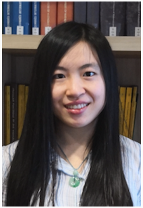
Pure Exploration in Multi-Armed Bandits

Zixin Zhong (University of Alberta)

Vincent Y. F. Tan (National University of Singapore)



National University of Singapore
Tutorial 2 in IJCAI 2022
25 July 2022

Outline

1. **What is multi-armed bandits (MAB)?**
   - Classification of MAB problems
   - Example — Cascading bandits
2. **Explore state-of-the-art findings of pure exploration**
   - BAI: fixed-confidence setting
   - BAI: fixed-budget setting
3. **Summary and discussions**

Outline

1. **What is multi-armed bandits (MAB)?**
2. Explore state-of-the-art findings of pure exploration
3. Summary and discussions

Motivation: data-driven optimization

- Subdomain of reinforcement learning, online learning problem.
- Application:
    - Internet advertisement placement
    - Restaurant recommendation
    - Clinical trials
    - ……

Multi-armed bandit problem (MAB)

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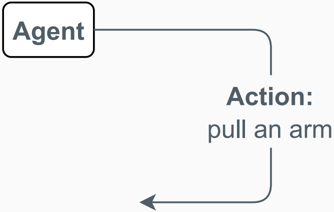
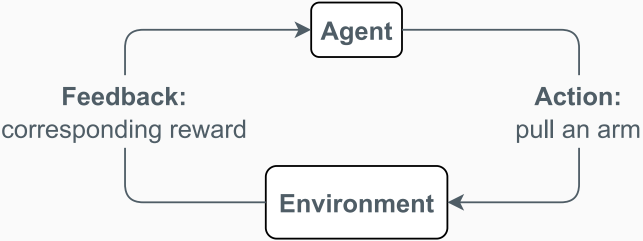


Agent

Action:
pull an arm

Multi-armed bandit problem (MAB)



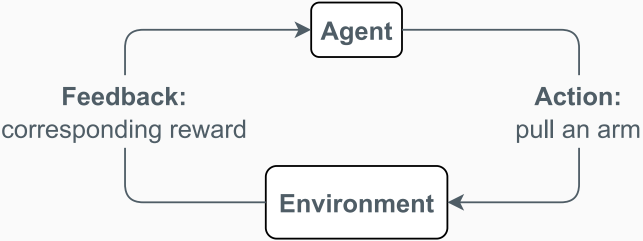
Agent

Feedback:
corresponding reward

Action:
pull an arm

Environment

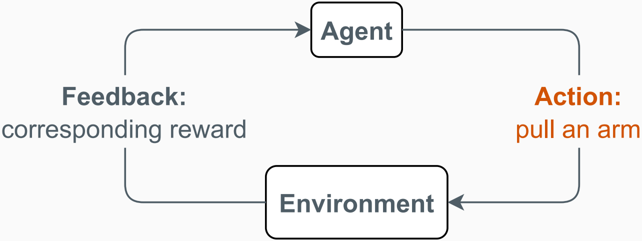
Multi-armed bandit problem (MAB)



Objectives

1. Maximize the cumulative reward over a fixed horizon.
2. Find the best arm (largest expected reward).

Multi-armed Bandit problem (MAB)



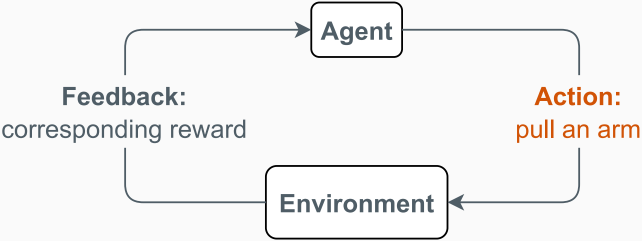
Agent

Feedback:
corresponding reward

Action:
pull an arm

Environment

Multi-armed Bandit problem (MAB)



Agent

Feedback:
corresponding reward

Action:
pull an arm

Environment

Challenge

- Exploitation: to pull "confident" arms to maximize reward.
- Exploration: to pull "unconfident" arms to find better ones.

Outline

1. **What is multi-armed bandits (MAB)?**
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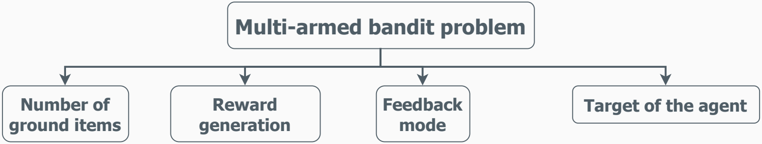
Classification



Multi-armed bandit problem

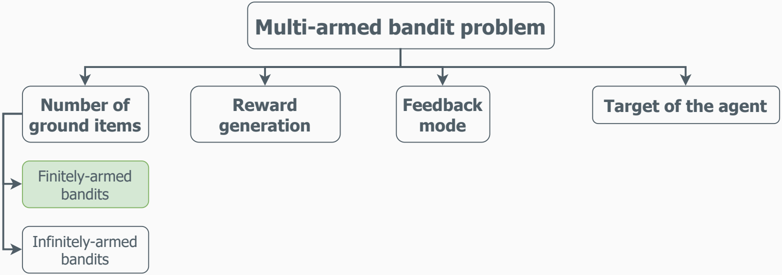
Number of ground items

Reward generation

Feedback mode

Target of the agent

Classification



Multi-armed bandit problem

Number of ground items

Reward generation

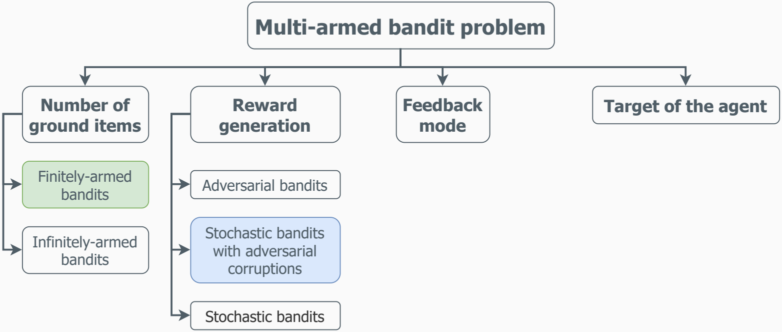
Feedback mode

Target of the agent

Finitely-armed bandits

Infinitely-armed bandits

Classification



Multi-armed bandit problem

Number of ground items

- Finitely-armed bandits
- Infinitely-armed bandits

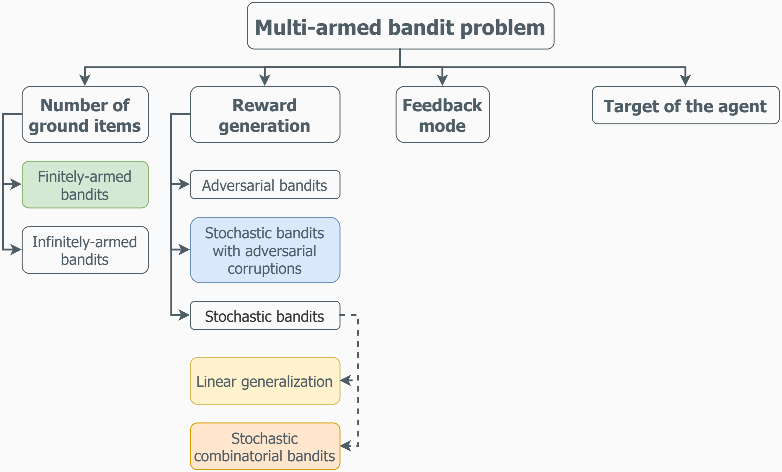
Reward generation

- Adversarial bandits
- Stochastic bandits with adversarial corruptions
- Stochastic bandits

Feedback mode

Target of the agent

Classification



Multi-armed bandit problem

Number of ground items

Finitely-armed bandits

Infinitely-armed bandits

Reward generation

Adversarial bandits

Stochastic bandits with adversarial corruptions

Stochastic bandits

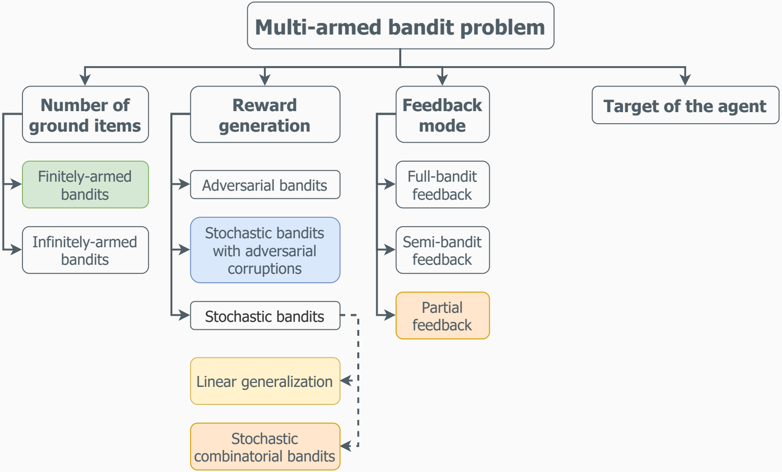
Linear generalization

Stochastic combinatorial bandits

Feedback mode

Target of the agent

Classification



Multi-armed bandit problem

Number of ground items

- Finitely-armed bandits
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Reward generation

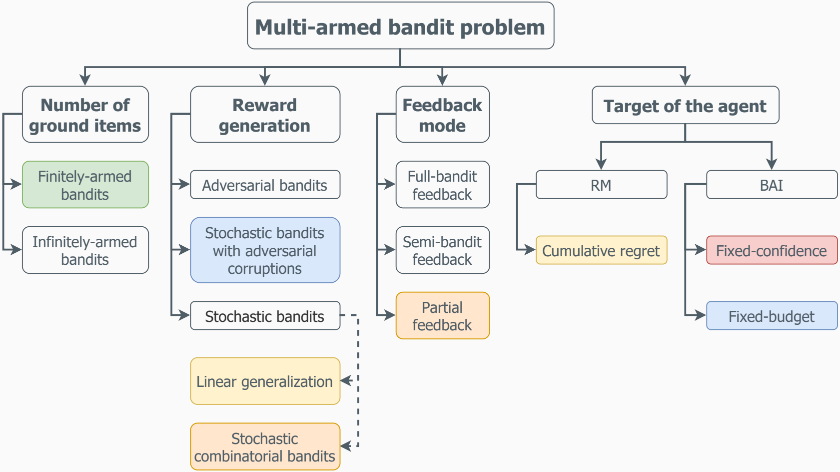
- Adversarial bandits
- Stochastic bandits with adversarial corruptions
- Stochastic bandits
  - Linear generalization
  - Stochastic combinatorial bandits

Feedback mode

- Full-bandit feedback
- Semi-bandit feedback
- Partial feedback

Target of the agent

Classification



Formulation of MAB models

♠ **Ground set** — $\mathcal{S}$ consists of available arms.

♠ **Dynamics** — At each time step $t = 1, 2, \ldots$

1. **Reward** $W_t(i)$ is associated with arm i.
2. Agent **pulls** arm A_t
3. Agent observes the corresponding **feedback** $O_t = f(\{W_t(i) : i \in A_t\})$.

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♠ **Number of arms**

- Finite-armed bandits (Audibert et al., 2009; Agrawal and Goyal, 2012)

  Ground set $\mathcal{S}$ of L arms is indexed by $[L] = \{1, 2, \ldots, L\}$.
- Infinite-armed bandits (Berry et al., 1997)

  Related to the topic of Bayesian optimization

Reward generation

STOCHASTIC BANDITS

- Each arm $i \in [L]$ is associated with an unknown distribution $\nu(i)$, mean $w(i)$, and variance $\sigma^2(i)$.
- $\{W_t(i)\}_{t=1}^T$ is the i.i.d. sequence of rewards associated with arm i during the T time steps.

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♠ Linear generalization (Abe and Long, 1999)

- $w(i) = x(i)^\top \beta$
- Feature vector $x(i) \in \mathbb{R}^d$ is known for each arm i, latent vector $\beta \in \mathbb{R}^d$ is not known.
- Reduces to standard bandits when $x(i) = e_i$, standard basis.

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- Reduces to standard bandits when $x(i) = e_i$, standard basis.

♠ Stochastic combinatorial bandits

- Stardard setting: $|A_t| = 1$.
- Combinatorial setting: $|A_t| \geq 1$.

Feedback mode

- ♠ FULL-BANDIT FEEDBACK

- ♠ SEMI-BANDIT FEEDBACK

- ♠ PARTIAL FEEDBACK

Feedback mode

♠ FULL-BANDIT FEEDBACK

Agent only observes the **sums** of the realizations of all pulled arms (Rejwan and Mansour, 2020; Kuroki et al., 2020).

♠ SEMI-BANDIT FEEDBACK

♠ PARTIAL FEEDBACK

Feedback mode

- ♠ Full-bandit feedback

  Agent only observes the sums of the realizations of all pulled arms (Rejwan and Mansour, 2020; Kuroki et al., 2020).

- ♠ Semi-bandit feedback

  Agent observes realizations of all pulled arms (Mannor and Tsitsiklis, 2004; Kalyanakrishnan et al., 2012).

- ♠ Partial feedback

Feedback mode

♠ FULL-BANDIT FEEDBACK

Agent only observes the sums of the realizations of all pulled arms (Rejwan and Mansour, 2020; Kuroki et al., 2020).

♠ SEMI-BANDIT FEEDBACK

Agent observes realizations of all pulled arms (Mannor and Tsitsiklis, 2004; Kalyanakrishnan et al., 2012).

♠ PARTIAL FEEDBACK

Agent only observes the realizations of a subset of pulled arms (Kveton et al., 2015b; Li et al., 2016).

Reward generation

- ♠ STOCHASTIC BANDITS

Reward generation

- ♠ STOCHASTIC BANDITS
- ♠ STOCHASTIC BANDITS WITH ADVERSARIAL CORRUPTIONS

  (Shen, 2019; Jun et al., 2018)

At each time step $t = 1, \ldots, T$:

1. Stochastic reward $W_t(i) \in [0, 1]$ is i.i.d. drawn for each arm i.

Reward generation

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- ♠ STOCHASTIC BANDITS WITH ADVERSARIAL CORRUPTIONS

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At each time step $t = 1, \ldots, T$:

1. Stochastic reward $W_t(i) \in [0, 1]$ is i.i.d. drawn for each arm i.
2. Agent pulls arm i_t.
3. Adversary observes $\{W_t(i)\}_{i \in [L]}$ as well as i_t, and corrupts $W_t(i_t)$ with c_t:

$$\tilde{W}_t(i_t) = W_t(i_t) + c_t \in [0, 1].$$

   but the norm of $\{c_t\}_{t=1}^{T}$ is suitably constrained.

4. Agent observes the corrupted reward $\tilde{W}_t(i_t)$.

Reward generation

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- ♠ ADVERSARIAL/NON-STOCHASTIC BANDITS

  (Auer et al., 2002b; Cesa-Bianchi and Lugosi, 2006)

  - Rewards $\{W_t(i)\}_{t=1}$ of each arm i are not necessarily drawn independently from the same distribution.

Reward generation

♠ STOCHASTIC BANDITS

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Stochastically constrained adversarial bandits (Zimmert and Seldin, 2021)

- $W_t(i)$ is a r.v. with mean $w_t(i)$, and gaps $\Delta_{i,j} = W_t(i) - W_t(j)$ are fixed.

Target of the agent

♠ Cumulative regret minimization

♠ Simple regret minimization

♠ Pure exploration/best arm identification (BAI)

Fixed-confidence setting

Fixed-budget setting

Target of the agent

♠ CUMULATIVE REGRET MINIMIZATION

Maximize the cumulative reward, i.e.,minimize the regret (the gap between the maximum cumulative reward and the reward obtained by the agent) (Agrawal and Goyal, 2012; Russo and Van Roy, 2014; Lai, 1987).

♠ SIMPLE REGRET MINIMIZATION

♠ PURE EXPLORATION/BEST ARM IDENTIFICATION (BAI)

Fixed-confidence setting

Fixed-budget setting

Target of the agent

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♠ SIMPLE REGRET MINIMIZATION

Maximize the mean reward of the chosen arm by the end of a fixed time horizon T (Carpentier and Valko, 2015).

♠ PURE EXPLORATION/BEST ARM IDENTIFICATION (BAI)

Fixed-confidence setting

Fixed-budget setting

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♠ PURE EXPLORATION/BEST ARM IDENTIFICATION (BAI)

Fixed-confidence setting Given a risk parameter δ, the agent aims to identify the best arm with probability $1 - \delta$ in minimal time steps (Jamieson and Nowak, 2014; Kalyanakrishnan et al., 2012).

Fixed-budget setting

Target of the agent

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Fixed-budget setting Given a budget constraint T, the agent aims to maximize the confidence of the chosen arm by the end of a fixed time horizon T (Auer et al., 2002a; Audibert and Bubeck, 2010; Carpentier and Locatelli, 2016).

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   - Example — Cascading bandits
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Example — Cascading bandits (Kveton et al., 2015a)

♠ Online recommender system

- seek to select a small list of items to the user over time.

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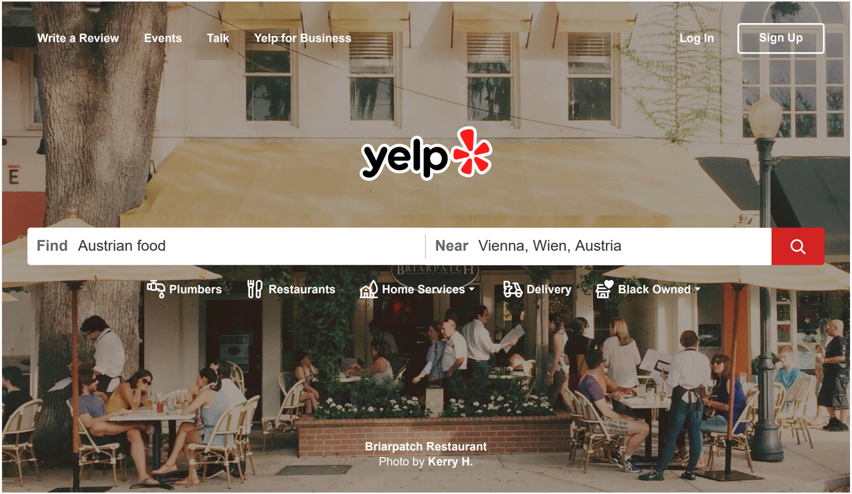
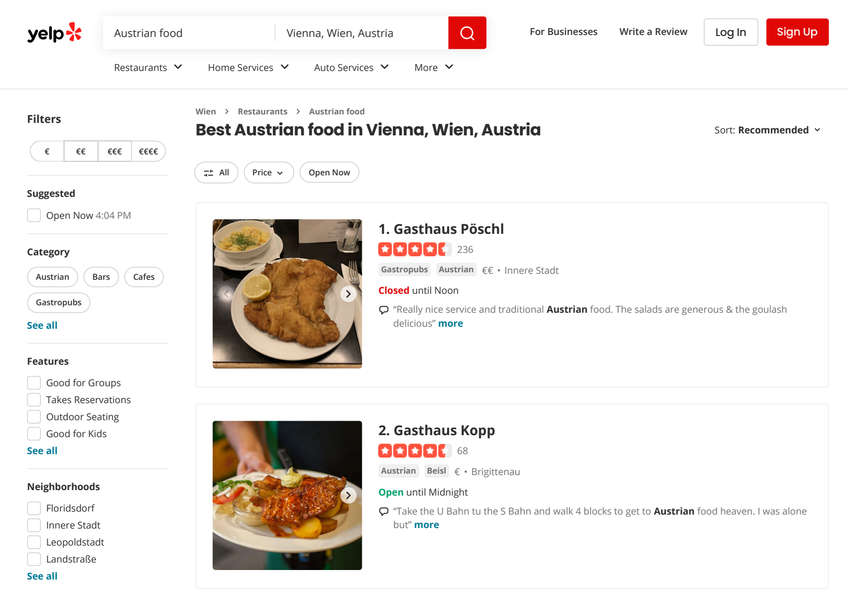


Find Austrian food

Near Vienna, Wien, Austria

Briarpatch Restaurant
Photo by **Kerry H.**

Example — Cascading bandits (Kveton et al., 2015a)



Best Austrian food in Vienna, Wien, Austria

1. Gasthaus Pöschl

★★★★½ 236

Gastropubs Austrian €€ • Innere Stadt

Closed until Noon

"Really nice service and traditional **Austrian** food. The salads are generous & the goulash delicious" **more**

2. Gasthaus Kopp

★★★★½ 68

Austrian Beisl € • Brigittenau

Open until Midnight

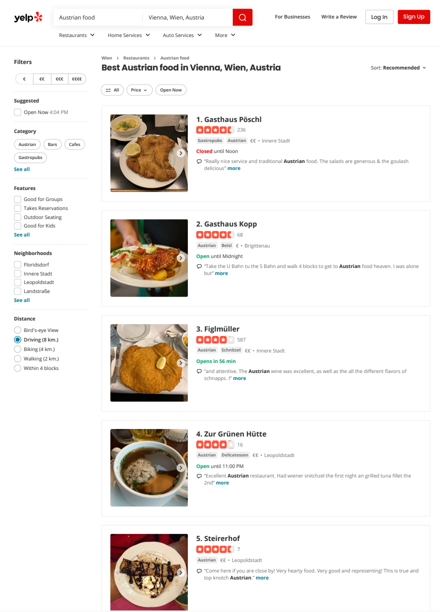
"Take the U Bahn tu the S Bahn and walk 4 blocks to get to **Austrian** food heaven. I was alone but" **more**

Example — Cascading bandits (Kveton et al., 2015a)

♠ Online recommender system

- Seek to select a small list of items to the user over time.
- How to maximize the ‘reward’ over several rounds of recommendation?

  — Regret Minimization (RM)



Filters

€ | €€ | €€€ | €€€€

Suggested

☐ Open Now 4:04 PM

Category

Austrian Bars Cafes Gastropubs

See all

Features

☐ Good for Groups
☐ Takes Reservations
☐ Outdoor Seating
☐ Good for Kids

See all

Neighborhoods

☐ Floridsdorf
☐ Innere Stadt
☐ Leopoldstadt
☐ Landstraße

See all

Distance

○ Bird's-eye View
● Driving (8 km.)
○ Biking (4 km.)
○ Walking (2 km.)
○ Within 4 blocks

Wien › Restaurants › Austrian food

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3. Figlmüller
587
Austrian Schnitzel €€ • Innere Stadt
Opens in 56 min
“and attentive. The **Austrian** wine was excellent, as well as the all the different flavors of schnapps. I” more

4. Zur Grünen Hütte
16
Austrian Delicatessen €€ • Leopoldstadt
Open until 11:00 PM
“Excellent **Austrian** restaurant. Had wiener snitchzel the first night an grilled tuna fillet the 2nd” more

5. Steirerhof
7
Austrian €€ • Leopoldstadt
“Come here if you are close by! Very hearty food. Very good and representing! This is true and top knotch **Austrian**.” more

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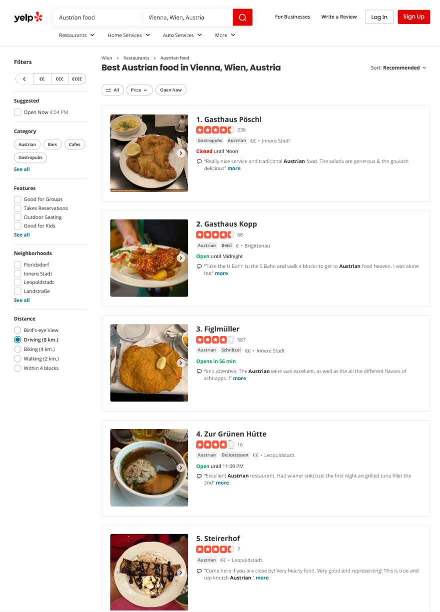
- How to select an attractive list of items after several rounds of recommendation?

  — Pure Exploration/
  Best Arm Identification (BAI)



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Example — Cascading bandits (Kveton et al., 2015a)

Ground set

A finite set of all available arms $[L] := \{1, \ldots, L\}$.

Click probability/weight of item $i \in [L]$

Arm i attracts the user with probability $w(i) \in [0, 1]$.

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Whether arm i is clicked at time t

This is revealed by a random variable $W_t(i) \sim \mathrm{Bern}\,(w(i))$.

- $W_t(i) = 1$ iff the user observes and clicks on i at time t.
- $W_t(i) = 0$ iff the user observes but does not click on i at time t.

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◆ $W_t(i)$'s are only observed for some arms.

Example — Cascading bandits (Kveton et al., 2015a)

For each time step $t = 1, 2, \ldots$

1. The agent selects a list of K arms $S_t := (i_1^t, \ldots, i_K^t) \in [L]^{(K)}$ to the user, where $[L]^{(K)} = \{$all K-permutations of $[L]\}$;

Example — Cascading bandits (Kveton et al., 2015a)

$$L = 9$$

For each time step $t = 1, 2, \ldots$

1. The agent selects a list of K arms $S_t := (i_1^t, \ldots, i_K^t) \in [L]^{(K)}$ to the user, where $[L]^{(K)} = \{$all K-permutations of $[L]\}$;

Example — Cascading bandits (Kveton et al., 2015a)

Recommendation

For each time step $t = 1, 2, \dots$

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Example — Cascading bandits (Kveton et al., 2015a)

Recommendation

$$K = 5$$

For each time step $t = 1, 2, \dots$

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Example — Cascading bandits (Kveton et al., 2015a)

Recommendation

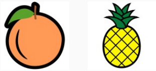
Attractiveness
$W_t(i)$

For each time step $t = 1, 2, \ldots$

1. The agent selects a list of K arms $S_t := (i_1^t, \ldots, i_K^t) \in [L]^{(K)}$ to the user, where $[L]^{(K)} = \{$all K-permutations of $[L]\}$;
2. The user examines the arms from i_1^t to i_K^t:
    - If she is attracted by an item, clicks on it;
    - If not, she skips to the next item and checks if it is attractive;
    - Process stops when she clicks on one item or when she comes to the end of the list.

Example — Cascading bandits (Kveton et al., 2015a)

Recommendation



Attractiveness ×

$W_t(i)$ 0

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Example — Cascading bandits (Kveton et al., 2015a)

Recommendation

Attractiveness	×	×	
$W_t(i)$	0	0	

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Recommendation				
Attractiveness	×	×	×	
$W_t(i)$	0	0	0	

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Recommendation				
Attractiveness	$\times$	$\times$	$\times$	$\surd$
$W_t(i)$	0	0	0	1

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Example — Cascading bandits (Kveton et al., 2015a)

Recommendation					
Attractiveness	$\times$	$\times$	$\times$	$\surd$	$?$
$W_t(i)$	0	0	0	1	$?$

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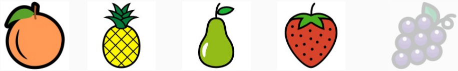
Recommendation					
Attractiveness	×	×	×	√	?
$W_t(i)$	0	0	0	1	?

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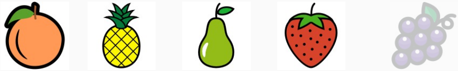
♠ **Combinatorial** bandits ♡ **Partial** feedback

Example — Cascading bandits (Kveton et al., 2015a)

Recommendation



Attractiveness	×	×	×	√	?
$W_t(i)$	0	0	0	1	?

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♠ **Combinatorial** bandits ♡ **Partial** feedback ♣ **Standard** setting & **Linear** generalization

Outline

1. What is multi-armed bandits (MAB)?

2. **Explore state-of-the-art findings of pure exploration**

3. Summary and discussions

Pure exploration/BAI settings

Fixed-confidence setting

- Given a risk parameter δ, the agent aims to identify the best arm with probability $1 - \delta$ in minimal time steps.
  (Jamieson and Nowak, 2014; Kalyanakrishnan et al., 2012)

Fixed-budget setting

- Given a budget constraint T, the agent aims to maximize the confidence of the chosen arm by the end of a fixed time horizon T.
  (Auer et al., 2002a; Audibert and Bubeck, 2010; Carpentier and Locatelli, 2016)

Pure exploration in stochastic bandits

- Ground set $\mathcal{S} = [L]$ consists of L available arms.
- Each arm $i \in [L]$ is associated with an unknown distribution $\nu(i)$, mean $w(i)$, and variance $\sigma^2(i)$.
- $\{W_t(i)\}_{t=1}^T$ is the i.i.d. sequence of rewards associated with arm i during the T time steps.

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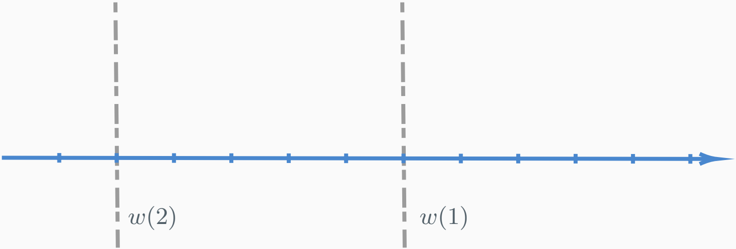

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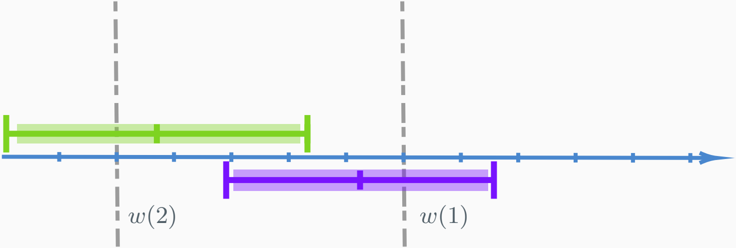

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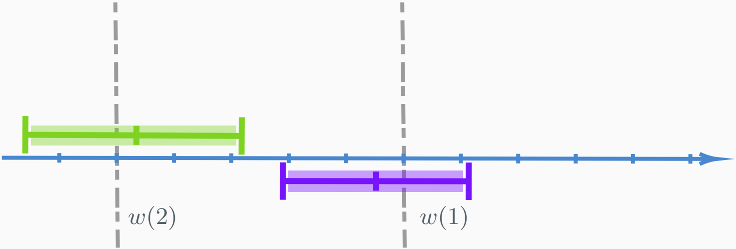

Pure exploration in stochastic bandits

- Optimal arm

$$1 = i^* = \arg\max_{i \in [L]} w(i)$$

  - Without loss of generality, assume

$$w(1) > w(2) \geq w(3) \geq \ldots \geq w(L).$$

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- Hardness parameters

$$H_1 = \sum_{i=1}^{L} \frac{1}{\Delta_i^2}, \quad H_2 = \max_{i \in [L]} \frac{i}{\Delta_i^2}.$$

Concentration inequalities: can we estimate $w(i)$ well?

Theorem 2.1 (Standard multiplicative variant of the Chernoff-Hoeffding bound; Dubhashi and Panconesi (2009), Theorem 1.1)

Suppose that $X_1, \ldots, X_T$ *are independent* $[0,1]$*-valued random variables, and let* $X = \sum_{t=1}^{T} X_t$*. Then for any* $\varepsilon \in (0,1)$*,*

$$\Pr(X - \mathbb{E}[X] \geq \varepsilon \mathbb{E}[X]) \leq \exp\left(-\frac{\varepsilon^2}{3}\mathbb{E}X\right),$$

$$\Pr(X - \mathbb{E}[X] \leq -\varepsilon \mathbb{E}[X]) \leq \exp\left(-\frac{\varepsilon^2}{3}\mathbb{E}X\right).$$

BAI algorithm

A deterministic and non-anticipatory online algorithm consists in a triple $\pi := ((\pi_t)_t, \mathcal{T}^\pi, \phi^\pi)$

- sampling rule $(\pi_t)_t$: which arm S_t^π to pull at time step t
- stopping rule $\mathcal{T}^\pi$: when to stop
- recommendation rule ϕ^π: which arm $\hat{S}^\pi$ to choose eventually

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$\mathcal{T}^\pi$

- Fixed-confidence setting: Time complexity of π (to minimize).
- Fixed-budget setting: $\mathcal{T}^\pi = \mathcal{T}$ (fixed).

Outline

1. What is multi-armed bandits (MAB)?

2. **Explore state-of-the-art findings of pure exploration**
    - BAI: fixed-confidence setting
    - BAI: fixed-budget setting

3. Summary and discussions

BAI: fixed-confidence

- δ-PAC algorithm: find the optimal arm with probability at least $1 - \delta$

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Theoretical study

▲ Propose a δ-PAC algorithm and upper bound its time complexity

▼ Derive a lower bound on the time complexity of any δ-PAC algorithm

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Simple pure exploration in stochastic bandits

- to identify the best arm with the largest mean:

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♠ Successive elimination

Successive Elimination, Median Elimination (Even-Dar et al., 2002)

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♠ Track optimal allocation

Track & Stop (Garivier and Kaufmann, 2016)

SUCCESSIVE ELIMINATION(δ) **(Even-Dar et al., 2002)**

Algorithm 1: SUCCESSIVE ELIMINATION(δ) (Even-Dar et al., 2002)

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Let $\hat{w}_{\max}^t = \max_{i \in [L]} \hat{w}_i^t$ and confidence radius $\alpha_t = \sqrt{\frac{\log(cLt^2/\delta)}{t}}$.
For each arm $i \in S$ such that $\hat{w}_{\max}^t - \hat{w}_i^t \geq 2\alpha_t$, set $S = S \setminus \{i\}$.
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6: For each arm $i \in S$ such that $\hat{w}_{\max}^t - \hat{w}_i^t \geq 2\alpha_t$, set $S = S \setminus \{i\}$.
7: $t = t + 1$.
8: If $|S| > 1$, the Go to Step 4, Else output $S$.
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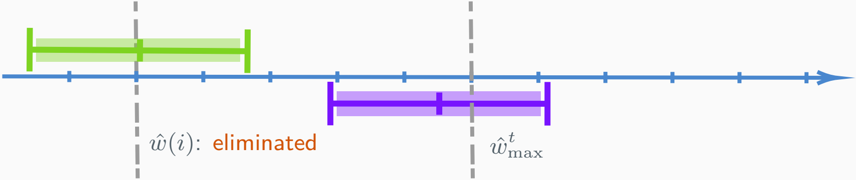

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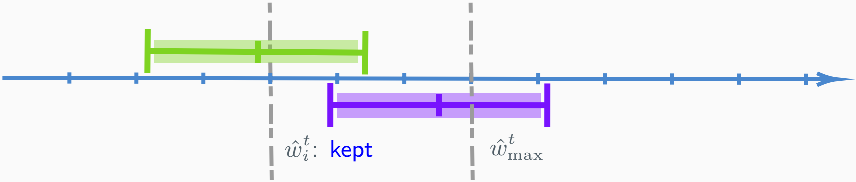

Successive Elimination(δ) (Even-Dar et al., 2002)

Step 1. Concentration inequality:

$$\Pr(|\hat{w}_i^t - w(i)| > \alpha_t, \forall i \in S, \forall t) \leq \delta.$$

SUCCESSIVE ELIMINATION(δ) **(Even-Dar et al., 2002)**

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Step 2. Assume $\{|\hat{w}_i^t - w(i)| > \alpha_t, \forall i, \forall t\}$ holds. Recall that we eliminate arm i when $\hat{w}_{\max}^t - \hat{w}_i^t \ge 2\alpha_t$. Since

$$\hat{w}_{\max}^t - \hat{w}_i^t \ge \hat{w}_1^t - \hat{w}_i^t \ge w(1) - \alpha_t - (w(i) + \alpha_t) = w(1) - w(i) - 2\alpha_2,$$

we eliminate a suboptimal arm $i \neq 1$ when

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Step 3. When each arm has been sampled for

$$t_i = O\left(\frac{\log(L/(\delta\Delta_i))}{\Delta_i^2}\right)$$

times, we have $\alpha_t \leq \Delta_i/4$ and arm i will be eliminated.

Hence, the time complexity would be

$$t_2 + \sum_{i=2}^{L} t_i = O\left(\sum_{t=1}^{L} \frac{\log(L/(\delta\Delta_i))}{\Delta_i^2}\right) = \tilde{O}(H_1), \quad H_1 = \sum_{i=1}^{L} \frac{1}{\Delta_i^2} \text{ (hardness)}.$$

MEDIAN ELIMINATION(ϵ, δ) **(Even-Dar et al., 2002)**

- With probability $1 - \delta$, identify an ϵ-optimal arm i: $w(i) \geq \max_{j \in [L]} w(j) - \epsilon$.

Algorithm 2: MEDIAN ELIMINATION(ϵ, δ) (Even-Dar et al., 2002)

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Algorithm 2: MEDIAN ELIMINATION(ϵ, δ) (Even-Dar et al., 2002)

```
1: Input: Survival set $S = [L]$. Set $\epsilon_1 = \epsilon/4$, $\delta_1 = \delta/2$, $\ell = 1$.
2: Sample each arm $i \in S$ for $\frac{1}{(\epsilon_\ell/2)^2} \log(3/\delta_\ell)$ times, and let $\hat{w}_i^t$ denote its average reward.
```

MEDIAN ELIMINATION(ϵ, δ) **(Even-Dar et al., 2002)**

♠ With probability $1-\delta$, identify an ϵ-optimal arm i: $w(i) \geq \max_{j \in [L]} w(j) - \epsilon$.

Algorithm 2: MEDIAN ELIMINATION(ϵ, δ) (Even-Dar et al., 2002)

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1: Input: Survival set $S = [L]$. Set $\epsilon_1 = \epsilon/4$, $\delta_1 = \delta/2$, $\ell = 1$.
2: Sample each arm $i \in S$ for $\frac{1}{(\epsilon_\ell/2)^2} \log(3/\delta_\ell)$ times, and let $\hat{w}_i^t$ denote its average reward.
3: Find the median of $\hat{w}_i^\ell$, denoted by $m_\ell :=$ median$\big(\{\hat{w}_i^\ell : i \in S_\ell\}\big)$.
4: Let $S_{\ell+1} = S_\ell \setminus \{i : \hat{w}_i^\ell < m_\ell\}$.
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6: If $|S| = 1$, Then output $S$.
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Applying the same concentration inequality, we can show the time complexity of MEDIAN ELIMINATION(ϵ, δ) is

$$O\left(\frac{L \log(1/\delta)}{\epsilon^2}\right).$$

Lower bound (Garivier and Kaufmann, 2016)

For any δ-PAC algorithm and any bandit instance μ,

$$\mathbb{E}_{\mu}[\tau_{\delta}] \geq T^{*}(\mu) \log\left(\frac{4}{\delta}\right)$$

where

$$T^{*}(\mu)^{-1} := \sup_{w \in \Sigma_L} \inf_{\lambda \in \mathrm{Alt}(\mu)} \left(\sum_{i=1}^{L} w_i d(\mu_i, \lambda_i) \right).$$

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- For any instance $\mu = (\mu_1, \ldots, \mu_L) \in \mathcal{S}$
  - $\mathcal{S} = \{(\mu_1, \ldots, \mu_L) : \exists i^*(\mu) \in [L] \ s.t. \ \mu_{i^*(\mu)} > \mu_i \quad \forall i \neq i^*(\mu)\}$
  - Unique optimal arm: $i^*(\mu) = \arg\max_{i \in [L]} \mu_i$
  - "Alternative set": $\mathrm{Alt}(\mu) := \{\lambda \in \mathcal{S} : i^*(\lambda) \neq i^*(\mu)\}$
- Set of probability distributions on $[L]$

$$\Sigma_L = \left\{ (w_1, \ldots, w_L) \in (0,1]^L : \sum_{i=1}^{L} w_i = 1 \right\}$$

Proof strategy of lower bound

- Let $\lambda \in \mathrm{Alt}(\mu)$ and define event $E = \{\tau_\delta < \infty, i_{\mathrm{out}}(\mu) \neq i^*(\lambda)\} \in \mathcal{F}_{\tau_\delta}$. Then

$$
\begin{aligned}
2\delta &\geq \mathbb{P}_\mu(\tau_\delta < \infty \text{ and } i_{\mathrm{out}}(\mu) \neq i^*(\mu)) + \mathbb{P}_\mu(\tau_\delta < \infty \text{ and } i_{\mathrm{out}}(\mu) \neq i^*(\lambda)) \\
&\geq \mathbb{P}_\mu(E^c) + \mathbb{P}_\lambda(E) \\
&\geq \frac{1}{2} \exp\left(- \sum_{i=1}^{L} \mathbb{E}_\mu[T_i(\tau_\delta)] D(\mu_i, \lambda_i) \right). \qquad \text{Bretagnolle–Huber inequality}
\end{aligned}
$$

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$$\begin{aligned} \frac{\mathbb{E}_\mu[\tau_\delta]}{T^*(\mu)} &= \mathbb{E}_\mu[\tau_\delta] \sup_{w \in \Sigma_L} \inf_{\lambda \in \mathrm{Alt}(\mu)} \sum_{i=1}^{L} w_i D(\mu_i, \lambda_i) \\ &\geq \cancel{\mathbb{E}_\mu[\tau_\delta]} \inf_{\lambda \in \mathrm{Alt}(\mu)} \sum_{i=1}^{L} \frac{\mathbb{E}_\mu[T_i(\tau_\delta)]}{\cancel{\mathbb{E}_\mu[\tau_\delta]}} D(\mu_i, \lambda_i) \\ &= \inf_{\lambda \in \mathrm{Alt}(\mu)} \sum_{i=1}^{L} \mathbb{E}_\mu[T_i(\tau_\delta)] D(\mu_i, \lambda_i) \geq \log \frac{4}{\delta}. \end{aligned}$$

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TRACK & STOP algorithm (Garivier and Kaufmann, 2016)

We thus have the asymptotic lower bound on the time complexity:

$$\liminf_{\delta \to 0} \frac{\mathbb{E}_\mu[\tau_\delta]}{\log(1/\delta)} \geq T^*(\mu).$$

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A matching upper bound can be achieved by TRACK & STOP

$$\mathbb{P}_\mu\left(\limsup_{\delta \to 0} \frac{\tau_\delta}{\log(1/\delta)} \leq T^*(\mu) \right) = 1,$$

or

$$\limsup_{\delta \to 0} \frac{\mathbb{E}_\mu[\tau_\delta]}{\log(1/\delta)} \leq T^*(\mu).$$

TRACK & STOP algorithm (Garivier and Kaufmann, 2016)

Algorithm 3: TRACK & STOP (Garivier and Kaufmann, 2016)

```
Let $N_i(t) = \sum_{u=1}^{t} 1\{S_u = i\}$ be the number of pulls of arm $i$,
    $\hat{\mu}_i(t) = \frac{1}{N_i(t)} \sum_{u=1}^{t} W_t(i) 1\{S_u = i\}$ be the empirical mean of arm $i$.
Set $\hat{\mu}(t) = (\hat{\mu}_1(t), \hat{\mu}_2(t), \ldots, \hat{\mu}_L(t))$.
Sample each arm once and update $t = L$, $N_i(L)$, $\hat{\mu}_i(L)$.
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Set $\hat{\mu}(t) = (\hat{\mu}_1(t), \hat{\mu}_2(t), \ldots, \hat{\mu}_L(t))$.
Sample each arm once and update $t = L$, $N_i(L)$, $\hat{\mu}_i(L)$.
while Stopping condition (Generalized Likelihood Ratio statistic) is not satisfied do
    Sample arm $S_{t+1}$ by C-Tracking/D-Tracking rule.
    Let $t = t + 1$, and update $N_i(t)$, $\hat{\mu}_i(t)$.
end while
Output $\hat{i} = \arg\max_{i \in [L]} \hat{\mu}_i(t)$.
```

TRACK & STOP (Garivier and Kaufmann, 2016)

Sampling rule

C-Tracking: $S_{t+1} \in \arg\max_{i \in [L]} \sum_{\tau=0}^{t} w_i^{\epsilon_\tau}(\hat{\mu}(\tau)) - N_i(t)$

D-Tracking: $S_{t+1} \in \begin{cases} \arg\min_{i \in U_t} N_i(t) & \text{if } U_t \neq \emptyset \quad \text{(forced exploration)} \\ \arg\max_{i \in [L]} t w_i^{\epsilon_t}(\hat{\mu}(t)) - N_i(t) & \text{else} \quad \text{(directed tracking)} \end{cases}$

Track & Stop (Garivier and Kaufmann, 2016)

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$$w^*(\mu) = \arg\max_{w\in\Sigma_L} \inf_{\lambda\in\mathrm{Alt}(\mu)} \left(\sum_{i=1}^{L} w_i d(w_i, \lambda_i) \right),$$

- Proportion of arm draws of any strategy matches the lower bound

$\epsilon_t = (L^2 + t)^{-1/2}/2$,

$w^\epsilon(\mu)$: L^∞ projection of $w^*(\mu)$ onto $\Sigma_L^{(\epsilon)} = \left\{ (w_1, \ldots, w_L) \in [\epsilon, 1]^L : \sum_{i=1}^{L} = 1 \right\}$

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Outline

1. What is multi-armed bandits (MAB)?

2. **Explore state-of-the-art findings of pure exploration**
   - BAI: fixed-confidence setting
   - BAI: fixed-budget setting

3. Summary and discussions

BAI: fixed-budget

Theoretical study

▲ Propose a BAI algorithm in a fixed time horizon and upper bound its failure probability

▼ Derive a lower bound on the failure probability of any algorithm

- Evaluate theoretical findings with experiments

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Simple pure exploration in stochastic bandits

- to identify the best arm with the largest mean: $i^* = \arg\max_{i \in [L]} w(i)$

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♠ UCB-based

$\mathrm{UCB\text{-}E}(a)$ (Audibert and Bubeck, 2010)

♠ Successive elimination

Sequential Halving (Karnin et al., 2013)

UCB-E(a) (Audibert and Bubeck, 2010)

Algorithm 4: UCB-E(a) (Audibert and Bubeck, 2010)

```
Input: time budget $T$, size of ground set of items $L$, parameter $a$.
For all $i \in [L]$, compute $N_{i,0}$, $\hat{w}_{i,0}$, $C_{i,0}$, $U_{i,0}$:
    $$N_{i,t} = \sum_{u=1}^{t} 1\{i_u = i\}, \ \hat{w}_{i,t} = \frac{1}{N_{i,t}} \sum_{u=1}^{t} W_{i,t} \cdot 1\{i_u = i\},$$
    $$C_{i,t} = \sqrt{\frac{a}{t}} \text{ if } t \geq 1, \qquad C_{i,0} = +\infty, \qquad U_{i,t} = \hat{g}_{i,t} + C_{i,t}.$$
for $t = 1, \ldots, T$ do
    Pull item $i_t = \arg\max_{i \in [L]} U_{i,t-1}$.
    Update $N_{i_t,t}$, $\hat{w}_{i_t,t}$, $C_{i,t}$, and $U_{i,t}$ for all $i$.
end for
Output $i_{\text{out}} = \arg\max_{i \in [L]} \hat{w}_{i,T}$.
```

UCB-E(a) (Audibert and Bubeck, 2010)

Step 1: Concentration. Let $\mathcal{E}_i := \{\forall t \geq L, |\hat{w}_{i,t} - w(i)| \leq C_{i,t}/5\}$ for all $i \in [L]$. We apply concentration inequality to show that

$$\Pr\left(\bigcap_{i=1}^{L} \mathcal{E}_i\right) \geq 1 - 2TL\exp\left(-\frac{2a}{25}\right).$$

In the following, we prove that conditioned on the event $\bigcap_{i=1}^{L} \mathcal{E}_i$, we have $i_{\mathrm{out}} = 1$, which concludes the proof.

We assume $\bigcap_{i=1}^{L} \mathcal{E}_i$ holds from now on. Since i_{out} is the item with the largest empirical mean, for all $i \neq i_{\mathrm{out}}$, we have

$$\hat{w}_{i_{\mathrm{out}},T} \geq \hat{w}_{i,t}, \quad \hat{w}_{i_{\mathrm{out}},T} \geq w(i_{\mathrm{out}}) - C_{i_{\mathrm{out}},T}/5, \quad w(i) + C_{i,T}/5 \geq \hat{w}_{i,t}.$$

Consequently, to show $i_{\mathrm{out}} = 1$, it is sufficient to show that

$$\frac{C_{i,T}}{5} \leq \frac{\Delta_i}{2} \;\Leftrightarrow\; N_{it} \geq \frac{4}{25}\frac{a}{\Delta_i^2} \quad \forall i \in [L]. \tag{1}$$

$\mathrm{UCB\text{-}E}(a)$ (Audibert and Bubeck, 2010)

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Step 2: Upper bound $N_{i,T}$ $(i \neq 1)$. To begin with, we prove by induction that

$$N_{i,t} \leq \frac{36}{25}\frac{a}{\Delta_i^2} \quad \forall\, i \neq 1. \tag{2}$$

$\mathrm{UCB\text{-}E}(a)$ (Audibert and Bubeck, 2010)

Step 3: Lower bound $N_{i,T}$ $(i \neq 1)$. Next, we again prove by induction that

$$N_{i,t} \geq \frac{4}{25} \min\left\{ \frac{a}{\Delta_i^2}, \frac{25}{36}(N_{1,t} - 1) \right\} \quad \forall i \neq 1. \tag{3}$$

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Step 4: Lower bound on $N_{1,T}$. Recall that we want to show (1). (i) To show (1) holds for all $i \neq 1$, (3) indicates that it is sufficient to show that

$$\frac{25}{36}(N_{1,t} - 1) \geq \frac{a}{\Delta_i^2} \quad \forall i \neq 1.$$

(ii) In order to show (1) holds for all $i = 1$, we apply (2), $t = \sum_{i=1}^{L} N_{i,t}$ and

$$\frac{36}{25} H_1 a \leq T - L \ \Leftrightarrow a \leq \frac{25(T-L)}{36 H_1}, \quad H_1 = \sum_{i=1}^{L} \frac{1}{\Delta_i^2}.$$

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Step 5: Conclusion. The failure probability is

$$2TL \exp\left(-\frac{2a}{25}\right) \quad \forall\, a \leq \frac{25(T-L)}{36H_1}$$

and achieves the minimum,

$$2TL \exp\left(-\frac{T-L}{18H_1}\right) \quad \text{when } a = \frac{25(T-L)}{36H_1}.$$

$\mathrm{UCB\text{-}E}(a)$ (Audibert and Bubeck, 2010)

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and achieves the minimum, however, requiring prior knowledge: hardness H_1

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SEQUANTIAL HALVING (SH) **(Karnin et al., 2013)**

Algorithm 5: SEQUANTIAL HALVING (SH) (Karnin et al., 2013)

```
Input: time budget $T$, size of ground set $L$.
Set $M = \lceil \log_2 L \rceil$, $N = \lfloor T/M \rfloor$, $T_0 = 0$, $A_0 = [L]$.
```

SEQUANTIAL HALVING (SH) **(Karnin et al., 2013)**

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```
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Set $M = \lceil \log_2 L \rceil$, $N = \lfloor T/M \rfloor$, $T_0 = 0$, $A_0 = [L]$.
```

M : number of phases

N : length of each phase

T_m : last time step of phase m

A_m : active set after phase m

SEQUANTIAL HALVING (SH) **(Karnin et al., 2013)**

Algorithm 5: SEQUANTIAL HALVING (SH) (Karnin et al., 2013)

```
Input: time budget $T$, size of ground set $L$.
Set $M = \lceil \log_2 L \rceil$, $N = \lfloor T/M \rfloor$, $T_0 = 0$, $A_0 = [L]$.
for phase $m = 1, 2, \ldots, M$ do
    Set $T_m = T_{m-1} + N, q_m = 1/|A_{m-1}|, n_m = \lfloor q_m N \rfloor$.
    for $t = T_{m-1} + 1, \ldots, T_m$ do
        Pull $i \in A_{m-1}$ with for $n_m$ times in order and observe $W_t(i)$.
    end for
```

SEQUANTIAL HALVING (SH) **(Karnin et al., 2013)**

Algorithm 5: SEQUANTIAL HALVING (SH) (Karnin et al., 2013)

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    end for
    For all $i \in A_{m-1}$, set
    $S_m(i) = \sum_{t=T_{m-1}+1}^{T_m} W_t(i_t) \cdot \mathbb{I}\{i_t = i\},\ \hat{w}_m(i) = \frac{S_m(i)}{n_m}$.
    Let $A_m$ contain the $\lceil L/2^m \rceil$ items with the highest $\hat{w}_m(i)$'s in $A_{m-1}$.
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    Let $A_m$ contain the $\lceil L/2^m \rceil$ items with the highest $\hat{w}_m(i)$'s in $A_{m-1}$.
end for
Output the single item $i_{\text{out}} \in A_M$.
```

Sequantial Halving (SH) (Karnin et al., 2013)

Step 1: Assume that the best arm was not eliminated prior to phase m. Then

$$\Pr(\hat{w}_m(1) < \hat{w}_m(i)) \leq \exp\left(-\frac{1}{2}n_m\Delta_i^2\right) \quad \forall\, i \in S_m \setminus \{1\}.$$

Step 2: The probability that the best arm is eliminated in phase m is at most

$$3\exp\left(-\frac{T}{8\log_2 L}\cdot\frac{\Delta_{i_m}^2}{i_m}\right)$$

where $i_m = L/2^{m+2}$.

Step 3: The failure probability can be bounded as follows:

$$\begin{aligned} 3\sum_{m=1}^{\log_2 L}\exp\left(-\frac{T}{8\log_2 L}\cdot\frac{\Delta_{i_m}^2}{i_m}\right) &\leq 3\sum_{m=1}^{\log_2 L}\exp\left(-\frac{T}{8\log_2 L}\cdot\frac{1}{\max_i i\Delta_i^{-2}}\right) \\ &= O\left(\log_2 L\exp\left(-\frac{T}{8H_2\log_2 L}\right)\right) \end{aligned}$$

when the hardness is measured by

$$H_2 = \max_{i\in[L]}\frac{i}{\Delta_i^2}.$$

BAI: fixed-budget

Algorithm/Instance	Reference	Failure probability e_T
$\text{UCB-E}\left(\frac{25(T-L)}{36H_1}\right)$	Audibert and Bubeck (2010)	$2TL\exp\left(-\frac{T-L}{18H_1}\right)$
SR	Audibert and Bubeck (2010)	$L(L-1)\exp\left(-\frac{T-L}{(1/2+\sum_{i=2}^{L}1/i)H_2}\right)$
$\textsc{UGapEb}\left(\frac{T-L}{16H_2}\right)$	Gabillon et al. (2012)	$2TL\exp\left(-\frac{T-L}{8H_2}\right)$
SAR	Bubeck et al. (2013)	$2L^2\exp\left(-\frac{T-L}{8(1/2+\sum_{i=2}^{L}1/i)H_2}\right)$
SH	Karnin et al. (2013)	$3\log_2 L\cdot\exp\left(-\frac{T}{8H_1\log_2 L}\right)$
$\text{NSE}(p)$	Shahrampour et al. (2017)	$(L-1)\exp\left(-\frac{2(T-L)}{H_p'C_p}\right)$
Stochastic Bandits	Carpentier and Locatelli (2016)	$\frac{1}{6}\exp\left(-\frac{400T}{H_2\log L}\right)$ (Lower Bound)

Shahrampour et al. (2017): $H_p' := \max_{i\neq 1}\frac{i^p}{\Delta_i^2}, \quad C_p := 2^{-p}+\sum_{i=2}^{L} i^{-p}\ \forall p>0.$

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- $H_2 \le H_1 \le H_2\log(2L)$ (Audibert and Bubeck, 2010)
- Whether SH or $\mathrm{NSE}(p)$ performs better depends on the instance, and SH does not involve a tunable parameter

BAI: fixed-budget + corruptions (Zhong et al., 2021)

STOCHASTIC BANDITS

- Each arm $i \in [L]$ is associated with an unknown distribution $\nu(i)$, mean $w(i)$, and variance $\sigma(i)^2$.
- $\{W_t(i)\}_{t=1}^{T}$ is the i.i.d. sequence of rewards associated with arm i during the T time steps.

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⇒ STOCHASTIC BANDITS WITH ADVERSARIAL CORRUPTIONS

▲ Propose algorithms with near-optimal performance guarantees

▼ Demonstrate (near-)optimality by designing an appropriate corruption strategy

Case 1: Biases and Contaminations in Clinical Trials

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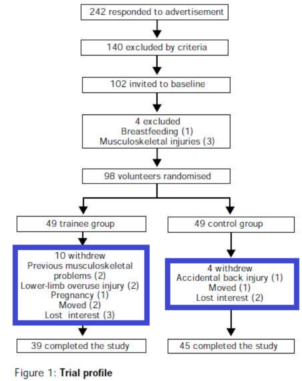

Figure 1: Loss-to-follow-up, boxed in blue.

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Case 2: Fake Users in Online Recommendation Systems

- Paid reviews:
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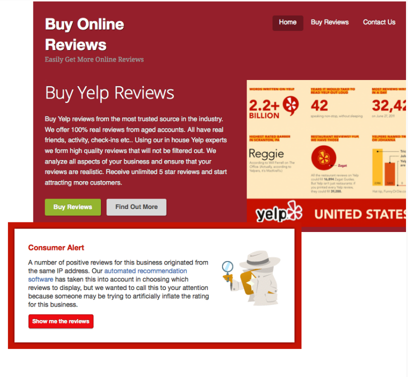

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Consumer Alert

A number of positive reviews for this business originated from the same IP address. Our automated recommendation software has taken this into account in choosing which reviews to display, but we wanted to call this to your attention because someone may be trying to artificially inflate the rating for this business.

Figure 2: Buying fake reviews, and warnings about fake reviews.

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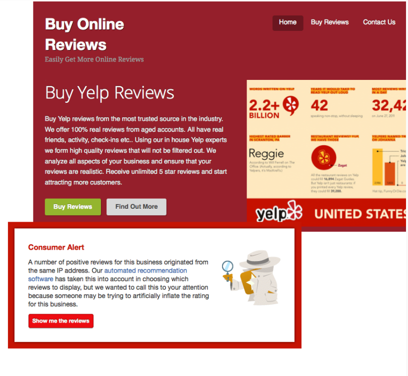

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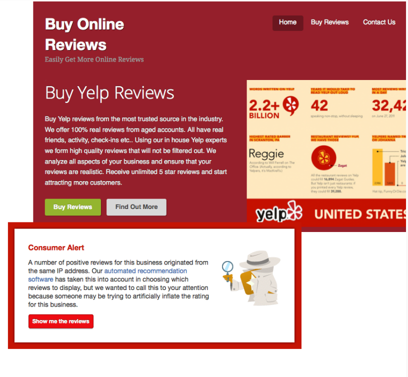

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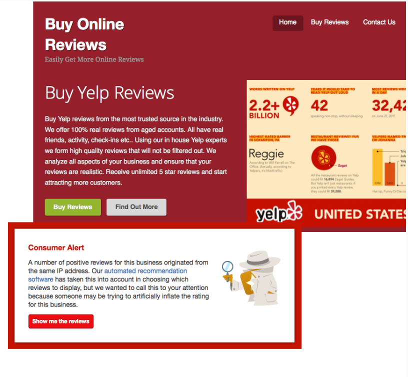

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Dynamic (Gupta et al., 2019)

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♠ At the end, the agent returns $i_{\text{out}} \in [L]$ as the recommendation.

Objective

- Assume $w(1) > w(2) \geq \ldots \geq w(L)$.
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♠ **Goal**: design an (ϵ_C, δ)-PAC algorithm π with both ϵ_C and δ small.

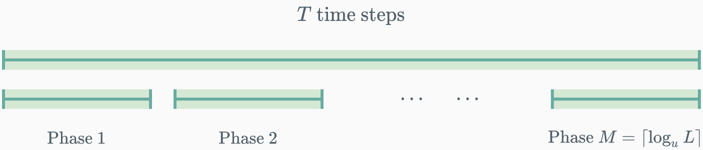
- $\epsilon_C < \Delta_{1,2}$: an (ϵ_C, δ)-PAC algorithm identifies the optimal item with probability at least $1 - \delta$.

PROBABILISTIC SEQUENTIAL SHRINKING **Algorithm**

Probabilistic Sequential Shrinking **Algorithm**

T time steps

Probabilistic Sequential Shrinking **Algorithm**



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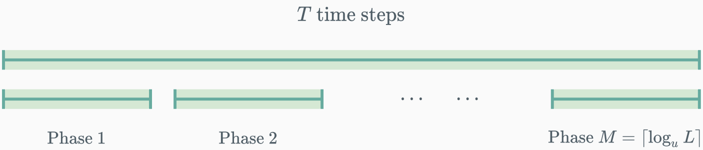

Active set A_0
$A_0 = [L]$

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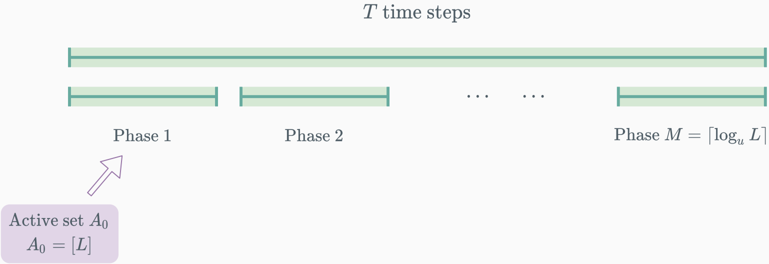

T time steps

$\cdots \quad \cdots$

Phase 1

Phase 2

Phase $M = \lceil \log_u L \rceil$

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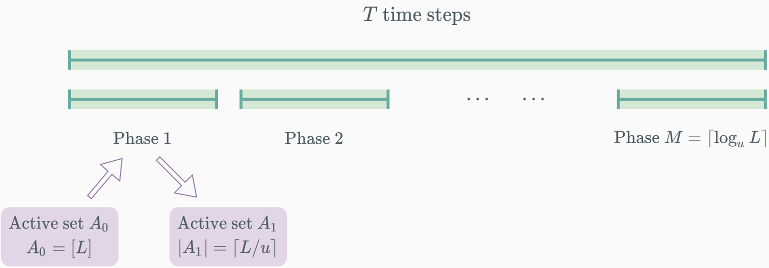

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⋯ ⋯

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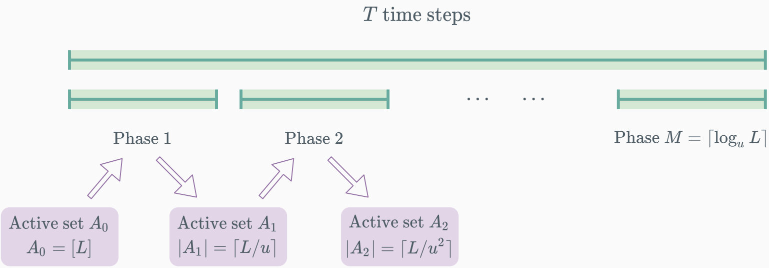
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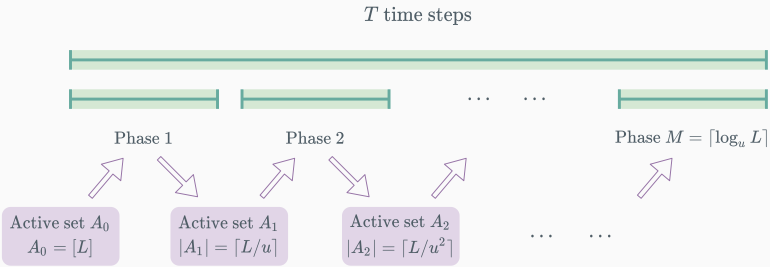

T time steps

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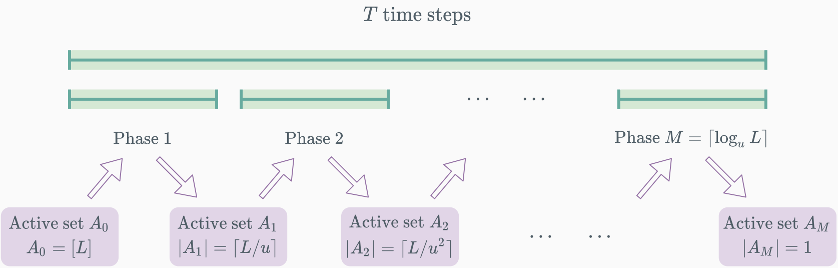

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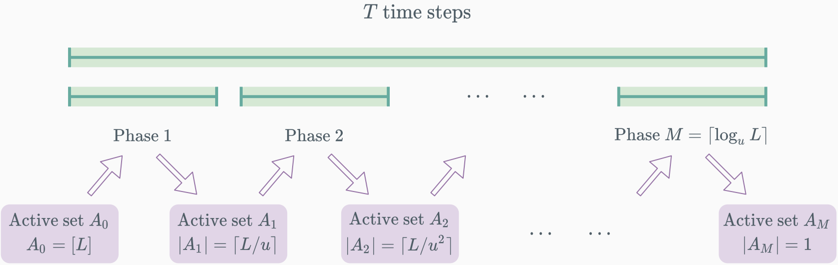

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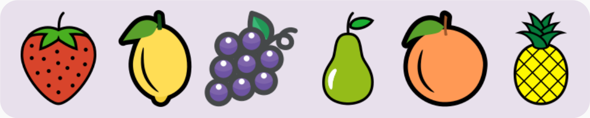
♠ How to shrink the active set?

PSS: Shrink the active set



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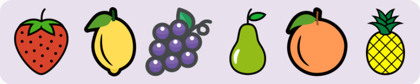

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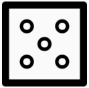

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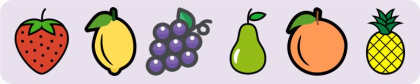

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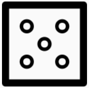

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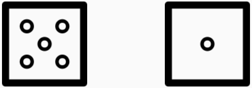

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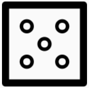
PSS: Shrink the active set

- Pull each active item with the same probability



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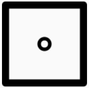
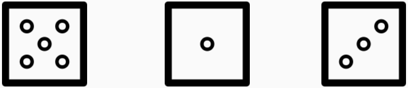


$\tilde{W}_2(1) = 0.3$

PSS: Shrink the active set

- Pull each active item with the same probability



$\tilde{W}_1(5) = 0.5$ $\tilde{W}_2(1) = 0.3$

PSS: Shrink the active set

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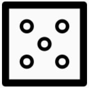

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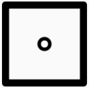

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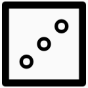
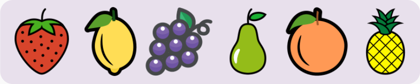
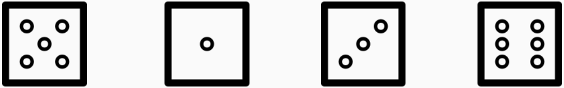


$\tilde{W}_3(3) = 0.9$

PSS: **Shrink the active set**



- Pull each active item with the same probability



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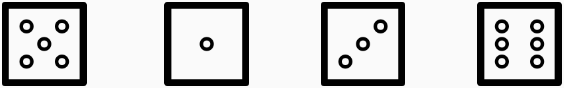

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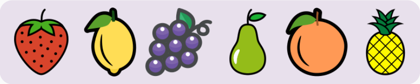

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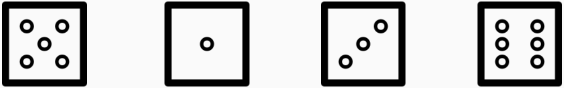

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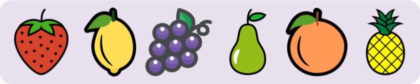

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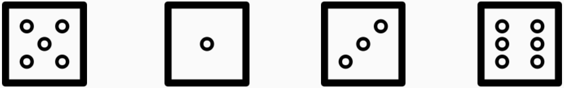

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  only keep items with high empirical means during the current phase

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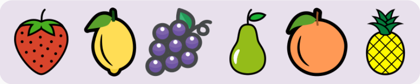

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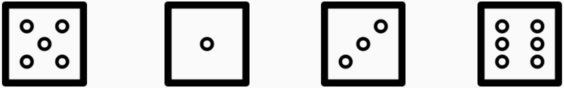

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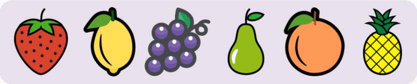

$\hat{W}_m(i)$	0.4	0.1	0.87	0.3	0.35	0.8

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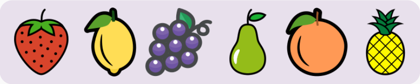

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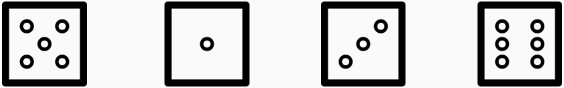

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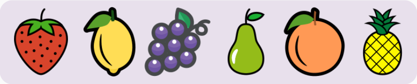

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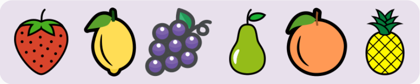

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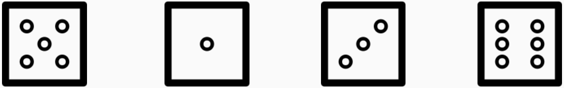

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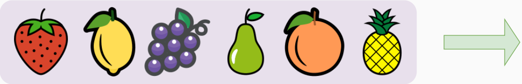

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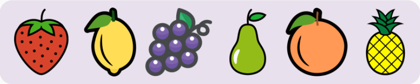

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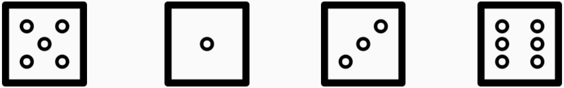

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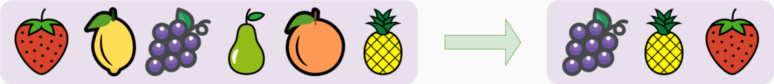

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Comparison to deterministic algorithms: UP, SH

PSS(L) and UNIFORM PULL (UP)

- PSS(L): pulls each item for T/L times in expectation.
- UP: pulls each item for $\lfloor T/L \rfloor$ times with a deterministic schedule.

$\Rightarrow$ PSS(L): randomized version of UP.

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PSS(2) and SEQUENTIAL HALVING (SH) (Karnin et al., 2013)

- **Similarity**: both divide the whole horizon into $\lceil \log_2 L \rceil$ phases and halve the active set during each phase.
- **Difference**:
  - at each time step of phase m, PSS(2) chooses item $i \in A_{m-1}$ with probability $1/|A_{m-1}|$ and pulls it;
  - during phase m, SH pulls each item in A_{m-1} for exactly $\lfloor T/(\lceil \log_2 L \rceil \cdot |A_{m-1}|) \rfloor$ times according to a deterministic schedule.

$\Rightarrow$ PSS(2): randomized version of SH.

Comparison among upper bounds

Comparison in stochastic bandits with adversarial corruptions

Algorithm	Order of error bound ϵ_C	Order of failure probability δ
PSS(u)	$\frac{C \log_u L}{T}$	$L(\log_u L) \exp\left[-\frac{T}{192\tilde{H}_2(w,L,u)\log_u L}\right]$

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SH	$\frac{CL \log_2 L}{T}$	$L(\log_2 L) \exp\left[-\frac{T}{192\tilde{H}_2(w,L,u)\log_2 L}\right]$

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SH	$\frac{CL\log_2 L}{T}$	$L(\log_2 L)\exp\left[-\frac{T}{192\tilde{H}_2(w,L,u)\log_2 L}\right]$
PSS(L)	$\frac{C}{T}$	$L\exp\left(-\frac{T}{192L/\Delta_{1,2}^2}\right)$
UP	$\frac{CL}{T}$	$L\exp\left(-\frac{T}{192L/\Delta_{1,2}^2}\right)$

- $\tilde{H}_2(w,L,u)=\max_{i\neq 1}\frac{\min\{u\cdot i,\ L\}}{\Delta_{1,i}^2}$: quantify difficulty of BAI.
- $H_2(w)=\max_{i\neq 1}\frac{i}{\Delta_i^2}, \tilde{H}_2(w,L,1)=H_2(w), \tilde{H}_2(w,L,u)\leq u\cdot H_2(w).$

Corruption Strategy and Impossibility Result

Theorem 2.2

Fix $\lambda \in (0,1)$ *and* $\Delta \in (0,1/2)$. *For any online algorithm, there is a BAI with an adversarial corruption instance over* T *steps, corruption budget* $C = 1 + (1+\lambda)2\Delta T$, *and optimality gap* Δ, *such that*

$$\mathbb{P}[\Delta_{1,i_{\text{out}}} > 0] = \mathbb{P}[\Delta_{1,i_{\text{out}}} \geq \Delta] = \mathbb{P}[i_{\text{out}} \neq 1] \\ \geq \frac{1}{2} \cdot \left[1 - \exp\left(-\frac{2\lambda^2 \Delta T}{3}\right)\right].$$

- $\dfrac{C}{T} > 2\Delta_{1,2}$: It is impossible for any algorithm to identify the optimal item with high probability.
- $\dfrac{C}{T} \leq \dfrac{\Delta_{1,L}}{8\lceil \log_u L \rceil}$: our work (Theorem 4.1) provides a guarantee for PSS(u).

$\Rightarrow$ The upper bound in our work (Theorem 4.1) is within a factor of $O(\log L)$ away from the largest possible upper bound on C/T in Theorem 2.2.

Outline

1. What is multi-armed bandits (MAB)?

2. Explore state-of-the-art findings of pure exploration

3. **Summary and discussions**

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- Problem formulation
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  - With adversarial corruptions: PROBABILISTIC SEQUENTIAL SHRINKING
- More existing works ...
  - *Multiple pure exploration*: to identify multiple arms
    CLUCB by Chen et al. (2014), EST1 and CSAR by Rejwan and Mansour (2020)
  - *Pure exploration in linear bandits*
    (Jedra and Proutiere; Yang and Tan, 2021)
  - • • •

Further exploration

- Fill the gap between upper and lower bounds for BAI under the fixed-budget setting?

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Further exploration

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- Identification of the arm with the highest median reward (Altschuler et al., 2019):
  More studies taking the median of rewards as the criterion are yet to be done.
- BAI in adversarial bandits (Shen, 2019; Zhong et al., 2021):
  Optimal attack strategies against regret minimization (Jun et al., 2018; Liu and Lai, 2020)
  Optimal attack strategies against pure exploration?

Q&A

Thanks for listening!

`https://zixinzh.github.io/homepage/conf_tutorial/`

Emails: `vtan@nus.edu.sg`, `zixin.zhong@u.nus.edu`

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