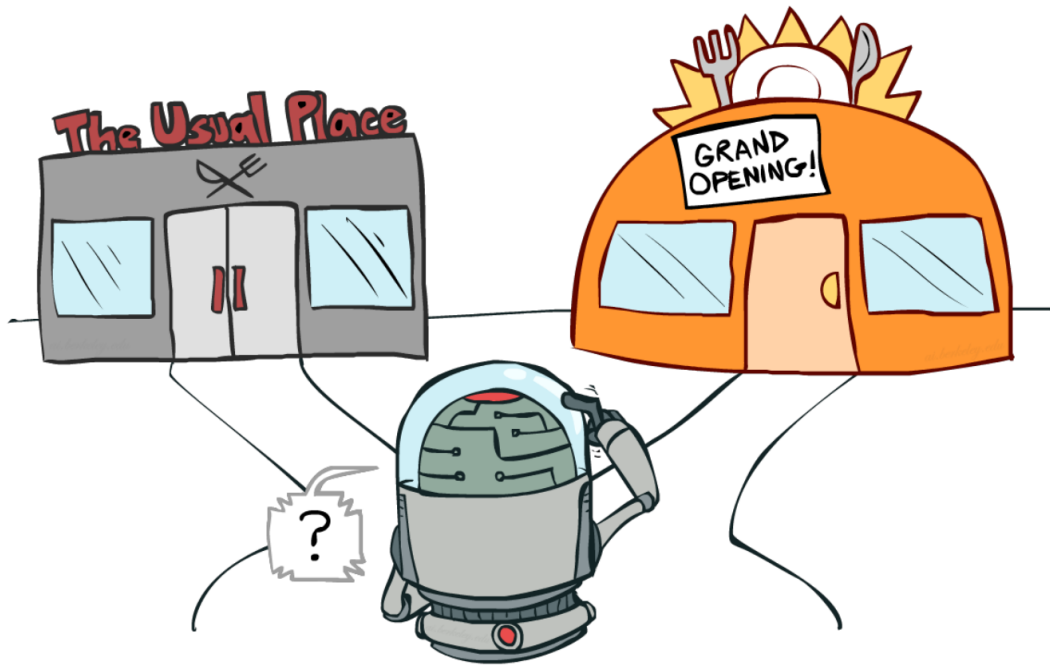


Image source: UC Berkeley CS188

Another Idea: “Optimism in the Face of Uncertainty”

In words:

Act according to the **best plausible world**.

At time t , suppose that arm a has been drawn for $N_t(a)$ times, with empirical mean $\hat{R}_t(a)$.

What can we say about the true mean $R(a)$?

$$|R(a) - \hat{R}_t(a)| \leq \sqrt{\frac{2 \log(2/\delta)}{N_t(a)}} \quad \text{w.p.} \geq 1 - \delta$$

What's the most optimistic mean estimation for arm a ?

$$\hat{R}_t(a) + \sqrt{\frac{2 \log(2/\delta)}{N_t(a)}}$$

Upper Confidence Bound (UCB)

UCB (Parameter: δ)

In the first A rounds, draw each arm once.

For the remaining rounds: in round t , draw

$$a_t = \operatorname{argmax}_a \hat{R}_t(a) + \sqrt{\frac{2 \log(2/\delta)}{N_t(a)}}$$

where $\hat{R}_t(a)$ is the empirical mean of arm a using samples up to time $t - 1$.

$N_t(a)$ is the number of samples of arm a up to time $t - 1$.

Regret Bound of UCB

Theorem. Regret Bound of UCB

UCB ensures with high probability,

$$\text{Regret} \lesssim \sqrt{AT} .$$

UCB Regret Bound Analysis

Visualizing UCB

True mean: [0.2, 0.4, 0.6, 0.7]

Contextual Bandits

Based on reward function and uncertainty estimation

Bandits 1

Summary for value-based approaches

Summary: Exploration

$\hat{R}_t(a)$: mean estimation for arm a at time t
 $N_t(a)$: number of samples for arm a at time t

Explore-then-Exploit

$$a_t = \begin{cases} \text{uniform}(\mathcal{A}) & t \leq T_0 \\ \operatorname{argmax}_a \hat{R}_{T_0}(a) & t > T_0 \end{cases}$$

ϵ -Greedy

$$a_t = \begin{cases} \text{uniform}(\mathcal{A}) & \text{with prob. } \epsilon \\ \operatorname{argmax}_a \hat{R}_t(a) & \text{with prob. } 1 - \epsilon \end{cases}$$

Boltzmann Exploration

$$\pi_t(a) \propto \exp(\lambda_t \hat{R}_t(a))$$

Inverse Gap Weighting

$$\pi_t(a) = \frac{1}{\gamma_t - \lambda_t \hat{R}_t(a)}$$

UCB

$$a_t = \operatorname{argmax}_a \hat{R}_t(a) + \sqrt{\frac{2 \log(2/\delta)}{N_t(a)}}$$

Summary: Exploration

	Regret Bound	Approach
Explore-then-Exploit ϵ -Greedy Boltzmann Exploration Inverse Gap Weighting	$A^{1/3} T^{2/3}$ $A^{1/3} T^{2/3}$ \times \sqrt{AT}	Mean estimation + decision rule
Upper Confidence Bound Thompson Sampling Arm Elimination	\sqrt{AT}	Mean and uncertain estimation + decision rule