Sequential Decision Making

Lecture 2 : Stochastic bandits

Emilie Kaufmann



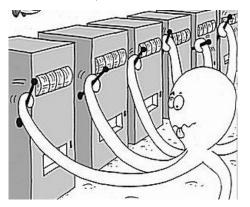




M2 Data Science, 2022/2023

Why bandits?

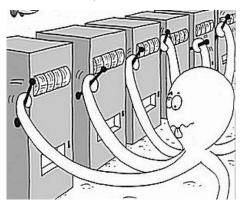
▶ Make money in a casino? (one-armed bandit = slot machine)



an agent facing arms in a Multi-Armed Bandit

Why bandits?

▶ Make money in a casino? (one-armed bandit = slot machine)



an agent facing arms in a Multi-Armed Bandit



Sequential resource allocation

Clinical trials

K treatment 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







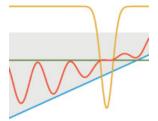


Which add should be displayed for a user, based on the previous clicks of previous (similar) users?

Useful reference



TOR LATTIMORE CSABA SZEPESVÁRI



The Bandit Book

by [Lattimore and Szepesvari, 2019]

The Multi-Armed Bandit Setup

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











At round t, an agent :

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

Sequential sampling strategy (bandit algorithm) :

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

Goal (for now!) : 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 :

- \triangleright chooses an arm A_t
- ightharpoonup receives a reward $R_t = X_{A_t,t} \sim \nu_{A_t}$

Sequential sampling strategy (bandit algorithm) :

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

Goal (for now!) : 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
- $lackbox{ observes a response } R_t \in \{0,1\}: \mathbb{P}(R_t=1|A_t=a)=\mu_a$

Goal: maximize the expected number of patients healed

Online content optimization

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











For the *t*-th visitor of a website.

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

Goal: maximize the sum of ratings

Outline

- 1 Performance measure and first strategies
- 2 Best achievable regret
- 3 Mixing Exploration and Exploitation
 - Upper Confidence Bound algorithms
- 4 Bayesian algorithms
 - Thompson Sampling

Regret of a bandit algorithm

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

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

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

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

What regret rate can we achieve?

- ightharpoonup consistency : $rac{\mathcal{R}_{
 u}(\mathcal{A},T)}{T}
 ightarrow 0$
- → 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

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

Proof.



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

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

A strategy with small regret should :

- ightharpoonup select not too often arms for which $\Delta_a > 0$
- ightharpoonup ... 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

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

Two naive strategies

▶ Idea 1 : Uniform Exploration

Draw each arm T/K times

where

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

▶ Idea 2 : Follow The Leader

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

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

is an estimate of the unknown mean μ_a .

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

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

- 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*

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

⇒ EXPLORATION followed by EXPLOITATION

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

- 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*

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

⇒ EXPLORATION followed by EXPLOITATION

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

$$\mathcal{R}_{\nu}(\text{ETC}, T) = \Delta \mathbb{E}[N_2(T)]$$

$$= \Delta \mathbb{E}[m + (T - 2m)\mathbb{1}(\hat{a} = 2)]$$

$$\leq \Delta m + (\Delta T) \times \mathbb{P}(\hat{\mu}_{2,m} \geq \hat{\mu}_{1,m})$$

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

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

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

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

⇒ EXPLORATION followed by EXPLOITATION

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

$$\mathcal{R}_{\nu}(\text{ETC}, T) = \Delta \mathbb{E}[N_2(T)]$$

$$= \Delta \mathbb{E}[m + (T - 2m)\mathbb{1}(\hat{a} = 2)]$$

$$\leq \Delta m + (\Delta T) \times \mathbb{P}(\hat{\mu}_{2,m} \geq \hat{\mu}_{1,m})$$

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

Intermezzo: Concentration Inequalities

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

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

Hoeffding inequality

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

$$\mathbb{P}\left(\frac{Z_1 + \dots + Z_s}{s} \ge \mu + x\right) \le e^{-\frac{sx^2}{2\sigma^2}}$$

Proof: Cramér-Chernoff method

- \triangleright 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

Intermezzo: Concentration Inequalities

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

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

Hoeffding inequality

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

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

Proof: Cramér-Chernoff method

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

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

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

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

⇒ EXPLORATION followed by EXPLOITATION

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

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

$$\mathcal{R}_{\nu}(T) = \Delta \mathbb{E}[N_2(T)]$$

$$= \Delta \mathbb{E}[m + (T - 2m)\mathbb{1}(\hat{a} = 2)]$$

$$< \Delta m + (\Delta T) \times \mathbb{P}(\hat{\mu}_{2m} > \hat{\mu}_{1m})$$

 $\hat{\mu}_{a,m}$: empirical mean of the first m observations from arm $a \to \text{Hoeffding's inequality}$

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

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

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

⇒ EXPLORATION followed by EXPLOITATION

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

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

$$\mathcal{R}_{\nu}(T) = \Delta \mathbb{E}[N_2(T)]$$

$$= \Delta \mathbb{E}[m + (T - 2m)\mathbb{1}(\hat{a} = 2)]$$

$$< \Delta m + (\Delta T) \times \exp(-m\Delta^2/2)$$

 $\hat{\mu}_{a,m}$: empirical mean of the first m observations from arm $a \to \text{Hoeffding's inequality}$

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

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

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

⇒ EXPLORATION followed by EXPLOITATION

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

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

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

$$\mathcal{R}_{
u}(\mathtt{ETC},\,\mathcal{T}) \leq rac{2}{\Delta} \left[\log \left(rac{\mathcal{T}\Delta^2}{2}
ight) + 1
ight].$$

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

- 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*

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

⇒ EXPLORATION followed by EXPLOITATION

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

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

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

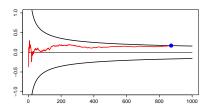
$$\mathcal{R}_{
u}(\mathtt{ETC}, \mathcal{T}) \leq rac{2}{\Delta} \left[\log \left(rac{\mathcal{T}\Delta^2}{2}
ight) + 1
ight].$$

- + logarithmic regret!
- requires the knowledge of T and Δ

Sequential Explore-Then-Commit

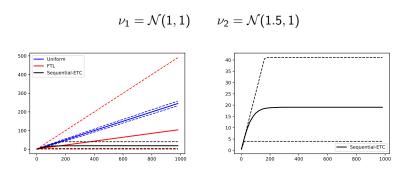
explore uniformly until a random time of the form

$$au = \inf \left\{ t \in \mathbb{N} : |\hat{\mu}_1(t) - \hat{\mu}_2(t)| > \sqrt{rac{c \log(T/t)}{t}}
ight\}$$



- $\hat{a}_{\tau} = \operatorname{argmax}_{\hat{a}} \hat{\mu}_{a}(\tau)$ and $(A_{t+1} = \hat{a}_{\tau})$ for $t \in \{\tau + 1, \dots, T\}$
- → [Garivier et al., 2016] for two Gaussian arms, for c=8, same regret as ETC, without the knowledge of Δ

Numerical illustration



Expected regret estimated over N = 500 runs for Sequential-ETC versus two naive baselines.

(dashed lines: empirical 0.05% and 0.95% quantiles of the regret)

Outline

- 1 Performance measure and first strategies
- 2 Best achievable regret
- 3 Mixing Exploration and Exploitation
 - Upper Confidence Bound algorithms
- 4 Bayesian algorithms
 - Thompson Sampling

Examples of regret rates

For two-armed bandits with bounded rewards, $\Delta = |\mu_1 - \mu_2|$

$$\mathcal{R}_{
u}(\mathtt{ETC},T)\lesssim rac{2}{\Delta}\log\left(T\Delta^{2}
ight).$$

problem-dependent logarithmic regret bound

Remark: blows up when Δ tends to zero...

$$\mathcal{R}_{\nu}(\text{ETC}, T) \lesssim \min \left[\frac{2}{\Delta} \log \left(T \Delta^{2} \right), \Delta T \right]$$

$$\leq \sqrt{T} \max_{u>0} \left(\min \left[\frac{2}{u} \log(u^{2}); u \right] \right)$$

$$< C\sqrt{T}.$$

problem-independent square-root regret bound

The Lai and Robbins lower bound

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

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

Key tool: Kullback-Leibler divergence.

Kullback-Leibler divergence

$$\mathrm{kl}(\mu,\mu') := \mathsf{KL}\left(
u_{\mu},
u_{\mu'}
ight) = \mathbb{E}_{X \sim
u_{\mu}}\left[\log rac{d
u_{\mu}}{d
u_{\mu'}}(X)
ight]$$

Theorem

For uniformly good algorithm,

$$\mu_{a} < \mu_{\star} \Rightarrow \liminf_{T \to \infty} \frac{\mathbb{E}_{\mu}[N_{a}(T)]}{\log T} \geq \frac{1}{\mathrm{kl}(\mu_{a}, \mu_{\star})}$$

[Lai and Robbins, 1985]

- 20

The Lai and Robbins lower bound

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

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

Key tool: Kullback-Leibler divergence.

Kullback-Leibler divergence

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

Theorem

For uniformly good algorithm,

$$\mu_{\mathsf{a}} < \mu_{\star} \Rightarrow \liminf_{T \to \infty} \frac{\mathbb{E}_{\mu}[N_{\mathsf{a}}(T)]}{\log T} \ge \frac{1}{\mathrm{kl}(\mu_{\mathsf{a}}, \mu_{\star})}$$

[Lai and Robbins, 1985]

The Lai and Robbins lower bound

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

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

Key tool: Kullback-Leibler divergence.

Kullback-Leibler divergence

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

Theorem

For uniformly good algorithm,

$$\mu_{\mathsf{a}} < \mu_{\star} \Rightarrow \liminf_{T \to \infty} \frac{\mathbb{E}_{\boldsymbol{\mu}}[N_{\mathsf{a}}(T)]}{\log T} \geq \frac{1}{\mathrm{kl}(\mu_{\mathsf{a}}, \mu_{\star})}$$

[Lai and Robbins, 1985]

- 20

Some room for better algorithms!

A particular case of parameteric and bounded distributions :

$$\nu_1 = \mathcal{B}(\mu_1)$$
 $\nu_2 = \mathcal{B}(\mu_2)$

- ▶ Regret of ETC : $\mathcal{R}_{\nu}(\mathrm{ETC}, T) \lesssim \frac{2}{\Delta} \log (T\Delta^2)$
- ▶ Lower bound : $\mathcal{R}_{\nu}(\mathcal{A}, T) \gtrsim \frac{\Delta}{\mathrm{kl}(\mu_2, \mu_1)} \log \left(T \Delta^2 \right)$

Pinsker's inequality : $kl(\mu_2, \mu_1) \ge 2(\mu_1 - \mu_2)^2$.

→ Explore-Then-Commit does not match the lower bound...

Outline

- 1 Performance measure and first strategies
- 2 Best achievable regret
- 3 Mixing Exploration and Exploitation
 - Upper Confidence Bound algorithms
- 4 Bayesian algorithms
 - Thompson Sampling

A simple strategy : ϵ -greedy

The ϵ -greedy rule [Sutton and Barto, 1998] is the simplest way to alternate exploration and exploitation.

ϵ -greedy strategy

At round t,

ightharpoonup with probability ϵ

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

ightharpoonup with probability $1-\epsilon$

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

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

$$\Delta_{\min} = \min_{a:u_a < u_a} \Delta_a$$

A simple strategy : ϵ -greedy

A simple fix:

ϵ_t -greedy strategy

At round t,

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

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

ightharpoonup with probability $1 - \epsilon_t$

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

Theorem [Auer et al., 2002]

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

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

Outline

- 1 Performance measure and first strategies
- 2 Best achievable regret
- 3 Mixing Exploration and Exploitation
 - Upper Confidence Bound algorithms
- 4 Bayesian algorithms
 - Thompson Sampling

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 :

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

 $egin{aligned} LCB = \mbox{Lower Confidence Bound} \\ UCB = \mbox{Upper Confidence Bound} \end{aligned}$

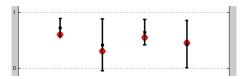


FIGURE - Confidence intervals on the means after t rounds

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

Optimistic bandit model =
$$\operatorname*{argmax}_{\boldsymbol{\mu} \in \mathcal{C}(t)} \operatorname*{max}_{\boldsymbol{\sigma} = 1, \dots, K} \boldsymbol{\mu}_{\boldsymbol{\sigma}}$$

▶ That is, select

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

We need $UCB_a(t)$ such that

$$\mathbb{P}\left(\mu_{\mathsf{a}} \leq \mathrm{UCB}_{\mathsf{a}}(t)\right) \gtrsim 1 - t^{-1}.$$

→ tool : concentration inequalities

Example : rewards are σ^2 sub-Gaussian

Hoeffding inequality, reloaded

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

$$\mathbb{P}\left(\frac{Z_1 + \dots + Z_s}{s} < \mu - x\right) \le e^{-\frac{sx^2}{2\sigma^2}}$$

We need $UCB_a(t)$ such that

$$\mathbb{P}\left(\mu_{\mathsf{a}} \leq \mathrm{UCB}_{\mathsf{a}}(t)\right) \gtrsim 1 - t^{-1}.$$

→ tool : concentration inequalities

Example : rewards are σ^2 sub-Gaussian

Hoeffding inequality, reloaded

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

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

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

- $N_a(t) = \sum_{s=1}^t \mathbb{1}_{(A_s=a)}$ 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

$$\mathbb{P}\left(\mu_{\mathsf{a}} \leq \hat{\mu}_{\mathsf{a}}(t) + \sigma \sqrt{\frac{\beta \log(t)}{N_{\mathsf{a}}(t)}}\right) \geq 1 - \frac{1}{t^{\frac{\beta}{2} - 1}}$$

- $N_a(t) = \sum_{s=1}^t \mathbb{1}_{(A_s=a)}$ 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

$$\mathbb{P}\left(\mu_{\mathsf{a}} \leq \hat{\mu}_{\mathsf{a}}(t) + \sigma \sqrt{\frac{\beta \log(t)}{N_{\mathsf{a}}(t)}}\right) \geq 1 - \frac{1}{t^{\frac{\beta}{2} - 1}}$$

Proof.

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

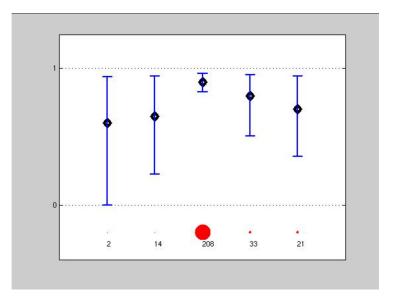
A first UCB algorithm

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

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

- ▶ popularized by [Auer et al., 2002] for bounded rewards : UCB1, for $\alpha = 2$
- ▶ the analysis of UCB(α) was further refined to hold for $\alpha > 1/2$ in that case [Bubeck, 2010, Cappé et al., 2013]

A UCB algorithm in action



Regret of $UCB(\alpha)$ for bounded rewards

Theorem

For every $\alpha>1$ and every sub-optimal arm a, there exists a constant $\mathcal{C}_{\alpha}>0$ such that

$$\mathbb{E}_{\boldsymbol{\mu}}[N_{\mathsf{a}}(T)] \leq \frac{4\alpha}{(\mu_{\star} - \mu_{\mathsf{a}})^2} \log(T) + C_{\alpha}.$$

Proof:



Context : σ^2 sub-Gaussian rewards

$$ext{UCB}_{a}(t) = \hat{\mu}_{a}(t) + \sqrt{rac{2\sigma^{2}(\log(t) + c\log\log(t))}{N_{a}(t)}}$$

Theorem [Cappé et al.'13]

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

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

Context : σ^2 sub-Gaussian rewards

$$ext{UCB}_{a}(t) = \hat{\mu}_{a}(t) + \sqrt{rac{2\sigma^{2}(\log(t) + c\log\log(t))}{N_{a}(t)}}$$

Theorem [Cappé et al.'13]

For c > 3, the UCB algorithm associated to the above index satisfy

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

► Gaussian rewards :

$$\mathcal{R}_{\nu}(\mathrm{UCB},T)\lesssim \left(\sum_{a:u_a\leq u_a} rac{2\sigma^2}{\Delta_a}
ight)\log(T).$$

→ matching the Lai and Robbins lower bound! asymptotically optimal

Context : σ^2 sub-Gaussian rewards

$$UCB_{a}(t) = \hat{\mu}_{a}(t) + \sqrt{\frac{2\sigma^{2}(\log(t) + c\log\log(t))}{N_{a}(t)}}$$

Theorem [Cappé et al.'13]

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

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

► Bernoulli rewards :

$$\mathcal{R}_{\nu}(\mathrm{UCB}, T) \lesssim \left(\sum_{a: \mu_a < \mu_a} \frac{1}{2\Delta_a}\right) \log(T)$$

→ optimal?

Context : σ^2 sub-Gaussian rewards

$$ext{UCB}_{a}(t) = \hat{\mu}_{a}(t) + \sqrt{rac{2\sigma^{2}(\log(t) + c\log\log(t))}{N_{a}(t)}}$$

Theorem [Cappé et al.'13]

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

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

Bernoulli rewards :

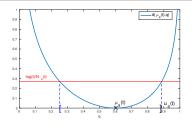
$$\mathcal{R}_{
u}(\mathrm{UCB},T)
eq \left(\sum_{eta: \mu_{a} < \mu_{\star}} rac{\Delta_{a}}{\mathrm{kl}(\mu_{a},\mu_{\star})}
ight) \log(T)$$

→ not matching the Lai and Robbins lower bound

The kl-UCB algorithm

Exploits the KL-divergence in the lower bound!

$$\mathrm{UCB}_{\mathsf{a}}(t) = \max \left\{ q \in [0,1] : \mathrm{kl}\left(\hat{\mu}_{\mathsf{a}}(t),q\right) \leq \frac{\log(t)}{N_{\mathsf{a}}(t)} \right\}.$$



A tighter concentration inequality [Garivier and Cappé, 2011]

For rewards that belong to a 1-d exponential family (e.g. Bernoulli)

$$\mathbb{P}(\mathrm{UCB}_{\mathsf{a}}(t) > \mu_{\mathsf{a}}) \gtrsim 1 - \frac{1}{t \log(t)}$$

An asymptotically optimal algorithm

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

$$\mathrm{UCB}_{\mathsf{a}}(t) = \max \left\{ q \in [0,1] : \mathrm{kl}\left(\hat{\mu}_{\mathsf{a}}(t), q\right) \leq \frac{\log(t) + c \log\log(t)}{N_{\mathsf{a}}(t)} \right\}.$$

Theorem [Cappé et al., 2013]

If $c \geq 3$, for every arm such that $\mu_a < \mu_{\star}$,

$$\mathbb{E}_{\mu}[N_{a}(T)] \leq \frac{1}{\mathrm{kl}(\mu_{a}, \mu_{\star})} \log(T) + C_{\mu} \sqrt{\log(T)}.$$

asymptotically optimal for rewards in a 1-d exponential family :

$$\mathcal{R}_{m{\mu}}(ext{kl-UCB}, T) \simeq \left(\sum_{a: \mu < \mu} rac{\Delta_a}{ ext{kl}(\mu_a, \mu_\star)}
ight) \log(T).$$

Outline

- 1 Performance measure and first strategies
- 2 Best achievable regret
- 3 Mixing Exploration and Exploitation
 - Upper Confidence Bound algorithms
- 4 Bayesian algorithms
 - Thompson Sampling

Frequentist versus Bayesian bandit

$$\nu_{\boldsymbol{\mu}} = (\nu^{\mu_1}, \dots, \nu^{\mu_K}) \in (\mathcal{P})^K.$$

► 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 $a: (Y_{a,s})_s \overset{\text{i.i.d.}}{\sim} \nu^{\mu_a}$	arm $a:(Y_{a,s})_s \mu\stackrel{\text{i.i.d.}}{\sim} \nu^{\mu_a}$

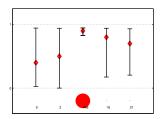
▶ The regret can be computed in each case

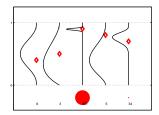
Frequentist regret	Bayesian regret
(regret)	(Bayes risk)
$\mathcal{R}_{oldsymbol{\mu}}(\mathcal{A}, T) = \mathbb{E}_{oldsymbol{\mu}}\!\!\left[\!\sum_{t=1}^{T} \left(\mu_{\star} - \mu_{A_t} ight)\!\right]$	$\mathbb{R}^{\pi}(\mathcal{A}, T) = \mathbb{E}_{\mu \sim \pi} \left[\sum_{t=1}^{T} (\mu_{\star} - \mu_{A_{t}}) \right]$ $= \int \mathcal{R}_{\mu}(\mathcal{A}, T) d\pi(\mu)$

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 $\pi_a^t = \mathcal{L}(\mu_a Y_{a,1},\ldots,Y_{a,N_a(t)})$





Example: Bernoulli bandits

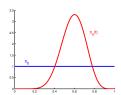
Bernoulli bandit model $\mu = (\mu_1, \dots, \mu_K)$

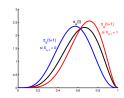
- **Bayesian view** : μ_1, \dots, μ_K are random variables prior distribution : $\mu_a \sim \mathcal{U}([0,1])$
- → posterior distribution :

$$\pi_{a}(t) = \mathcal{L}(\mu_{a}|R_{1}, \dots, R_{t})$$

$$= \operatorname{Beta}\left(\underbrace{S_{a}(t)}_{\#ones} + 1, \underbrace{N_{a}(t) - S_{a}(t)}_{\#zeros} + 1\right)$$

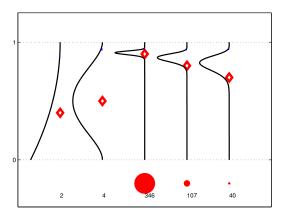
 $S_a(t) = \sum_{s=1}^t R_s \mathbb{1}_{(A_s=a)}$ sum of the rewards.





Bayesian algorithm

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



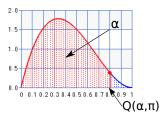
First example : Bayes-UCB

- $ightharpoonup \Pi_0 = (\pi_1(0), \dots, \pi_K(0))$ be a prior distribution over (μ_1, \dots, μ_K)
- ▶ $\Pi_t = (\pi_1(t), \dots, \pi_K(t))$ be the posterior distribution over the means (μ_1, \dots, μ_K) after t observations

Bayes-UCB selects at time t + 1

$$A_{t+1} = \underset{a=1,\dots,K}{\operatorname{argmax}} \ Q\left(1 - \frac{1}{t(\log t)^c}, \pi_a(t)\right)$$

where $Q(\alpha, \pi)$ is the quantile of order α of the distribution π .



First example: Bayes-UCB

- $ightharpoonup \Pi_0 = (\pi_1(0), \dots, \pi_K(0))$ be a prior distribution over (μ_1, \dots, μ_K)
- ▶ $\Pi_t = (\pi_1(t), \dots, \pi_K(t))$ be the posterior distribution over the means (μ_1, \dots, μ_K) after t observations

Bayes-UCB selects at time t+1

$$A_{t+1} = \operatorname*{argmax}_{a=1,\dots,K} \ Q\left(1 - \frac{1}{t(\log t)^c}, \pi_a(t)\right)$$

where $Q(\alpha, \pi)$ is the quantile of order α of the distribution π .

Bernoulli reward with uniform prior:

- $\pi_a(t) = \text{Beta}(S_a(t) + 1, N_a(t) S_a(t) + 1)$

First example: Bayes-UCB

- $ightharpoonup \Pi_0 = (\pi_1(0), \dots, \pi_K(0))$ be a prior distribution over (μ_1, \dots, μ_K)
- ▶ $\Pi_t = (\pi_1(t), \dots, \pi_K(t))$ be the posterior distribution over the means (μ_1, \dots, μ_K) after t observations

Bayes-UCB selects at time t+1

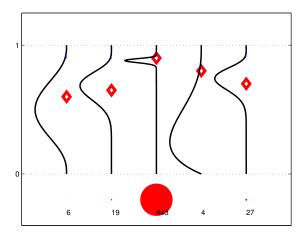
$$A_{t+1} = \underset{a=1,\dots,K}{\operatorname{argmax}} \ Q\left(1 - \frac{1}{t(\log t)^c}, \pi_a(t)\right)$$

where $Q(\alpha, \pi)$ is the quantile of order α of the distribution π .

Gaussian rewards with Gaussian prior:

$$\blacktriangleright \pi_a(0) \stackrel{i.i.d}{\sim} \mathcal{N}(0,\kappa^2)$$

Bayes UCB in action



▶ Bayes-UCB is also asymptotically optimal for Bernoulli distribution

Outline

- 1 Performance measure and first strategies
- 2 Best achievable regret
- 3 Mixing Exploration and Exploitation
 - Upper Confidence Bound algorithms
- 4 Bayesian algorithms
 - Thompson Sampling

Thompson Sampling

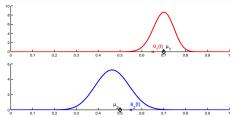
A very old idea: [Thompson, 1933].

Two equivalent interpretations :

- "select an arm at random according to its probability of being the best"

Thompson Sampling: a randomized Bayesian algorithm

$$\left\{ \begin{array}{l} \forall \textit{a} \in \{1..K\}, \quad \theta_{\textit{a}}(t) \sim \pi_{\textit{a}}(t) \\ \textit{A}_{t+1} = \mathop{\mathsf{argmax}}_{\textit{a}=1...K} \theta_{\textit{a}}(t). \end{array} \right.$$



Thompson Sampling is asymptotically optimal

Problem-dependent regret

$$\forall \epsilon > 0, \quad \mathbb{E}_{\boldsymbol{\mu}}[N_{\boldsymbol{a}}(T)] \leq (1+\epsilon) \frac{1}{\mathrm{kl}(\mu_{\boldsymbol{a}}, \mu_{\star})} \log(T) + o_{\mu,\epsilon}(\log(T)).$$

This results 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]

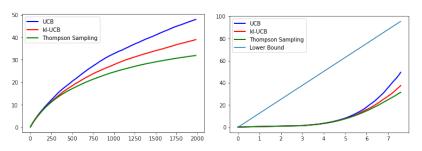
Problem-independent regret [Agrawal and Goyal, 2017]

For Bernoulli and Gaussian bandits, Thompson Sampling satisfies

$$\mathcal{R}_{\boldsymbol{\mu}}(\mathtt{TS},T) = O\left(\sqrt{KT\log(T)}\right).$$

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

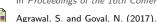
- ▶ the optimism-in-face-of-uncertainty principle (UCB)
- posterior sampling (Thompson Sampling)

What do they need?

- ▶ UCB : the hability 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!)



Further Optimal Regret Bounds for Thompson Sampling. In Proceedings of the 16th Conference on Artificial Intelligence and Statistics.



Near-optimal regret bounds for thompson sampling. J. ACM, 64(5):30:1-30:24.

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

Bubeck, S. (2010).

Jeux de bandits et fondation du clustering.

PhD thesis, Université de Lille 1.

Kullback-Leibler upper confidence bounds for optimal sequential allocation. Annals of Statistics, 41(3):1516-1541.

Machine Learning, 47(2):235-256.

Garivier, A. and Cappé, O. (2011).

Cappé, O., Garivier, A., Maillard, O.-A., Munos, R., and Stoltz, G. (2013).

The KL-UCB algorithm for bounded stochastic bandits and beyond. In Proceedings of the 24th Conference on Learning Theory.

Garivier, A., Kaufmann, E., and Lattimore, T. (2016). On explore-then-commit strategies.

In Advances in Neural Information Processing Systems (NeurIPS).

Kaufmann, E., Korda, N., and Munos, R. (2012).

Thompson Sampling: an Asymptotically Optimal Finite-Time Analysis. In *Proceedings of the 23rd conference on Algorithmic Learning Theory*.

i K

Korda, N., Kaufmann, E., and Munos, R. (2013).
Thompson Sampling for 1-dimensional Exponential family bandits.

In Advances in Neural Information Processing Systems.

Lai, T. and Robbins, H. (1985).

Asymptotically efficient adaptive allocation rules.

Advances in Applied Mathematics, 6(1):4–22.

Lattimore, T. and Szepesvari, C. (2019).

Bandit Algorithms.
Cambridge University Press.

Li, L., Chu, W., Langford, J., and Schapire, R. E. (2010).

A contextual-bandit approach to personalized news article recommendation.

) D.

Robbins, H. (1952).

Some aspects of the sequential design of experiments. Bulletin of the American Mathematical Society, 58(5):527–535.



Sutton, R. and Barto, A. (1998).

Reinforcement Learning: an Introduction.

MIT press.



Thompson, W. (1933).

On the likelihood that one unknown probability exceeds another in view of the evidence of two samples.

Biometrika, 25:285-294.