Sequential Learning

Multi-Armed Bandits

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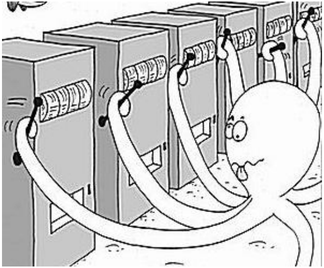
Stochastic bandit : a simple MDP

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)

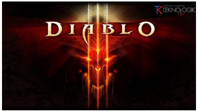





- What treatment should be allocated to the next patient based on responses observed on previous patients ?

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**) :

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

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

ν_1 ν_2 ν_3 ν_4 ν_5

At round t, an agent :

- chooses an arm A_t
- 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 : Maximize $\mathbb{E}\left[\sum_{t=1}^{T} R_t\right]$

➜ a particular reinforcement learning problem

Clinical trials

Historical motivation [Thompson, 1933]

$\mathcal{B}(\mu_1)$

$\mathcal{B}(\mu_2)$

$\mathcal{B}(\mu_3)$

$\mathcal{B}(\mu_4)$

$\mathcal{B}(\mu_5)$

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. $R_t \in \{1, \ldots, 5\}$)

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 : $\mu_a = \mathbb{E}_{X\sim\nu_a}[X]$.

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

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

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

What regret rate can we achieve ?

- consistency : $\frac{\mathcal{R}_\nu(\mathcal{A},T)}{T} \to 0$
- 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

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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 :

- 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

$\Rightarrow$ 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

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

- **Idea 2 :** Follow The Leader

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

where

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

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)

A better idea : Explore-Then-Commit

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

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

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

$\Rightarrow$ EXPLORATION followed by EXPLOITATION

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

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

$\hat{\mu}_{a,m}$: 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
$\rightarrow$ requires a concentration inequality

Intermezzo : Concentration Inequalities

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

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

Hoeffding inequality

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

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

Proof : Cramér-Chernoff method

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

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

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

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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
$$A_t \sim \mathcal{U}(\{1, \ldots, K\})$$
- with probability $1 - \epsilon$
$$A_t = \operatorname*{argmax}_{a=1,\ldots,K} \hat{\mu}_a(t).$$

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

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

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 $1 - \epsilon_t$

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

Theorem [Auer, 2002]

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

➜ requires the knowledge of a lower bound on $\Delta_{\min}$...

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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 :

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

LCB = Lower Confidence Bound
UCB = Upper Confidence Bound

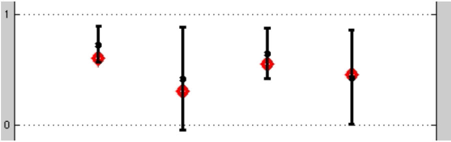

Figure – Confidence intervals on the means after t rounds

The optimism principle

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

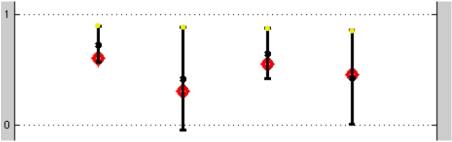

Figure – Confidence intervals on the means after t rounds

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

- That is, select

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

How to build confidence intervals ?

We need $\mathrm{UCB}_a(t)$ such that

$$\mathbb{P}\left(\mu_a \leq \mathrm{UCB}_a(t)\right) \gtrsim 1 - t^{-1}.$$

➜ tool : concentration inequalities

Example : rewards are σ^2 sub-Gaussian

Hoeffding inequality, reloaded

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

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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.

$$\mathbb{P}\left(\mu_a > \hat{\mu}_a(t) + \sigma\sqrt{\frac{\beta\log(t)}{N_a(t)}}\right) \le \mathbb{P}\left(\exists s \le t : \mu_a > \hat{\mu}_{a,s} + \sigma\sqrt{\frac{\beta\log(t)}{s}}\right)$$

$$\le \sum_{s=1}^{t}\mathbb{P}\left(\hat{\mu}_{a,s} < \mu_a - \sigma\sqrt{\frac{\beta\log(t)}{s}}\right) \le \sum_{s=1}^{t}\frac{1}{t^{\beta/2}} = \frac{1}{t^{\beta/2-1}}.$$

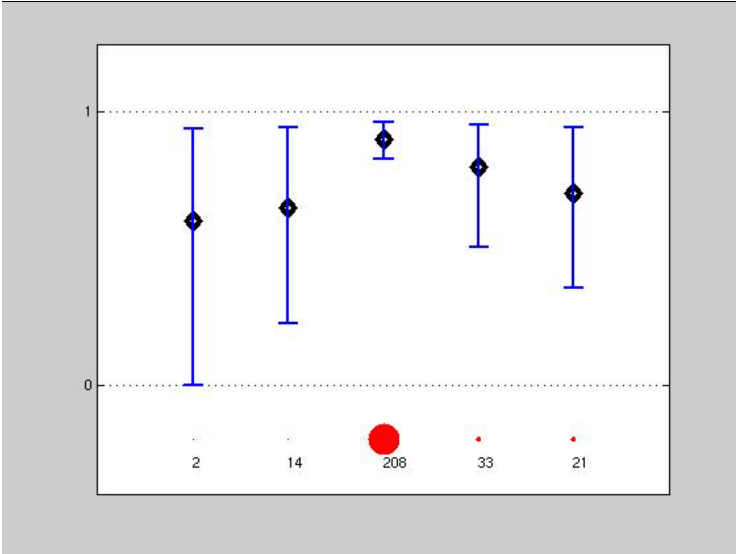
A first UCB algorithm

UCB(α) selects $A_{t+1} = \mathrm{argmax}_a \ \mathrm{UCB}_a(t)$ 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, 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

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

Theorem [Cappé et al.'13]

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

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

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 :

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

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 $[0,1]$:

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

for $\alpha = 1/2$.

Is UCB(α) the best possible algorithm ?

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

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

Key tool : Kullback-Leibler divergence.

Kullback-Leibler divergence

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

Lower bound [Lai et al., 1985]

For *uniformly good* algorithm,

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

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Kullback-Leibler divergence

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

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Kullback-Leibler divergence

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Comparing upper and lower bounds

For Gaussian bandits with variance σ^2,

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

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

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

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

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

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

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

$$\mathcal{R}_\nu(\mathcal{A}, T) \gtrsim \sum_{a:\mu_a<\mu_\star} \frac{2\sigma^2}{(\mu_\star - \mu_a)} \log(T)$$

➜ 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$(1/2)$:**

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

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

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

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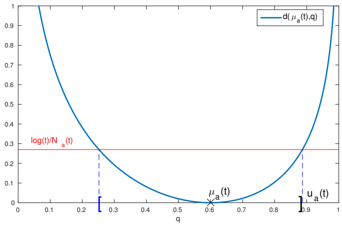
➜ UCB is *not* asymptotically optimal for Bernoulli bandits...

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

The kl-UCB algorithm

Exploits the KL-divergence in the lower bound !

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



A tighter concentration inequality [Garivier and Cappé, 2011]

For Bernoulli rewards

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

An asymptotically optimal algorithm

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

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

Theorem [Cappé et al., 2013]

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

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

- kl-UCB is asymptotically optimal for Bernoulli bandits :

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

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 $\nu_{\boldsymbol{\mu}} = (\nu_{\mu_1}, \ldots, \nu_{\mu_K})$.

- Two probabilistic models

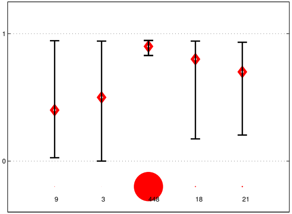
Frequentist model	**Bayesian model**
$\mu_1, \ldots, \mu_K$ unknown parameters	$\mu_1, \ldots, \mu_K$ drawn from a prior distribution : $\mu_a \sim \pi_a$
arm a : $(Y_{a,s})_s \overset{\text{i.i.d.}}{\sim} \nu_{\mu_a}$	arm a : $(Y_{a,s})_s \vert \boldsymbol{\mu} \overset{\text{i.i.d.}}{\sim} \nu_{\mu_a}$

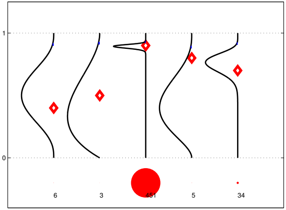
where $(Y_{a,s})$ is the sequence of successive rewards obtained from arm a

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





Example : Bernoulli bandits

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

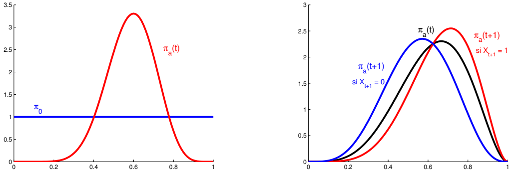
- **Bayesian view** : $\mu_1, \dots, \mu_K$ are random variables

  prior distribution : $\mu_a \sim \mathcal{U}([0,1])$

➜ posterior distribution :

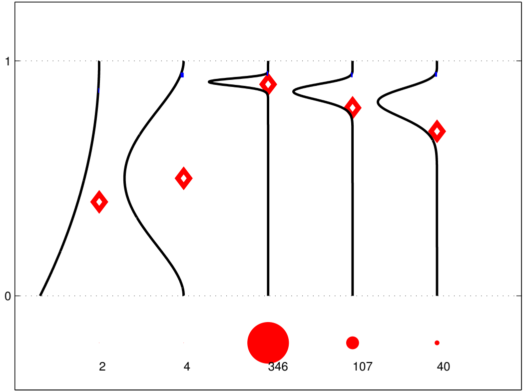
$$\begin{aligned} \pi_a(t) &= \mathcal{L}(\mu_a | R_1, \dots, R_t) \\ &= \mathrm{Beta}\Big(\underbrace{S_a(t)}_{\#ones} + 1, \underbrace{N_a(t) - S_a(t)}_{\#zeros} + 1\Big) \end{aligned}$$

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



Bayesian algorithm

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



Outline

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

A very old idea : [Thompson, 1933].

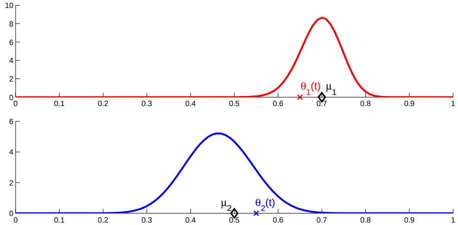
Two equivalent interpretations :

- "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"

$\neq$ optimistic

Thompson Sampling : a randomized Bayesian algorithm

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



Thompson Sampling is asymptotically optimal

Problem-dependent regret

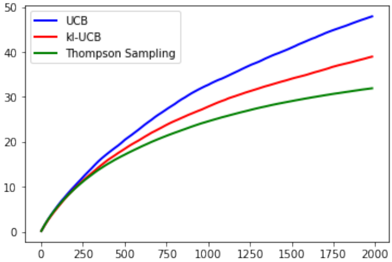
$$\forall \epsilon > 0, \quad \mathbb{E}_{\boldsymbol{\mu}}[N_a(T)] \leq (1+\epsilon)\frac{1}{\mathrm{kl}(\mu_a, \mu_\star)} \log(T) + o_{\mu,\epsilon}(\log(T)).$$

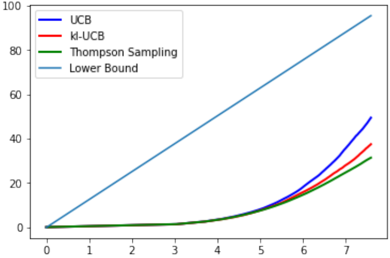
This results holds :

- 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]

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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