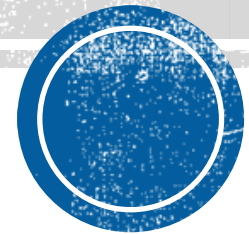


Stochastic multi-armed bandits



Shipra Agrawal

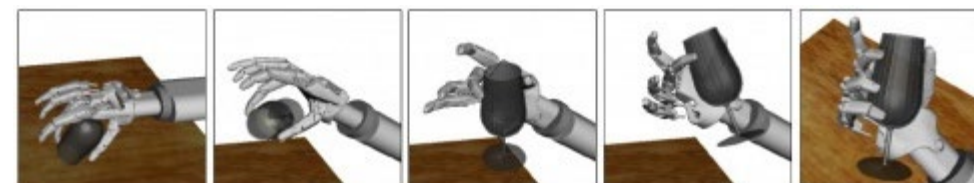
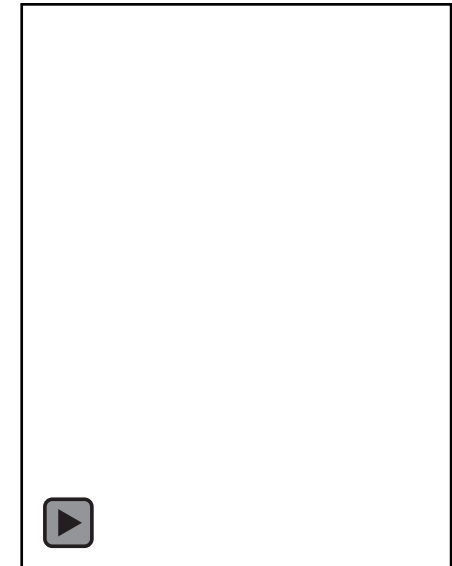
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Learning from sequential interactions

Tradeoff between

- information and rewards
- learning and optimization
- Exploration and exploitation



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Managing exploitation-exploitation tradeoff

The multi-armed bandit problem (Thompson 1933; Robbins 1952)

Multiple rigged slot machines in a casino.

Which one to put money on?

- Try each one out



WHEN TO STOP TRYING (EXPLORATION) AND START PLAYING (EXPLOITATION)?



Stochastic multi-armed bandit problem

- Online decisions
 - At every time step $t = 1, \dots, T$, pull one arm out of N arms
- Stochastic feedback
 - For each arm i , reward is generated **i.i.d.** from a **fixed but unknown distribution** support $[0,1]$, mean μ_i
- Bandit feedback
 - Only the reward of the pulled arm can be observed
- Minimize **regret** compared to the best arm

$$E[\sum_{t=1}^T (\mu^* - \mu_{i_t})] \quad \text{where } \mu^* = \max_j \mu_j$$



Other formulations: Bayesian bandits and Gittins index

- Prior distribution over parameters of each arm's reward distribution
 - E.g. if arm i has reward distribution $\text{Bernoulli}(\mu_i)$, there is a prior on distribution of μ_i
 - On observing a reward we have a posterior
- Expected reward/regret:
 - *Expectation over prior distribution*, in addition to reward distribution of arms
- Gittins Index [Gittins, 1979]
 - Optimal policy when maximizing *expected total discounted reward*
- Bayesian Regret minimization
 - e.g., see [Osband, Russo and Van Roy 2013, Russo and Van Roy 2014, 2015, 2016], [Bubeck and Liu 2013]

Outline

- Basic algorithmic techniques for the stochastic MAB problem
 - UCB
 - Thompson Sampling
- Useful Generalizations
 - Contextual bandits
 - Assortment optimization
 - Bandits with constraints
- Later: Bandit techniques for MDP/RL

Recall: Stochastic multi-armed bandit problem

- Online decisions
 - At every time step $t = 1, \dots, T$, pull one arm out of N arms
- Stochastic feedback
 - For each arm i , reward is generated **i.i.d.** from a **fixed but unknown distribution** support $[0,1]$, mean μ_i
- Bandit feedback
 - Only the reward of the pulled arm can be observed
- Minimize regret in time T

$$E[\sum_{t=1}^T (\mu^* - \mu_{i_t})]$$



The need for exploration

- Two arms **black** and **red**
 - Random rewards with unknown mean $\mu_1 = 1.1$, $\mu_2 = 1$
 - Optimal expected reward in T time steps is $1.1 \times T$
- Exploit only strategy: use the current best estimate (MLE/empirical mean) of unknown mean to pick arms
- Initial few trials can mislead into playing red action forever

1.1, 1, 0.2,
1, 1, 1, 1, 1, 1, 1,
- Expected regret in T steps is close to $0.1 \times T$

Exploration-Exploitation tradeoff

- Exploitation: play the empirical mean reward maximizer
- Exploration: play less explored actions to ensure empirical estimates converge

Lower bounds

- Expected regret in any time T ,

$$\text{Regret}(T) = \sum_i (\mu^* - \mu_{i_t}) = \sum_i \Delta_i E[k_i(T)]$$

Lower bounds

- [Lai and Robbins 1985](#) [Informal] For *any* given instance of the MAB problem, any “reasonable algorithm” will play a suboptimal arm at least $\Omega(\log(T))$ times for large T
- Worst case bound: For every algorithm, there exists an instance with $\Omega(\sqrt{NT})$ regret

UCB algorithm [Auer 2002]

- Empirical mean at time t for arm i
- Upper confidence bound (UCB)
- Optimism:
- Optimistic Algorithm
 - At each time step t , play the with best optimistic estimates

$$\hat{\mu}_{i,t} = \frac{\sum_{s=1:t, I_s=i} r_s}{n_{i,t}}$$

$$UCB_{i,t} = \hat{\mu}_{i,t} + \sqrt{\frac{4 \ln t}{n_{i,t}}}$$

$$UCB_{i,t} > \mu_i \text{ w.h.p.}$$

$$i_t = \arg \max_i UCB_{t,i}$$

UCB algorithm [Auer 2002]

Algorithm 1: UCB algorithm for the stochastic N-armed bandit problem

```
foreach  $t = 1, \dots, N$  do
| Play arm  $t$ 
end
foreach  $t = N + 1, N + 2, \dots, T$  do
| Play arm  $I_t = \arg \max_{i \in \{1, \dots, N\}} \text{UCB}_{i,t-1}$ .
| Observe  $r_t$ , compute  $\text{UCB}_{i,t}$ 
end
```



Regret analysis

- Recall Regret in any time T ,

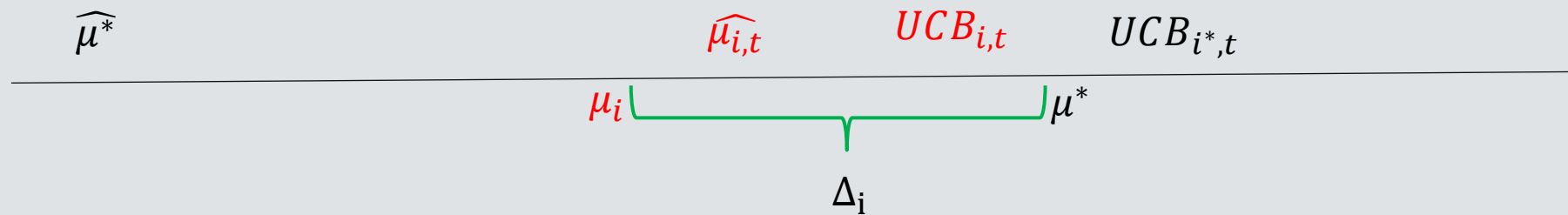
$$\text{Regret}(T) = \sum_i \Delta_{i_t} = \sum_i \Delta_i E[k_i(T)]$$

where $\Delta_i = \mu^* - \mu_i$

- Bound the number of mistakes $E[k_i(T)]$ for all suboptimal arms $i \neq i^*$
 - A bound of $E[k_i(T)] \leq \frac{C \ln T}{\Delta_i^2}$ for i each implies $\sum_{i \neq i^*} \frac{C \ln T}{\Delta_i}$ regret bound

Regret analysis

- Arm i will be played at time t only if $UCB_{i,t} > UCB_{i^*,t}$
- If $n_{i,t} > \frac{16\ln(T)}{\Delta_i^2}$: $\hat{\mu}_{i,t} < \mu_i + \frac{\Delta_i}{2}$, $UCB_{i,t} \leq \hat{\mu}_{i,t} + \frac{\Delta_i}{2}$



- No more plays of arm i (with high probability)
 - $\frac{16\ln(T)}{\Delta_i^2}$ bound on expected number of mistakes
 - $Regret(T) = \sum_i \Delta_{i_t} = \sum_i \Delta_i E[k_i(T)] \leq \sum_{i \neq i^*} \frac{16\ln(T)}{\Delta_i}$

Thompson Sampling [Thompson, 1933]

- Natural and Efficient heuristic
- Maintain belief about parameters (e.g., mean reward) of each arm
- Observe feedback, update belief of pulled arm i in Bayesian manner
- Pull arm with posterior probability of being best arm
 - NOT same as choosing the arm that is most likely to be best

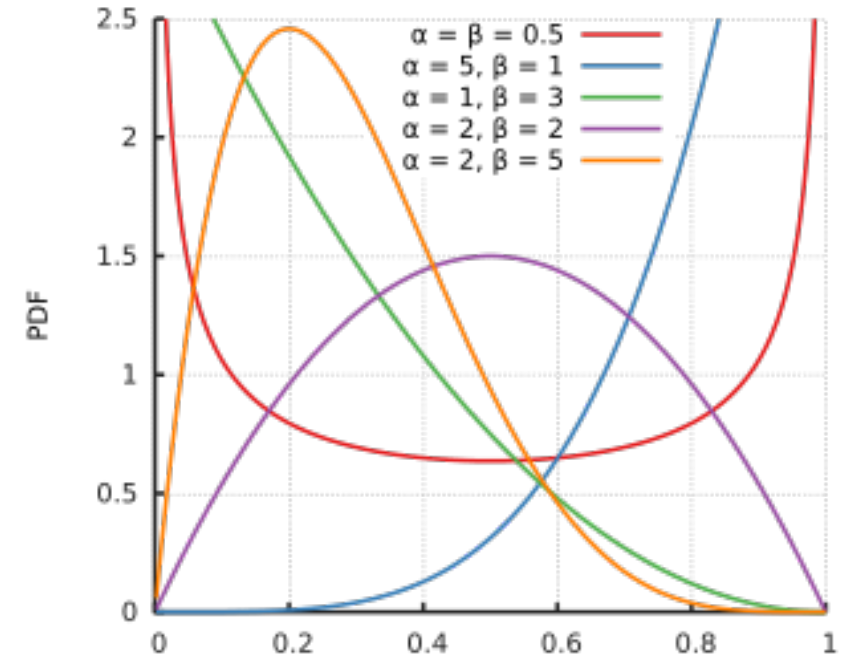


Bernoulli rewards, Beta priors

Uniform distribution $Beta(1,1)$

$Beta(\alpha, \beta)$ prior \Rightarrow Posterior

- $Beta(\alpha + 1, \beta)$ if you observe 1
- $Beta(\alpha, \beta + 1)$ if you observe 0



Start with $Beta(1,1)$ prior belief for every arm

In round t ,

- For every arm i , sample $\theta_{i,t}$ independently from posterior $Beta(S_{i,t} + 1, F_{i,t} + 1)$
- Play arm $i_t = \max_i \theta_{i,t}$
- Observe reward and update the Beta posterior for arm i_t



Arbitrary reward distribution mean μ , Gaussian prior

Standard normal prior $N(0,1)$

Gaussian likelihood $N(\mu, 1)$ of reward

Posterior after n independent observations: $N\left(\hat{\mu}, \frac{1}{n+1}\right)$

- $\hat{\mu}$ is the empirical mean

Start with $N(0, v^2)$ prior belief for every arm

In round t ,

- For every arm i , sample $\theta_{i,t}$ independently from posterior $N\left(\hat{\mu}_i, \frac{v^2}{n_i+1}\right)$
- Play arm $i_t = \max_i \theta_{i,t}$
- Observe reward and update empirical mean $\hat{\mu}_i$ and number of plays n_i for arm i_t



Regret bounds

Optimal instance-dependent bounds for Bernoulli rewards

- $\text{Regret}(T) \leq \ln(T)(1 + \epsilon) \sum_i \frac{\Delta_i}{KL(\mu^* || \mu_i)} + O\left(\frac{N}{\epsilon^2}\right)$ [A. and Goyal 2012, 2013]
 - Matches *asymptotic instance wise lower bound* [Lai Robbins 1985]
 - Closely related bounds by [Kaufmann et al. 2013]
 - Bayesian UCB algorithm also achieves this [Kaufmann et al. 2012]

Arbitrary bounded reward distribution (Beta and Gaussian priors)

- $\text{Regret}(T) \leq O(\ln(T) \sum_i \frac{1}{\Delta_i})$ [A. and Goyal 2013]
 - Matches the best available for UCB for general reward distributions

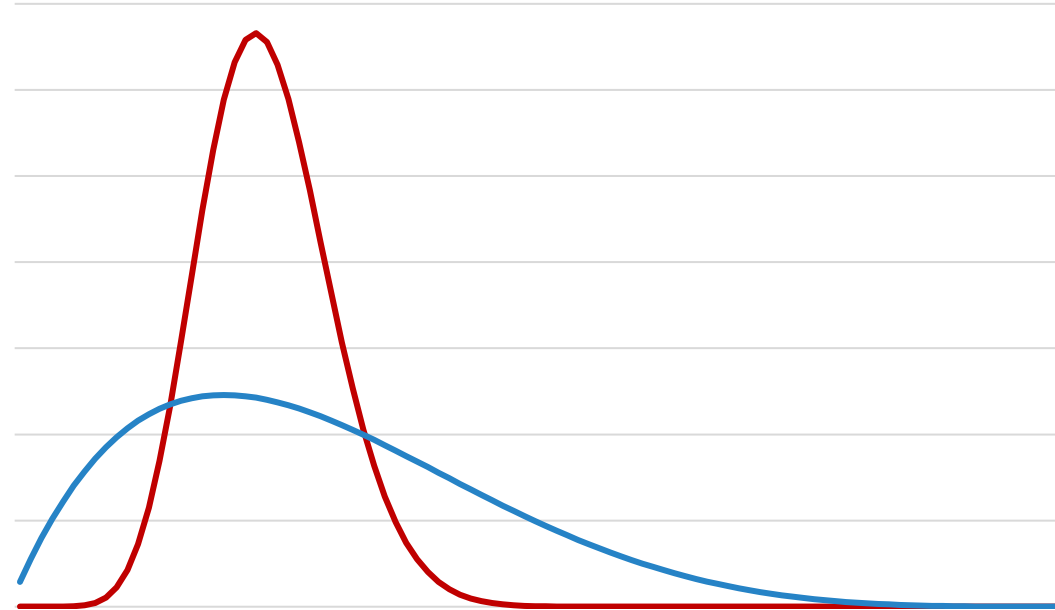
Instance-independent bounds (Beta and Gaussian priors)

- $\text{Regret}(T) \leq O(\sqrt{NT \ln T})$ [A. and Goyal 2013]
 - Lower bound $\Omega(\sqrt{NT})$
- Prior and likelihood mismatch allowed! – worst case regret bounds



Posterior Sampling: main idea [Thompson 1933]

- Maintain Bayesian posteriors for unknown parameters
- With more trials posteriors concentrate on the true parameters
 - Mode captures MLE: enables exploitation
- Less trials means more uncertainty in estimates
 - Spread/variance captures uncertainty: enables exploration



Why does it work? Two arms example

- Two arms, $\mu_1 \geq \mu_2$, $\Delta = \mu_1 - \mu_2$
- Every time arm 2 is pulled, Δ regret
- ➔ ▪ Bound the number of pulls of arm 2 by $\frac{\log(T)}{\Delta^2}$ to get $\frac{\log(T)}{\Delta}$ regret bound
- How many pulls of arm 2 are actually needed?



Easy situation

After $n \geq \frac{16 \log(T)}{\Delta^2}$ pulls of arm 2 and arm 1

- Empirical means are well separated

$$\text{Error } |\widehat{\mu}_i - \mu_i| \leq \sqrt{\frac{\log(T)}{n}} \leq \frac{\Delta}{4} \text{ whp}$$

(Using Azuma Hoeffding inequality)

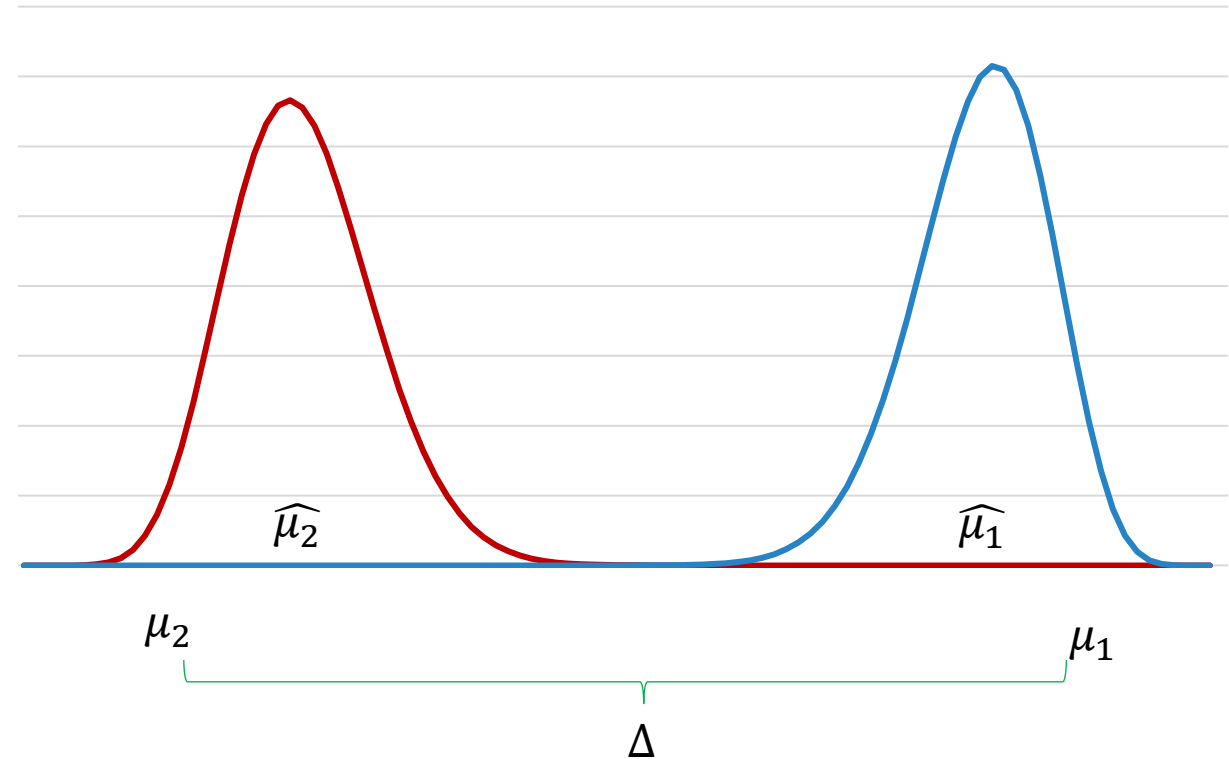
- Beta Posteriors are well separated

$$\text{Mean} = \frac{\alpha_i}{\alpha_i + \beta_i} = \widehat{\mu}_i$$

$$\text{standard deviation} \simeq \frac{1}{\sqrt{\alpha + \beta}} = \frac{1}{\sqrt{n}} \leq \frac{\Delta}{4}$$

The two arms can be distinguished!

No more arm 2 pulls.



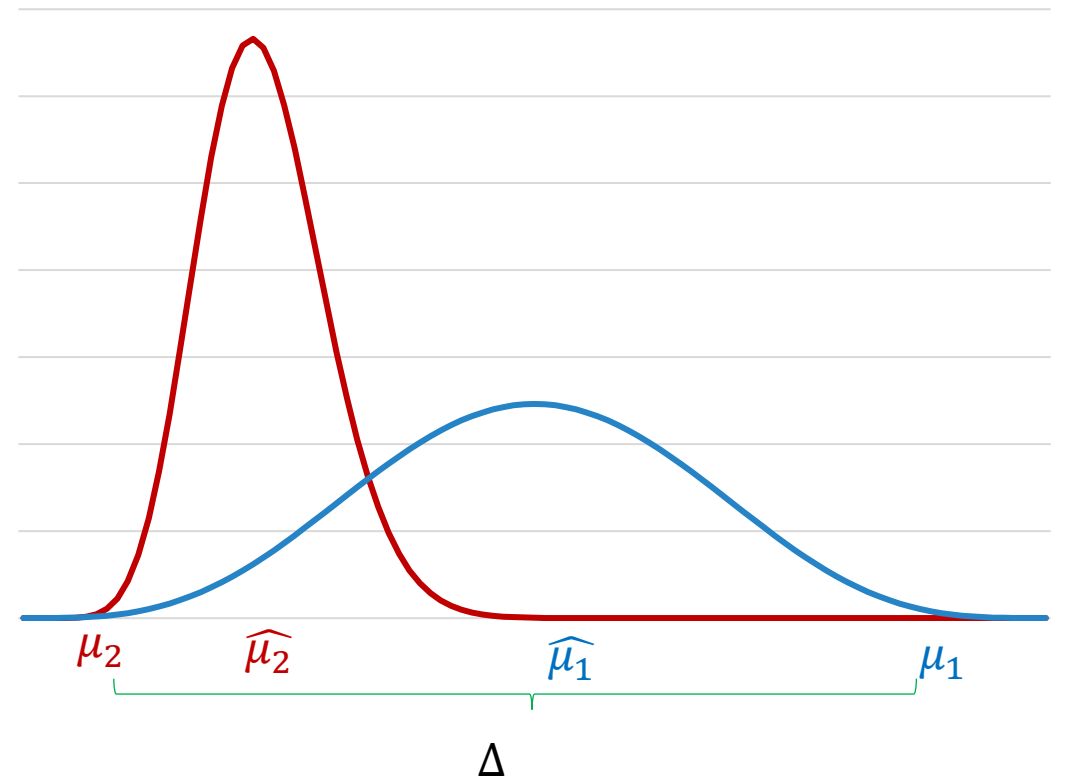
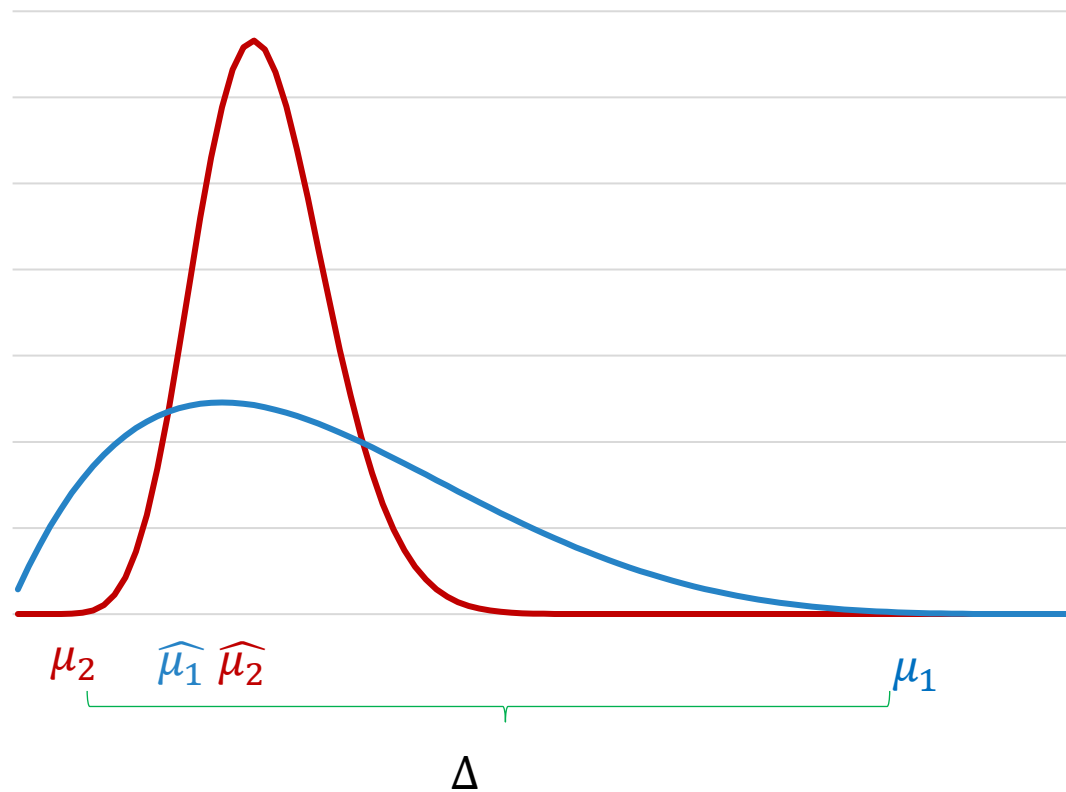
Easy situation

- Before arm 2 is pulled less than $n = \frac{16 \log(T)}{\Delta^2}$ times?
 - Regret is at most $n\Delta = \frac{16 \log(T)}{\Delta}$



Difficult situation

- After $\frac{16 \log(T)}{\Delta^2}$ pulls of arm 2, but *before* arm 1 is pulled enough



Main insight

- Arm 1 will be played roughly every constant number of steps in this situation
- It will take at most $constant \times \frac{\log T}{\Delta^2}$ steps (extra pulls of arm 2) to get out of this situation
- Total number of pulls of arm 2 before enough pulls of arm 1 is at most $O\left(\frac{\log T}{\Delta^2}\right)$
- Summary: variance of posterior enables exploration
- Optimal bounds (and for multiple arms) require more careful use of posterior structure



Multiple arms case

- Main observation: Given some high probability events

$$\Pr(i_t = a^* \mid F_{t-1}) \geq \frac{p}{1-p} \cdot \Pr(i_t = i \mid F_{t-1})$$

- p is the probability of anti-concentration of posterior sample for the best arm

- E.g., $p_a := \Pr(\theta_{i^*} \geq \mu_{i^*} - \frac{\Delta_i}{4})$

- Best arm gets played roughly every $\frac{1}{p}$ plays **of arm i**

- p can be lower bounded by Δ_i in general but it actually goes to 1 exponentially fast with increase in number of trials of best arm.
 - Cannot accumulate much regret from arm i without playing arm i^* sufficiently

Next: Useful Generalizations of the basic MAB problem

Recall: The basic Stochastic multi-armed bandit problem

- Online decisions
 - At every time step $t = 1, \dots, T$, pull one arm out of N arms
- Stochastic feedback
 - For each arm i , reward is generated **i.i.d. across time** from a **fixed but unknown distribution** support $[0,1]$, mean μ_i
- Bandit feedback
 - Only the reward of the pulled arm can be observed
- Minimize regret in time T

$$E[\sum_{t=1}^T (\mu^* - \mu_{i_t})]$$





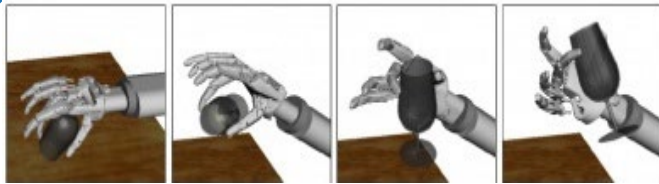
- Personalization
 - Linear contextual bandits



- Customer Choice behavior
 - Dynamic assortment selection



- Revenue management and resource allocation
 - Budget/supply constraints, nonlinear utilities



- Reinforcement learning
 - State-dependent response



- Inventory management, Dynamic Pricing
 - Learning continuous state MDPs

#1: Handling context in MAB

- Large number of products and customer types
- Utilize similarity?
- Content based recommendation (Supervised learning)
 - Customers and products described by their features
 - Similar features means similar preferences
 - Parametric models mapping customer and product features to customer preferences
 - E.g. linear regression
- Contextual bandits
 - Exploration-exploitation to learn the parametric models



Linear Contextual Bandits

- N arms, possibly very large N
- A d-dimensional context (feature vector) $x_{i,t}$ for every arm i , time t
- Linear parametric model
 - Unknown parameter **vector** μ
 - Expected reward for arm i at time t is $x_{i,t} \cdot \mu$
- Algorithm picks $x_t \in \{x_{1,t}, \dots, x_{N,t}\}$, observes $r_t = x_t \cdot \mu + \eta_t$
- Optimal arm depends on context: $x_t^* = \arg \max_i x_{i,t} \cdot \mu$
- Goal: Minimize regret
 - $\text{Regret}(T) = \sum_t (x_t^* \cdot \mu - x_t \cdot \mu)$



UCB for linear contextual bandits

Linear regression

- Least square solution $\hat{\mu}_t$ of set of $t - 1$ equations

$$x_s \cdot \mu = r_s, \quad s = 1, \dots, t - 1$$

- $\hat{\mu}_t \simeq B_t^{-1} (\sum_{s=1}^{t-1} x_s r_s)$ where $B_t = I + \sum_{s=1}^{t-1} x_s x_s'$
- B_t^{-1} covariance matrix of this estimator

High confidence interval for θ

- With high probability $\|\mu - \hat{\mu}_t\|_{B_t} \leq C \sqrt{d \log(Td)}$

[Rusmevichientong and Tsitsiklis 2010] [Abbasi-Yadkori et al 2011]



UCB algorithm

- At time t
 - Observe the contexts $x_{i,t}$ for different arms $i = 1, \dots, N$
 - Compute confidence interval for the unknown parameter
 - Choose the best arm according to the most optimistic parameter in C_t

$$C_t = \{z : \|z - \hat{\mu}\|_{B_t} \leq C\sqrt{d \log(Td)}\}$$

Algorithm 1: LinUCB algorithm

foreach $t = 1, \dots, T$ **do**

 Observe set $A_t \subseteq [N]$, and context $x_{i,t}$ for all $i \in A_t$.

 Play arm $I_t = \arg \max_{i \in A_t} \max_{z \in C_t} z^\top x_{i,t}$ with C_t as defined:

 Observe r_t . Compute C_{t+1}

end

Regret bounds

- LinUCB [Auer 2002] With probability $1 - \delta$, regret

$$\text{Regret}(T) \leq \tilde{O}(d\sqrt{T})$$

- Note : no dependence on number of arms
- Lower bound $\Omega(d\sqrt{T})$



Proof outline



Thompson Sampling for linear contextual bandits

Linear regression

- Least square error solution $\hat{\mu}_t$ of set of $t - 1$ equations

$$x_s \cdot \mu = r_s, \quad s = 1, \dots, t - 1$$

- $\hat{\mu}_t \simeq B_t^{-1} (\sum_{s=1}^{t-1} x_s r_s)$ where $B_t = I + \sum_{s=1}^{t-1} x_s x_s'$
- B_t^{-1} covariance matrix of this estimator

Gaussian posterior

- $N(0, I)$ starting prior on μ ,
- Reward distribution given $\mu, x_{i,t}$: $N(\mu^T x_{i,t}, 1)$,
- posterior on μ at time t is $N(\hat{\mu}_t, B_t^{-1})$



Thompson Sampling for linear contextual bandits

[A., Goyal 2013] Algorithm:

At Step t ,

- Sample $\tilde{\mu}_t$ from $N(\hat{\mu}_t, v^2 B_t^{-1})$
- Observe context x_t
- Pull arm with feature x_t where

$$x_t = \max_i x_{i,t} \cdot \tilde{\mu}_t$$



Regret bounds

- LinUCB [Auer 2002] With probability $1 - \delta$, regret

$$\text{Regret}(T) \leq \tilde{O}(d\sqrt{T})$$

- Thompson Sampling [A. and Goyal 2013] With probability $1 - \delta$, regret

$$\text{Regret}(T) \leq \tilde{O}(d^{3/2}\sqrt{T})$$

- *Any likelihood, unknown prior, only assumes bounded or sub-Gaussian noise*
- Note : no dependence on number of arms
- Lower bound $\Omega(d\sqrt{T})$



Many other contextual formulations

More general functions modeling expected reward on playing arm with context x

- Generalized linear bandits $g(\mu^T x)$

[Filippi et al. 2010]

- Convex bandits: $f(x)$ for f convex in x

[Agarwal et al. 2011][Bubeck et al. 2015, 2016, 2017]

- Lipschitz bandits : $f(x)$ for Lipschitz function f on a metric space

[Kleinberg 2004] [Kleinberg et al. 2008] [Slivkins 2011] [Bubeck et al. 2011]

#2: Assortment selection as multi-armed bandit

- Consider arms as products
- Limited display space, k products displayed at a time
- Probability that customer chooses product i from assortment S : $p_i(S)$
- Challenge: Customer response on one product is influenced by other products in the assortment
 - Feedbacks from individual arms are no longer independent





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Ve



Customer choice modeling

Multinomial logit choice model [Luce 1959, McFadden 1978]

- Probability of choosing product i (feature vector x_i) in assortment S

$$p_i(S) = \frac{e^{\theta_i}}{1 + \sum_{j \in S} e^{\theta_j}}$$

- Probability of no purchase

$$p_i(S) = \frac{1}{1 + \sum_{j \in S} e^{\theta_j}}$$

- Key property: Independence of irrelevant alternatives
- Fixed reward r_i for product i
- Given a $\theta = (\theta_1, \theta_2, \dots, \theta_N)$, the optimal assortment is efficiently computable [Rusmevichientong et al. 2010] [Davis et al. 2013]



The MNL bandit problem

[A., Avadhanula, Goyal, Zeevi, 2016]

N products, Unknown parameters $\theta_1, \theta_2, \dots, \theta_N$

At every step t ,

- recommend an *assortment* S_t of size at most K,
- *observe customer choice* i_t , revenue r_{i_t}
- update parameter estimates

Goal:

- optimize total expected revenue $E[\sum_{t=1}^T r_{i_t}]$
- or minimize regret compared to the optimal assortment $S^* = \operatorname{argmax}_S \sum_{i=1}^N r_i p_i(S)$



Main challenges and techniques

- Censored feedback
 - Feedback for product i effected by other products in assortment
 - Combinatorial choice: N^K possible assortments

[A., Avadhanula, Goyal, Zeevi, 2016, 2017]

- Technique to get unbiased estimate of individual parameters:
 - offer an assortment until no-purchase
 - Number of times i is purchased is unbiased estimate of its parameter e^{θ_i}
- Then, use standard UCB or Thompson Sampling techniques



Regret bounds

UCB based algorithm [A., Avadhanula, Goyal, Zeevi, 2016]

- $\tilde{O}(\sqrt{NT})$ regret bounds (under an assumption on no-purchase probability)
 - Parameter independent, no dependence on K
 - Matching lower bound of $\Omega(\sqrt{NT})$ [Chen and Wang 2017]

Thompson Sampling [A., Avadhanula, Goyal, Zeevi, 2017]

- Similar regret bounds, significantly more attractive empirical results

More recent work

- Contextual settings in [Chen et al. 2018][Ou et al 2018][Oh and Iyengar 2019]
- Nested logit models [Chen, Wang & Zhu, 2018]
- With resource constraints [Cheung & Simchi-Levi 2017]



#3: Bandits with constraints and non-linear aggregate utility

Regular bandits

- Total number of pulls constrained by T
 - No other global constraint on decisions across time
- Maximize sum of rewards



More global constraints

- Resource constraints in pricing and network revenue management
- Multiple Budget constraints in advertising campaigns
 - Nonlinear risk constraints
- Covering constraints in network routing and scheduling, sensor networks, crowdsourcing
- In pay-per-click advertising multiple performance criteria to be satisfied simultaneously
 - revenue, user satisfaction, diversity, minimum impressions



More than sum of rewards

- Smooth delivery in advertising
 - Minimize variance over time
- Demographics of clicks
 - maximizing minimum number of each type
- Nonlinear functions converting number of clicks to user satisfaction, or revenue
- Crowd sourcing: Need diversity among workers
- Sensor measurements: cover variety of locations
 - maximizing minimum number of successful sensor measurements from each location



Generalizing MAB

- Classic MAB
 - Observe reward r_t on pulling an arm i_t
 - Maximize $\sum_t r_t$
- Bandits with knapsacks (BwK) [Badanidiyuru, Kleinberg, Slivkins 2013, Besbes and Zeevi 2009, 2012]

Observe non-negative reward r_t and cost vector \mathbf{c}_t

$$\begin{aligned} & \text{maximize } \sum_t r_t \\ & \text{s. t. } \sum_t \mathbf{c}_{t,j} \leq B, \forall j \end{aligned}$$



Bandits with convex knapsacks and concave rewards (BwCR)

[Agrawal, Devanur 2014]

- Pulling an arm i_t generates a d dimensional vector \mathbf{v}_t , unknown mean V_{i_t}
- Total number of pulls constrained by T

+ Arbitrary convex global constraints on average of observations across time

$$\frac{1}{T} \sum_t \mathbf{v}_t \in S, \quad S \text{ is arbitrary convex set}$$

- Maximize arbitrary concave function $f\left(\frac{1}{T} \sum_t \mathbf{v}_t\right)$

Minimize distance $\text{dis}\left(\frac{1}{T} \sum_t \mathbf{v}_t, S\right)$ from convex set S



UCB like optimistic algorithm for BwCR

What is an optimistic estimate of the mean observation **vectors**?

- Need to estimate for every arm i and every coordinate j
- Non-decreasing f : upper bound (UCB)
 - The function value at the estimate will be more than actual
- Downward closed S : lower bound (LCB)
 - If actual mean is in S , the estimate will be in S
- In general
 - Most optimistic estimate in the confidence interval?



Optimistic algorithm for BwCR

- Play the (distribution over) arm that appears to be the best according to **the most optimistic estimates** in the confidence interval
 - Two levels of optimizations

- Actual mean lies in confidence intervals

$$H_t = \{\tilde{V}: \tilde{V}_{ij} \in [\text{LCB}_{t,ij}, \text{UCB}_{t,ij}]\}$$

- Play best distribution over arms according to **most optimistic estimate**

$$\mathbf{p}_t = \arg \max_{\mathbf{p}} \max_{\tilde{V} \in H_t} f \left(\sum_i p_i \tilde{V}_i \right)$$

s. t. $\min_{\tilde{U} \in H_t} \text{dis}(\sum_i p_i \tilde{U}_i, S) \leq 0$



Regret bounds

- [A. and Devanur 2014] UCB like optimistic algorithm that

- achieves near-optimal average regret

$$\text{Regret in objective} \leq \tilde{O}\left(L\sqrt{N/T}\right), \quad \text{Regret in constraints} \leq \tilde{O}\left(\sqrt{N/T}\right)$$

- achieves problem specific optimal bounds on regret for Bandits with knapsacks

$$\text{Regret} \leq \tilde{O}\left(\text{OPT}\sqrt{N/B} + \sqrt{N \text{OPT}}\right)$$

- is polynomial time implementable

- Recent Extensions to contextual bandits



