

Sequential Learning

Multi-Armed Bandits

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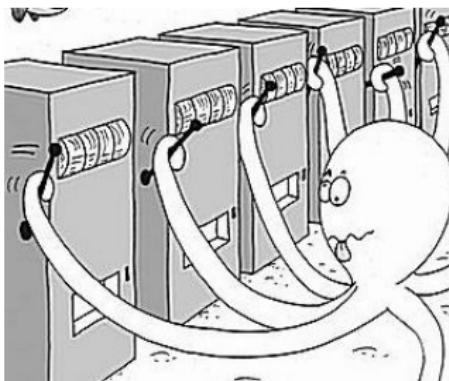


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Stochastic bandit : a simple MDP

A stochastic multi-armed bandit model can be viewed as an MDP with a single state s_0

- ▶ unknown reward distribution $\nu_{s_0, a}$ with mean $r(s_0, a)$
- ▶ transition $p(s_0 | s_0, a) = 1$
- ▶ the agent repeatedly chooses between the same set of actions



an **agent** facing **arms** in a Multi-Armed Bandit

Sequential resource allocation

Clinical trials

- ▶ K treatments for a given symptom (with unknown effect)



- ▶ What treatment should be allocated to the next patient based on responses observed on previous patients ?

Online advertisement

- ▶ K adds that can be displayed



- ▶ Which add should be displayed for a user, based on the previous clicks of previous (similar) users ?

The Multi-Armed Bandit Setup

K **arms** \leftrightarrow K rewards streams $(X_{a,t})_{t \in \mathbb{N}}$



At round t , an agent :

- ▶ chooses an arm A_t
- ▶ receives a reward $R_t = X_{A_t, t}$

Sequential sampling strategy (**bandit algorithm**) :

$$A_{t+1} = F_t(A_1, R_1, \dots, A_t, R_t).$$

Goal : Maximize $\sum_{t=1}^T R_t$.

The Stochastic Multi-Armed Bandit Setup

K arms \leftrightarrow K probability distributions : ν_a has mean μ_a



At round t , an agent :

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- ▶ receives a reward $R_t = X_{A_t, t} \sim \nu_{A_t}$

Sequential sampling strategy (**bandit algorithm**) :

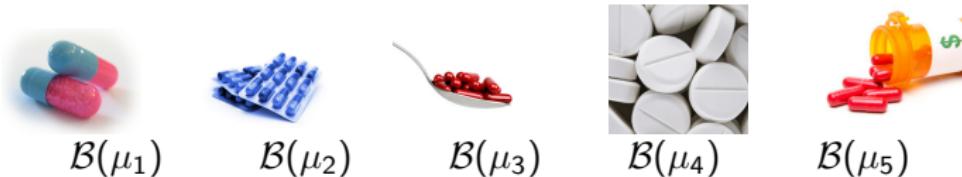
$$A_{t+1} = F_t(A_1, R_1, \dots, A_t, R_t).$$

Goal : Maximize $\mathbb{E} \left[\sum_{t=1}^T R_t \right]$

→ a particular reinforcement learning problem

Clinical trials

Historical motivation [Thompson, 1933]



For the t -th patient in a clinical study,

- ▶ chooses a **treatment** A_t
- ▶ observes a **response** $R_t \in \{0, 1\} : \mathbb{P}(R_t = 1 | A_t = a) = \mu_a$

Goal : maximize the expected number of patients healed

Online content optimization

Modern motivation (\$\$) [Li et al., 2010]
(recommender systems, online advertisement)



ν_1



ν_2



ν_3



ν_4



ν_5

For the t -th visitor of a website,

- ▶ recommend a movie A_t
- ▶ observe a rating $R_t \sim \nu_{A_t}$ (e.g. $R_t \in \{1, \dots, 5\}$)

Goal : maximize the sum of ratings

Outline

- 1 Performance measure and first strategies
- 2 Mixing Exploration and Exploitation
 - Upper Confidence Bound algorithms
- 3 Bayesian bandit algorithms
 - Thompson Sampling

Regret of a bandit algorithm

Bandit instance : $\nu = (\nu_1, \nu_2, \dots, \nu_K)$, mean of arm a : $\mu_a = \mathbb{E}_{X \sim \nu_a}[X]$.

$$\mu_* = \max_{a \in \{1, \dots, K\}} \mu_a \quad a_* = \operatorname{argmax}_{a \in \{1, \dots, K\}} \mu_a.$$

Maximizing rewards \leftrightarrow selecting a_* as much as possible
 \leftrightarrow minimizing the **regret** [Robbins, 1952]

$$\mathcal{R}_\nu(\mathcal{A}, T) := \underbrace{T\mu_*}_{\substack{\text{sum of rewards of} \\ \text{an oracle strategy} \\ \text{always selecting } a_*}} - \underbrace{\mathbb{E} \left[\sum_{t=1}^T R_t \right]}_{\substack{\text{sum of rewards of} \\ \text{the strategy } \mathcal{A}}}$$

What regret rate can we achieve ?

- consistency : $\frac{\mathcal{R}_\nu(\mathcal{A}, T)}{T} \rightarrow 0$
- can we be more precise ?

Regret decomposition

$N_a(t)$: number of selections of arm a in the first t rounds

$\Delta_a := \mu_\star - \mu_a$: sub-optimality gap of arm a

Regret decomposition

$$\mathcal{R}_\nu(\mathcal{A}, T) = \sum_{a=1}^K \Delta_a \mathbb{E}[N_a(T)].$$

Proof.



Regret decomposition

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Regret decomposition

$$\mathcal{R}_\nu(\mathcal{A}, T) = \sum_{a=1}^K \Delta_a \mathbb{E}[N_a(T)].$$

A strategy with small regret should :

- ▶ select not too often arms for which $\Delta_a > 0$
- ▶ ... which requires to try all arms to estimate the values of the Δ_a 's

⇒ Exploration / Exploitation trade-off

Two naive strategies

- ▶ **Idea 1** : Uniform Exploration

Draw each arm T/K times

⇒ EXPLORATION

$$\mathcal{R}_\nu(\mathcal{A}, T) = \left(\frac{1}{K} \sum_{a: \mu_a > \mu_*} \Delta_a \right) T$$

Two naive strategies

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⇒ EXPLORATION

$$\mathcal{R}_\nu(\mathcal{A}, T) = \left(\frac{1}{K} \sum_{a: \mu_a > \mu_*} \Delta_a \right) T$$

► Idea 2 : Follow The Leader

where

$$A_{t+1} = \operatorname{argmax}_{a \in \{1, \dots, K\}} \hat{\mu}_a(t)$$

$$\hat{\mu}_a(t) = \frac{1}{N_a(t)} \sum_{s=1}^t X_{a,s} \mathbb{1}_{(A_s=a)}$$

is an estimate of the unknown mean μ_a .

⇒ EXPLOITATION $\mathcal{R}_\nu(\mathcal{A}, T) \geq (1 - \mu_1) \times \mu_2 \times (\mu_1 - \mu_2) T$
(Bernoulli arms)

A better idea : Explore-Then-Commit

Given $m \in \{1, \dots, T/K\}$,

- ▶ draw each arm m times
- ▶ compute the empirical best arm $\hat{a} = \operatorname{argmax}_a \hat{\mu}_a(Km)$
- ▶ keep playing this arm until round T

$$A_{t+1} = \hat{a} \text{ for } t \geq Km$$

⇒ EXPLORATION followed by EXPLOITATION

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Analysis for two arms. $\mu_1 > \mu_2$, $\Delta := \mu_1 - \mu_2$.

$$\begin{aligned}\mathcal{R}_\nu(\text{ETC}, T) &= \Delta \mathbb{E}[N_2(T)] \\ &= \Delta \mathbb{E}[m + (T - 2m) \mathbb{1}(\hat{a} = 2)] \\ &\leq \Delta m + (\Delta T) \times \mathbb{P}(\hat{\mu}_{2,m} \geq \hat{\mu}_{1,m})\end{aligned}$$

$\hat{\mu}_{a,m}$: empirical mean of the first m observations from arm a

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$\hat{\mu}_{a,m}$: empirical mean of the first m observations from arm a
→ requires a concentration inequality

Intermezzo : Concentration Inequalities

Sub-Gaussian random variables : Z is σ^2 -subGaussian if

$$\mathbb{E}[Z] = \mu \quad \text{and} \quad \mathbb{E} \left[e^{\lambda(Z-\mu)} \right] \leq e^{\frac{\lambda^2 \sigma^2}{2}}. \quad (1)$$

Hoeffding inequality

Z_i i.i.d. satisfying (1). For all $s \geq 1$

$$\mathbb{P} \left(\frac{Z_1 + \cdots + Z_s}{s} \geq \mu + x \right) \leq e^{-\frac{sx^2}{2\sigma^2}}$$

Proof : Cramér-Chernoff method

- ▶ ν_a bounded in $[a, b] : (b - a)^2/4$ sub-Gaussian (Hoeffding's lemma)
- ▶ $\nu_a = \mathcal{N}(\mu_a, \sigma^2) : \sigma^2$ sub-Gaussian

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Assumption : ν_1, ν_2 are bounded in $[0, 1]$.

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Analysis for two arms. $\mu_1 > \mu_2$, $\Delta := \mu_1 - \mu_2$.

Assumption : ν_1, ν_2 are bounded in $[0, 1]$.

For $m = \frac{2}{\Delta^2} \log\left(\frac{T\Delta^2}{2}\right)$,

$$\mathcal{R}_\nu(\text{ETC}, T) \leq \frac{2}{\Delta} \left[\log\left(\frac{T\Delta^2}{2}\right) + 1 \right].$$

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+ logarithmic regret !

- requires the knowledge of T and Δ

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A simple strategy : ϵ -greedy

The ϵ -greedy rule [Sutton and Barto, 2018] is the simplest way to alternate exploration and exploitation.

ϵ -greedy strategy

At round t ,

- ▶ with probability ϵ

$$A_t \sim \mathcal{U}(\{1, \dots, K\})$$

- ▶ with probability $1 - \epsilon$

$$A_t = \operatorname{argmax}_{a=1, \dots, K} \hat{\mu}_a(t).$$

→ Linear regret : $\mathcal{R}_\nu(\epsilon\text{-greedy}, T) \geq \epsilon \frac{K-1}{K} \Delta_{\min} T$.

$$\Delta_{\min} = \min_{a: \mu_a < \mu_*} \Delta_a$$

A simple strategy : ϵ -greedy

A simple fix :

ϵ_t -greedy strategy

At round t ,

- ▶ with probability $\epsilon_t := \min\left(1, \frac{K}{d^2 t}\right)$

$$A_t \sim \mathcal{U}(\{1, \dots, K\})$$

- ▶ with probability $1 - \epsilon_t$

$$A_t = \operatorname{argmax}_{a=1, \dots, K} \hat{\mu}_a(t-1).$$

Theorem [Auer, 2002]

If $0 < d \leq \Delta_{\min}$, $\mathcal{R}_\nu(\epsilon_t\text{-greedy}, T) = O\left(\frac{K \log(T)}{d^2}\right)$.

→ requires the knowledge of a lower bound on Δ_{\min} ...

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The optimism principle

Step 1 : construct a set of statistically plausible models

- ▶ For each arm a , build a confidence interval on the mean μ_a :

$$\mathcal{I}_a(t) = [\text{LCB}_a(t), \text{UCB}_a(t)]$$

LCB = Lower Confidence Bound

UCB = Upper Confidence Bound

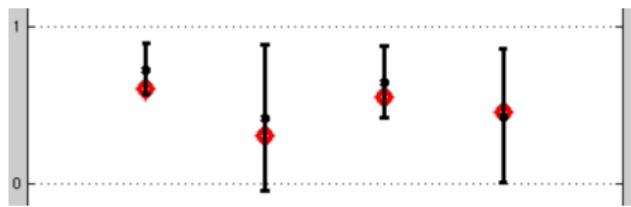


Figure – Confidence intervals on the means after t rounds

The optimism principle

Step 2 : act as if the best possible model were the true model
(optimism in face of uncertainty)

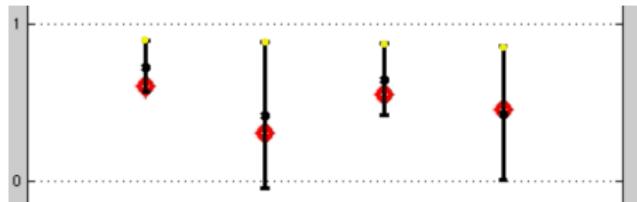


Figure – Confidence intervals on the means after t rounds

$$\text{Optimistic bandit model} = \operatorname{argmax}_{\mu \in \mathcal{C}(t)} \max_{a=1, \dots, K} \mu_a$$

- ▶ That is, select

$$A_{t+1} = \operatorname{argmax}_{a=1, \dots, K} \text{UCB}_a(t).$$

How to build confidence intervals ?

We need $UCB_a(t)$ such that

$$\mathbb{P}(\mu_a \leq UCB_a(t)) \gtrsim 1 - t^{-1}.$$

→ tool : concentration inequalities

Example : rewards are σ^2 sub-Gaussian

Hoeffding inequality, reloaded

Z_i i.i.d. satisfying (1). For all $s \geq 1$

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⚠ Cannot be used directly in a bandit model as **the number of observations from each arm is random !**

How to build confidence intervals ?

- ▶ $N_a(t) = \sum_{s=1}^t \mathbb{1}_{(A_s=a)}$ number of selections of a after t rounds
- ▶ $\hat{\mu}_{a,s} = \frac{1}{s} \sum_{k=1}^s Y_{a,k}$ average of the first s observations from arm a
- ▶ $\hat{\mu}_a(t) = \hat{\mu}_{a,N_a(t)}$ empirical estimate of μ_a after t rounds

Hoeffding inequality + union bound

$$\mathbb{P} \left(\mu_a \leq \hat{\mu}_a(t) + \sigma \sqrt{\frac{\beta \log(t)}{N_a(t)}} \right) \geq 1 - \frac{1}{t^{\frac{\beta}{2}-1}}$$

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Proof.

$$\begin{aligned} \mathbb{P} \left(\mu_a > \hat{\mu}_a(t) + \sigma \sqrt{\frac{\beta \log(t)}{N_a(t)}} \right) &\leq \mathbb{P} \left(\exists s \leq t : \mu_a > \hat{\mu}_{a,s} + \sigma \sqrt{\frac{\beta \log(t)}{s}} \right) \\ &\leq \sum_{s=1}^t \mathbb{P} \left(\hat{\mu}_{a,s} < \mu_a - \sigma \sqrt{\frac{\beta \log(t)}{s}} \right) \leq \sum_{s=1}^t \frac{1}{t^{\beta/2}} = \frac{1}{t^{\beta/2-1}}. \end{aligned}$$

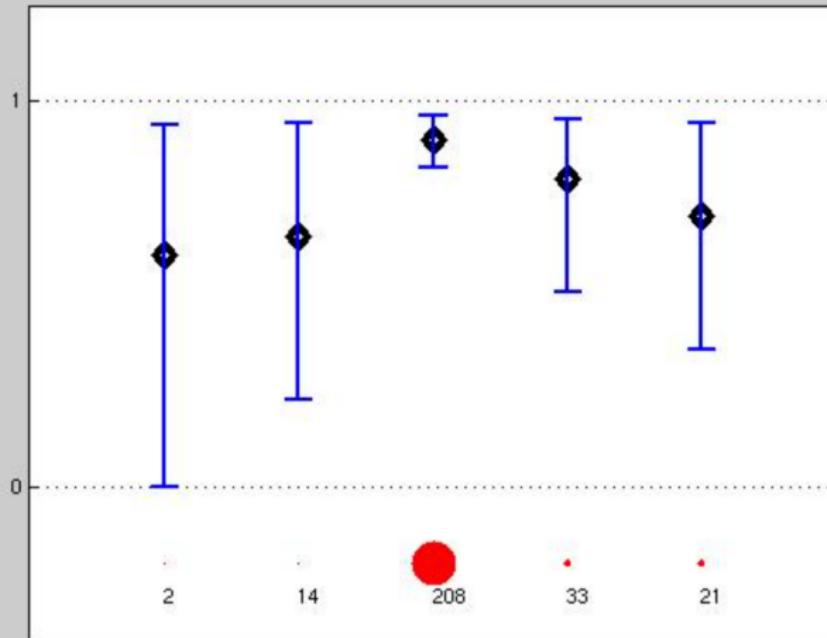
A first UCB algorithm

UCB(α) selects $A_{t+1} = \operatorname{argmax}_a \text{UCB}_a(t)$ where

$$\text{UCB}_a(t) = \underbrace{\hat{\mu}_a(t)}_{\text{exploitation term}} + \underbrace{\sqrt{\frac{\alpha \log(t)}{N_a(t)}}}_{\text{exploration bonus}}.$$

- ▶ popularized by [Auer, 2002] for bounded rewards : [UCB1](#), for $\alpha = 2$
- ▶ the analysis was UCB(α) was further refined to hold for $\alpha > 1/2$, still for bounded rewards [Bubeck, 2010]

A UCB algorithm in action



Regret of UCB(α)

Context : σ^2 sub-Gaussian rewards

$$\text{UCB}_a(t) = \hat{\mu}_a(t) + \sqrt{\frac{2\sigma^2(\log(t) + c \log \log(t))}{N_a(t)}}$$

Theorem [Cappé et al.'13]

For $c \geq 3$, the UCB algorithm associated to the above index satisfy

$$\mathbb{E}[N_a(T)] \leq \frac{2\sigma^2}{(\mu_* - \mu_a)^2} \log(T) + C_\mu \sqrt{\log(T)}.$$

if the rewards distributions are σ^2 sub-Gaussian.

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if the rewards distributions are σ^2 sub-Gaussian.

► regret bound for Gaussian distribution with variance σ^2 :

$$\mathcal{R}_\nu(\text{UCB}(\alpha), T) = 2\sigma^2 \left(\sum_{a: \mu_a < \mu_*} \frac{1}{\Delta_a} \right) \log(T) + \mathcal{O}(\sqrt{\log(T)})$$

for $\alpha = 2\sigma^2$.

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if the rewards distributions are σ^2 sub-Gaussian.

► regret bound for distributions that are bounded in $[0, 1]$:

$$\mathcal{R}_\nu(\text{UCB}(\alpha), T) = \frac{1}{2} \left(\sum_{a: \mu_a < \mu_*} \frac{1}{\Delta_a} \right) \log(T) + \mathcal{O}(\sqrt{\log(T)})$$

for $\alpha = 1/2$.

Is UCB(α) the best possible algorithm ?

Context : a **parametric bandit model** where each arm is parameterized by its mean $\nu = (\nu_{\mu_1}, \dots, \nu_{\mu_K})$, $\mu_a \in \mathcal{I}$.

$$\nu \leftrightarrow \mu = (\mu_1, \dots, \mu_K)$$

Key tool : **Kullback-Leibler divergence**.

Kullback-Leibler divergence

$$\text{kl}(\mu, \mu') := \text{KL}(\nu_\mu, \nu_{\mu'}) = \mathbb{E}_{X \sim \nu_\mu} \left[\log \frac{d\nu_\mu}{d\nu_{\mu'}}(X) \right]$$

Lower bound [Lai et al., 1985]

For *uniformly good* algorithm,

$$\mu_a < \mu_\star \Rightarrow \liminf_{T \rightarrow \infty} \frac{\mathbb{E}_\mu[N_a(T)]}{\log T} \geq \frac{1}{\text{kl}(\mu_a, \mu_\star)}$$

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Kullback-Leibler divergence

$$\text{kl}(\mu, \mu') := \frac{(\mu - \mu')^2}{2\sigma^2} \quad (\text{Gaussian bandits})$$

Lower bound [Lai et al., 1985]

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Kullback-Leibler divergence

$$\text{kl}(\mu, \mu') := \mu \log \left(\frac{\mu}{\mu'} \right) + (1 - \mu) \log \left(\frac{1 - \mu}{1 - \mu'} \right) \quad (\text{Bernoulli bandits})$$

Lower bound [Lai et al., 1985]

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Comparing upper and lower bounds

For Gaussian bandits with variance σ^2 ,

- ▶ **Upper bound for UCB($2\sigma^2$) :**

$$\mathcal{R}_\nu(\text{UCB}, T) \lesssim \sum_{a: \mu_a < \mu_*} \frac{2\sigma^2}{(\mu^* - \mu_a)} \log(T)$$

- ▶ **Lower bound :** for large values of T ,

$$\mathcal{R}_\nu(\mathcal{A}, T) \gtrsim \sum_{a: \mu_a < \mu_*} \frac{(\mu_* - \mu_a)}{\text{kl}(\mu_a, \mu_*)} \log(T)$$

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- UCB is **asymptotically optimal** for Gaussian bandits !

Comparing upper and lower bounds

For **Bernoulli bandits** (that are bounded in $[0, 1]$),

- ▶ **Upper bound for UCB(1/2) :**

$$\mathcal{R}_\nu(\text{UCB}, T) \lesssim \sum_{a: \mu_a < \mu_*} \frac{1}{2(\mu^* - \mu_a)} \log(T)$$

- ▶ **Lower bound :** for large values of T ,

$$\mathcal{R}_\nu(\mathcal{A}, T) \gtrsim \sum_{a: \mu_a < \mu_*} \frac{(\mu_* - \mu_a)}{\text{kl}(\mu_a, \mu_*)} \log(T)$$

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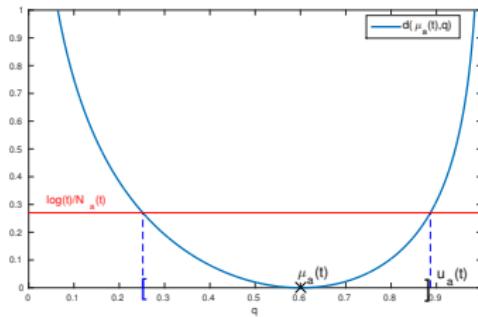
- UCB is *not* asymptotically optimal for Bernoulli bandits...

Pinsker's inequality : $\text{kl}(\mu, \mu') \geq 2(\mu - \mu')^2$

The kl -UCB algorithm

Exploits the KL-divergence in the lower bound !

$$\text{UCB}_a(t) = \max \left\{ q \in [0, 1] : \text{kl}(\hat{\mu}_a(t), q) \leq \frac{\log(t)}{N_a(t)} \right\}.$$



A tighter concentration inequality [Garivier and Cappé, 2011]

For Bernoulli rewards

$$\mathbb{P}(\text{UCB}_a(t) > \mu_a) \gtrsim 1 - \frac{1}{t \log(t)}.$$

An asymptotically optimal algorithm

kl-UCB selects $A_{t+1} = \operatorname{argmax}_a \text{UCB}_a(t)$ with

$$\text{UCB}_a(t) = \max \left\{ q \in [0, 1] : \text{kl}(\hat{\mu}_a(t), q) \leq \frac{\log(t) + c \log \log(t)}{N_a(t)} \right\}.$$

Theorem [Cappé et al., 2013]

If $c \geq 3$, for every arm such that $\mu_a < \mu_*$,

$$\mathbb{E}_\mu[N_a(T)] \leq \frac{1}{\text{kl}(\mu_a, \mu_*)} \log(T) + C_\mu \sqrt{\log(T)}.$$

► kl-UCB is **asymptotically optimal** for Bernoulli bandits :

$$\mathcal{R}_\mu(\text{kl-UCB}, T) \simeq \left(\sum_{a: \mu_a < \mu_*} \frac{\mu_* - \mu_a}{\text{kl}(\mu_a, \mu_*)} \right) \log(T).$$

Outline

- 1 Performance measure and first strategies
- 2 Mixing Exploration and Exploitation
 - Upper Confidence Bound algorithms
- 3 Bayesian bandit algorithms
 - Thompson Sampling

Frequentist versus Bayesian bandit

Context : parametric bandit model $\nu_{\mu} = (\nu_{\mu_1}, \dots, \nu_{\mu_K})$.

- ▶ Two probabilistic models

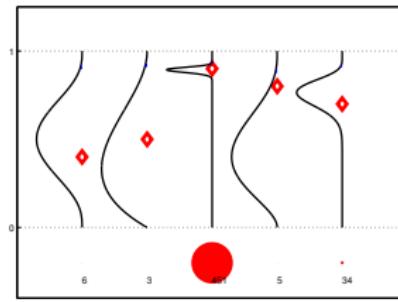
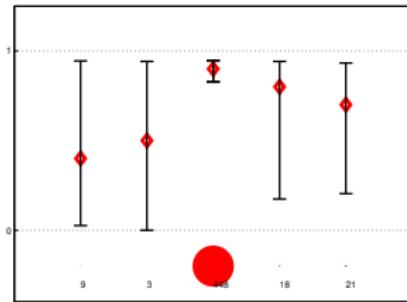
Frequentist model	Bayesian model
μ_1, \dots, μ_K unknown parameters	μ_1, \dots, μ_K drawn from a prior distribution : $\mu_a \sim \pi_a$
arm a : $(Y_{a,s})_s \stackrel{\text{i.i.d.}}{\sim} \nu_{\mu_a}$	arm a : $(Y_{a,s})_s \mu \stackrel{\text{i.i.d.}}{\sim} \nu_{\mu_a}$

where $(Y_{a,s})$ is the sequence of successive rewards obtained from arm a

Frequentist and Bayesian algorithms

- ▶ Two types of tools to build bandit algorithms :

Frequentist tools	Bayesian tools
MLE estimators of the means Confidence Intervals	Posterior distributions $\pi_a^t = \mathcal{L}(\mu_a Y_{a,1}, \dots, Y_{a,N_a(t)})$



Example : Bernoulli bandits

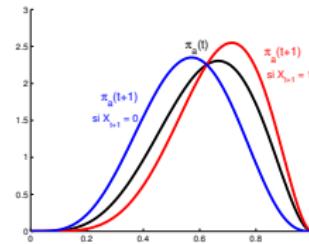
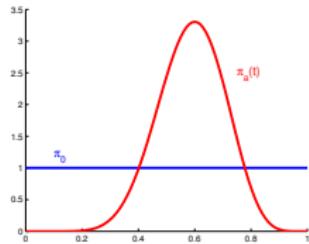
Bernoulli bandit model $\mu = (\mu_1, \dots, \mu_K)$

- ▶ **Bayesian view** : μ_1, \dots, μ_K are random variables
prior distribution : $\mu_a \sim \mathcal{U}([0, 1])$

- posterior distribution :

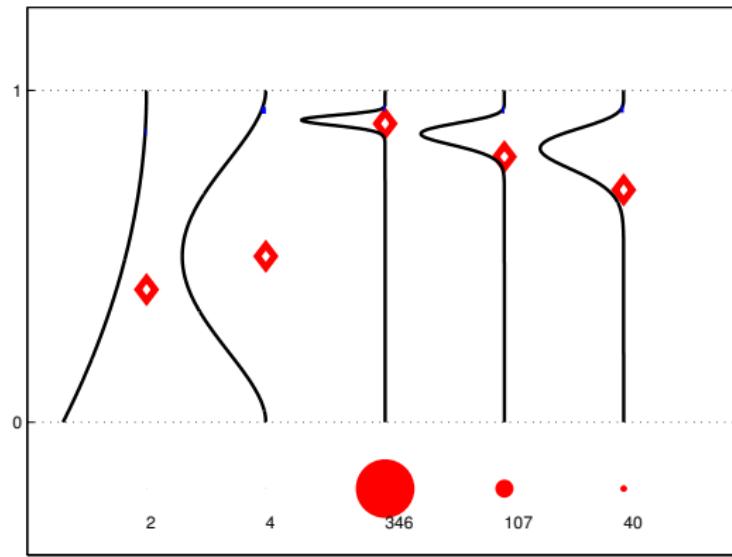
$$\begin{aligned}\pi_a(t) &= \mathcal{L}(\mu_a | R_1, \dots, R_t) \\ &= \text{Beta}\left(\underbrace{S_a(t)}_{\# \text{ones}} + 1, \underbrace{N_a(t) - S_a(t)}_{\# \text{zeros}} + 1\right)\end{aligned}$$

$S_a(t) = \sum_{s=1}^t R_s \mathbb{1}_{(A_s=a)}$ sum of the rewards.



Bayesian algorithm

A **Bayesian bandit algorithm** exploits the posterior distributions of the means to decide which arm to select.



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Thompson Sampling

A very old idea : [Thompson, 1933].

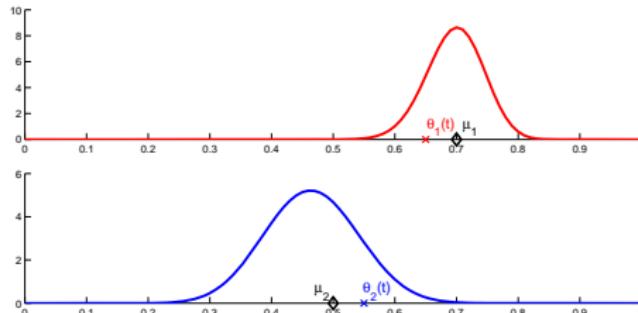
Two equivalent interpretations :

- ▶ “select an arm at random according to its probability of being the best”
- ▶ “draw a possible bandit model from the posterior distribution and act optimally in this sampled model”

≠ optimistic

Thompson Sampling : a randomized Bayesian algorithm

$$\begin{cases} \forall a \in \{1..K\}, \theta_a(t) \sim \pi_a(t) \\ A_{t+1} = \underset{a=1 \dots K}{\operatorname{argmax}} \theta_a(t). \end{cases}$$



Thompson Sampling is asymptotically optimal

Problem-dependent regret

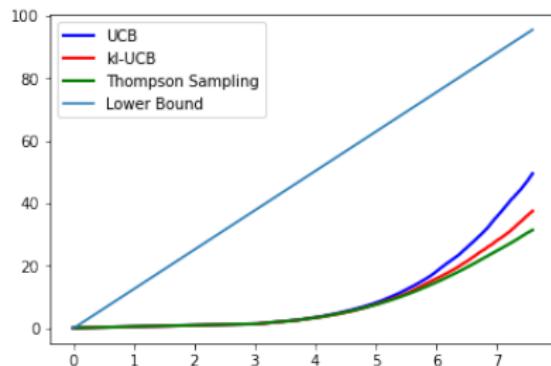
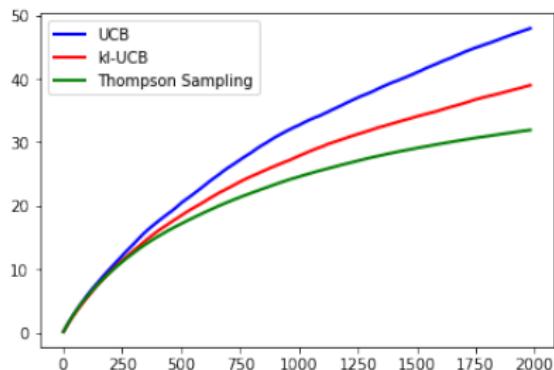
$$\forall \epsilon > 0, \quad \mathbb{E}_\mu[N_a(T)] \leq (1 + \epsilon) \frac{1}{\text{kl}(\mu_a, \mu_*)} \log(T) + o_{\mu, \epsilon}(\log(T)).$$

This result holds :

- ▶ for **Bernoulli bandits**, with a **uniform prior**
[Kaufmann et al., 2012, Agrawal and Goyal, 2013]
- ▶ for **Gaussian bandits**, with **Gaussian prior** [Agrawal and Goyal, 2017]
- ▶ for **exponential family bandits**, with **Jeffrey's prior**
[Korda et al., 2013]

Bayesian versus Frequentist algorithms

- ▶ Regret up to $T = 2000$ (average over $N = 200$ runs) as a function of T (resp. $\log(T)$)



$$\mu = [0.1 \ 0.15 \ 0.2 \ 0.25]$$

Summary

Several ways to solve the exploration/exploitation trade-off, mostly

- ▶ the optimism-in-face-of-uncertainty principle (**UCB**)
- ▶ posterior sampling (**Thompson Sampling**)

What do they need ?

- ▶ UCB : the capacity to build a **confidence region** for the unknown model parameters and compute the best possible model
- ▶ Thompson Sampling : the ability to define a **prior distribution** and sample from the corresponding posterior distribution
- these principles can be extended to more challenging bandit problems and to reinforcement learning

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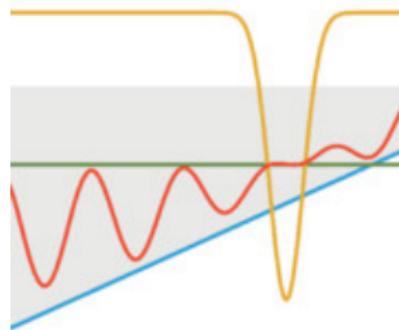
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Bandit Algorithms

TOR LATTIMORE
CSABA SZEPESVÁRI



The Bandit Book

by [Lattimore and Szepesvári, 2020]