Bandits

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Contextual Bandits and Non-Contextual Bandits

Context

Contextual Bandit

a_1 ?

$\boldsymbol{a_2}$ $\mathbf{0.5}$

a_3 ?

Policy: $\pi(a|\text{context})$

Non-Contextual Bandit

a_1 ?

$\boldsymbol{a_2}$ $\mathbf{0.5}$

a_3 ?

Policy: $\pi(a)$

Multi-Armed Bandits

Multi-Armed Bandits

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

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

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

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

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

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

- "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

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 $\hat{a} = \mathrm{argmax}_a \hat{R}(a)$ **(Exploit)**

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

Quantifying the Estimation Error

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

Key Question:

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

for some decreasing function of N

Empirical mean of N i.i.d. samples

True mean

Explore-then-Exploit Regret Bound Analysis

Assume $\underbrace{|\hat{R}(a) - R(a)|}$ $\leq f(N) = f\left(\frac{T_0}{A}\right)$

$R(a) \in [0, R_{max}]$

$$\text{Regret} = \sum_{t=1}^{T_0} \left(R(a^*) - R(a_t)\right) + \sum_{t=T_0+1}^{T} \left(R(a^*) - R(a_t)\right)$$

$$\leq T_0 R_{max} + \sum_{t=T_0+1}^{T} \Big(\underbrace{R(a^*) - \hat{R}(a^*)}_{\leq f(T_0/A)} + \underbrace{\hat{R}(a_t) - R(a_t)}\Big)$$

$a_t = \arg\max \hat{R}(a)$

$$\leq T_0 R_{max} + 2(T - T_0)\, f(T_0/A)$$

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 $1 - \delta$,

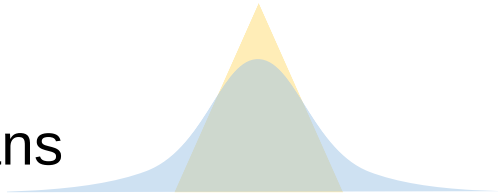
$$\left| \frac{1}{N} \sum_{i=1}^{N} X_i - \frac{1}{N} \sum_{i=1}^{N} \mathbb{E}[X_i] \right| \leq \sigma \sqrt{\frac{2 \log(2/\delta)}{N}} \;.$$

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

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



Regret Bound of Explore-then-Exploit

$a \lesssim b$ means
$a \leq \text{const.} \cdot b$
or $a = O(b)$

Theorem. Regret Bound of Explore-then-Exploit

Suppose that $R(a) \in [0,1]$ and w_t is 1-sub-Gaussian.

Then with probability at least $1 - A\delta$, Explore-then-Exploit ensures

$$\text{Regret} \leq T_0 + 2(T - T_0)\sqrt{\frac{2A\log(2/\delta)}{T_0}} \quad .$$

$$\text{Reg} \lesssim T_0 + 2T\sqrt{\frac{A}{T_0}}$$
$$\lesssim A^{1/3}T^{2/3}$$

By AM-GM: $\dfrac{T_0 + T\sqrt{\frac{A}{T_0}} + T\sqrt{\frac{A}{T_0}}}{3} \geq \sqrt[3]{T_0 \cdot T\sqrt{\frac{A}{T_0}} \cdot T\sqrt{\frac{A}{T_0}}} = A^{1/3}T^{2/3}$

To minimize $T_0 + 2T\sqrt{\frac{A}{T_0}}$, choose $T_0 = T\sqrt{\frac{A}{T_0}} \Rightarrow T_0 = A^{1/3}T^{2/3}$

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 $t > A$,

Draw

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

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 $t - 1$.

Regret Bound of ϵ-Greedy

Theorem. Regret Bound of ϵ-Greedy

With proper choice of ϵ, the expected regret of ϵ-Greedy is bounded by

$$\mathbb{E}[\text{Regret}] \leq \tilde{O}\left(A^{1/3}\, T^{2/3}\right).$$

Can We Do Better?

In explore-then-exploit and ϵ-greedy, every arm receives the same amount of exploration.

… Maybe, for those arms that look worse, the amount of exploration on them can be reduced?

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

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

Boltzmann Exploration

Boltzmann Exploration (Parameter: λ_t)

In each round, sample a_t according to

$$p_t(a) \propto \exp\left(\lambda_t \hat{R}_t(a)\right)$$

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

Cesa-Bianchi, Gentile, Lugosi, Neu. **Boltzmann Exploration Done Right**, 2017.
Bian and Jun. **Maillard Sampling: Boltzmann Exploration Done Optimally**. 2021.

Another adaptive exploration $p_t(a) = \frac{1}{\gamma - \lambda_t \hat{R}_t(a)}$ will work! (later in the course)

Another Idea: “Optimism in the Face of Uncertainty”

In words:

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

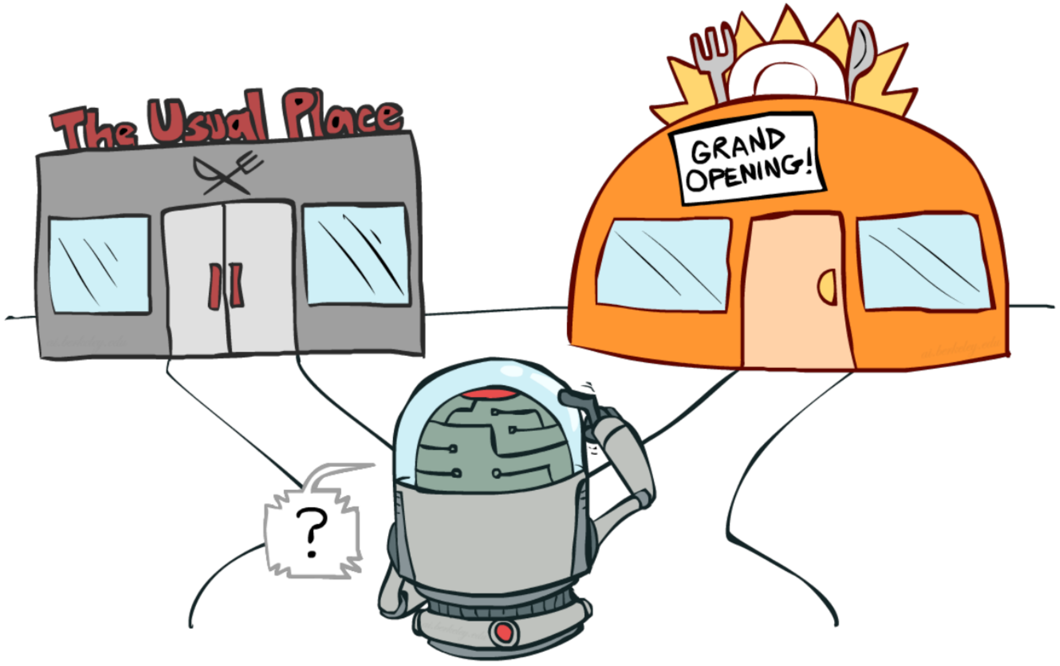


Image source: UC Berkeley AI course slide, lecture 11.

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 $R(a)$?

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

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

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

UCB

UCB (Parameter: δ)

In the first A rounds, draw each arm once.

For the remaining rounds: in round t, draw

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

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 $t-1$.

P Auer, N Cesa-Bianchi, P Fischer. **Finite-time analysis of the multiarmed bandit problem**, 2002.

Regret Bound of UCB

Theorem. Regret Bound of UCB

With probability at least $1 - AT\delta$,

$$\text{Regret} \le O\left(\sqrt{AT\log(1/\delta)}\right) = \tilde{O}(\sqrt{AT}) \ .$$

UCB Regret Bound Analysis

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

Assume $\left| R(a) - \hat{R}_t(a) \right| \leq \sqrt{\frac{2\log T/\delta}{N_t(a)}} \quad \forall t, a$

$$\text{Regret} \leq A + \sum_{t=A+1}^{T} \left(R(a^*) - R(a_t) \right)$$

$$\leq A + \sum_{t=A+1}^{T} \Big(\underbrace{R(a^*) - \tilde{R}_t(a^*)}_{\leq 0} + \underbrace{\tilde{R}_t(a_t) - R(a_t)}_{\underbrace{\tilde{R}_t(a_t) - \hat{R}_t(a_t)}_{= \sqrt{\frac{2\log(T/\delta)}{N_t(a_t)}}} + \underbrace{\hat{R}_t(a_t) - R(a_t)}_{\leq \sqrt{\frac{2\log(T/\delta)}{N_t(a_t)}}}} \Big)$$

$$\lesssim A + \sum_{t=A+1}^{T} 2\sqrt{\frac{2\log(T/\delta)}{N_t(a_t)}}$$

$$= A + \sum_a \sum_{t=A+1}^{T} \mathbb{I}\{a_t = a\} \cdot 2\sqrt{\frac{2\log(T/\delta)}{N_t(a)}} = A + \sum_a \underbrace{\left(1 + \frac{1}{\sqrt{2}} + \frac{1}{\sqrt{3}} + \cdots + \frac{1}{\sqrt{N_t(a)}} \right)}_{\lesssim \sqrt{N_t(a)}} \cdot 2\sqrt{2\log T/\delta}$$

$$\lesssim A + \sum_a \sqrt{N_t(a) \log 1/\delta}$$

$$\leq A + \sqrt{A \sum_a N_t(a) \log 1/\delta} \leq A + \sqrt{A T \log 1/\delta}$$

Exploration Strategies (Review)

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

$N_t(a)$: number of samples for arm a at time t

Explore-then-Exploit

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

ϵ-Greedy

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

Boltzmann Exploration

$$p_t(a) \propto \exp\left(\lambda_t \hat{R}_t(a)\right)$$

UCB

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

Comparison

	Regret Bound	Exploration
Explore-then-Exploit ϵ-Greedy	$A^{1/3}\, T^{2/3}$	Non-adaptive
Boltzmann Exploration	---	Adaptive
UCB Thompson Sampling	$\sqrt{AT}$	Adaptive

Visualizing UCB

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

Bayesian Setting for MAB

Assumptions:

- At the beginning, the environment draws a parameter $\theta^\star$ from some prior distribution $\theta^\star \sim P_{\text{prior}}$
- In every round, the reward vector $\boldsymbol{r_t} = (r_t(1), \ldots, r_t(A))$ is generated from $\boldsymbol{r_t} \sim P_{\theta^\star}$

E.g., Gaussian Case

- At the beginning, $\theta^\star(a) \sim \mathcal{N}(0, 1)$ for all $a \in \{1, \ldots, A\}$.
- In every round, the reward of arm a is generated by $r_t(a) \sim \mathcal{N}(\theta^\star(a), 1)$.

For the learner, P_{prior} is known; $\theta^\star$ is unknown; P_θ is known for any θ.

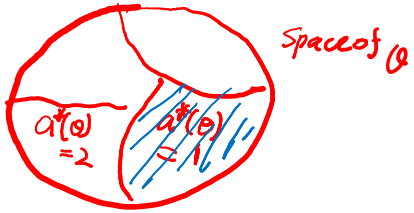
Thompson Sampling

William Thompson. **On the likelihood that one unknown probability exceeds another in view of the evidence of two samples**, 1933.

In words:

Randomly pick an arm according to the probability you **believe** it is the optimal arm.

At time t, after seeing $\mathcal{H}_t = (a_1, r_1(a_1), a_2, r_2(a_2), \dots, a_{t-1}, r_{t-1}(a_{t-1}))$, the learner has a **posterior distribution** for $\theta^\star$:



$$P(\theta^\star = \theta | \mathcal{H}_t) = \frac{P(\mathcal{H}_t, \theta^\star = \theta)}{P(\mathcal{H}_t)} = \frac{P_\theta(\mathcal{H}_t) P_{\text{prior}}(\theta)}{P(\mathcal{H}_t)} \propto P_\theta(\mathcal{H}_t) P_{\text{prior}}(\theta)$$

In math:

Sample a_t according to $p_t(a) = \int_\theta \; P(\theta|\mathcal{H}_t)\, \mathbb{I}\{a^\star(\theta) = a\} = \mathbb{E}_{\theta \sim P(\cdot \mid \mathcal{H}_t)}[\mathbb{I}\{a^\star(\theta) = a\}]$

Implementation: Sample $\theta_t \sim P(\cdot \mid \mathcal{H}_t)$, and choose $a_t = a^\star(\theta_t)$.

Thompson Sampling in the Gaussian Case

$\theta = (\theta(1), \cdots, \theta(A))$. $\mathcal{H}_t = (a_1, r_1(a_1), \cdots, a_{t-1}, r_{t-1}(a_{t-1}))$

const: const unrelated to θ

$$\Pr(\theta \mid \mathcal{H}_t) \propto P_{prior}(\theta)\, P_\theta(\mathcal{H}_t)$$

$$= \text{const.} \prod_a e^{-\frac{\theta(a)^2}{2}} \cdot \text{const.} \prod_{s=1}^{t-1} e^{-\frac{(\theta(a_s) - r_s(a_s))^2}{2}}$$

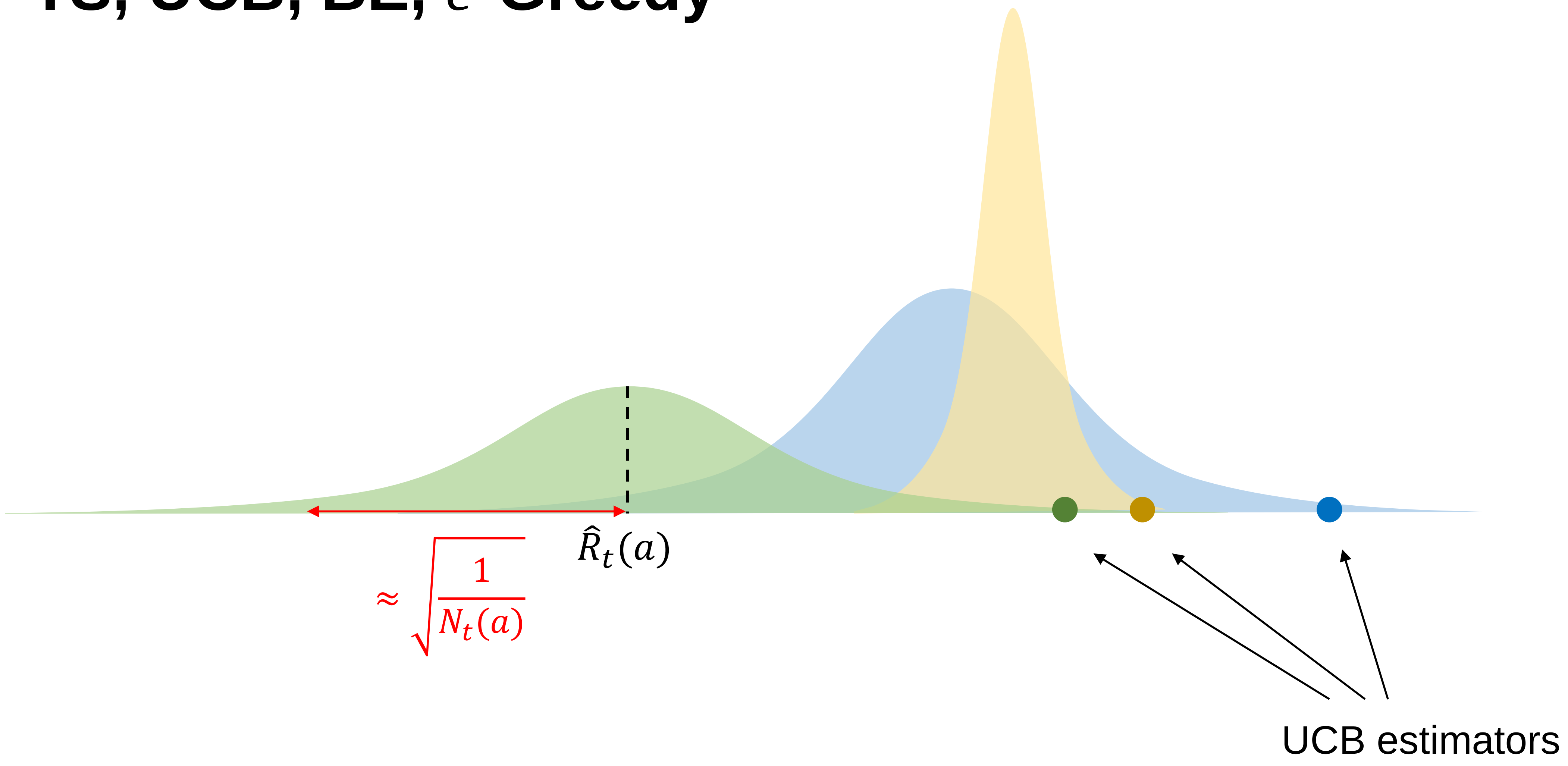
$$= \text{const} \prod_a e^{-\left[\frac{\theta(a)^2}{2} + \sum_{s=1}^{t-1} \mathbb{1}\{a_s = a\} \frac{(\theta(a) - r_s(a))^2}{2}\right]}$$

$$\underbrace{= \text{const} \prod_a e^{-\frac{(N_t(a)+1)(\theta(a) - \hat{R}_t(a))^2}{2}} \cdot \text{const.}}$$

$$\theta \sim \prod_a \mathcal{N}\left(\hat{R}_t(a), \frac{1}{N_t(a)+1}\right)$$

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

TS, UCB, BE, ϵ-Greedy



Mean estimation ($\hat{R}_t(a)$) + different exploration mechanism

More on Thompson Sampling

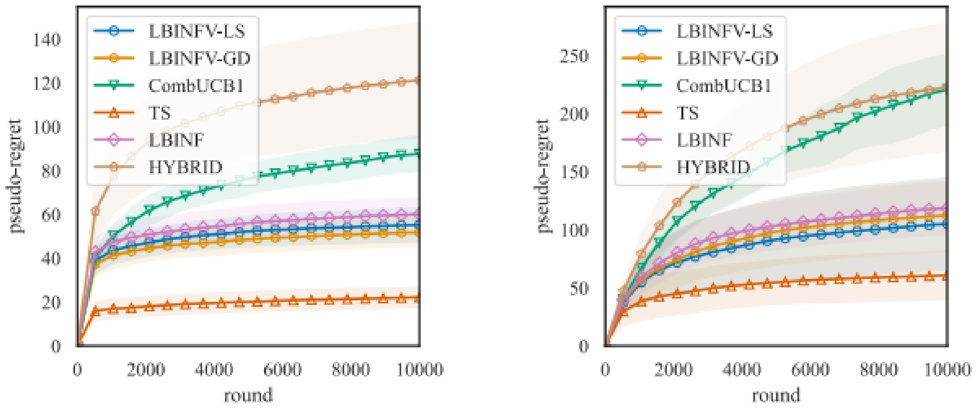
For **Bernoulli** reward, the commonly used prior is the **Beta** prior.

Regret bound analysis for Thompson sampling

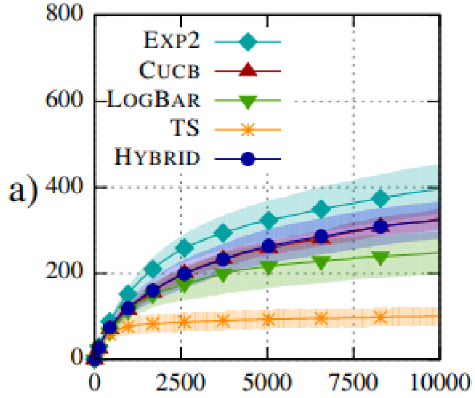
Shipra Agrawal, Navin Goyal. Near-optimal Regret Bounds for Thompson Sampling. 2017.

Daniel Russo and Ben Van Roy. An Information-Theoretic Analysis of Thompson Sampling. 2016.

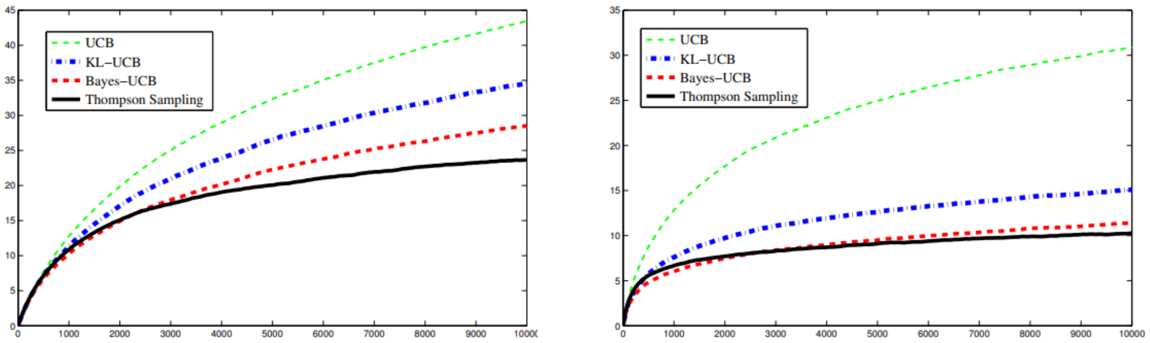
Superior Empirical Performance of TS



Tsuchiya, Ito, Honda. Further Adaptive Best-of-Both-Worlds Algorithm for Combinatorial Semi-Bandits. 2023



Zimmert, Luo, Wei. Beating Stochastic and Adversarial Semi-bandits Optimally and Simultaneously. 2019.



Kaufmann, Korda Munos. Thompson Sampling: An Asymptotically Optimal Finite Time Analysis. 2012.