Reinforcement Learning

Some Insights from the Bandit Literature

Emilie Kaufmann

M2 MVA, 2023/2024

RL : Taking a step back

RL $\leftrightarrow$ Learn a good policy in an unknown Markov Decision Process

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Good policy : according to some notion of value

$$V^{\pi}(s) \quad = \quad \mathbb{E}^{\pi}\left[\sum_{t=1}^{\infty}\gamma^{t-1}r_t \middle| s_1 = s\right]$$

RL : Taking a step back

RL $\leftrightarrow$ Learn a good policy in an unknown Markov Decision Process

Good policy : according to some notion of value

$$
\begin{aligned}
V^{\pi}(s) &= \mathbb{E}^{\pi}\left[\sum_{t=1}^{\infty}\gamma^{t-1}r_t \middle| s_1 = s\right] \\
\text{or} \quad V^{\pi}(s) &= \mathbb{E}^{\pi}\left[\sum_{t=1}^{H} r_t \middle| s_1 = s\right]
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$$

Learn : with what constraints ?

- learn a good policy using few interactions
- learn a good policy while maximizing rewards

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\end{aligned}
$$

Learn : with what constraints ?

- learn a good policy using few interactions (*sample complexity*)
- learn a good policy while maximizing rewards (*regret*)

Both notions have been mathematically formalized in the *(theoretical)* RL literature, and mostly studied for tabular MDPs

Outline of the last two sessions

- In-depth study of the simplest MDP : the multi-armed bandit
  - ➜ Stochastic bandit algorithms (and their theoretical guarantees)
  - ➜ Towards a more realistic model : contextual bandits
  - ➜ Regret or Sample complexity ?

- Bandit tools for reinforcement learning *(next week)*
  - ➜ (Bandit-based) exploration in RL
  - ➜ (Bandit-based) Monte-Carlo Tree Search
  - ➜ AlphaZero

Reinforcement Learning

Lecture 7 : Multi-armed bandits

Emilie Kaufmann

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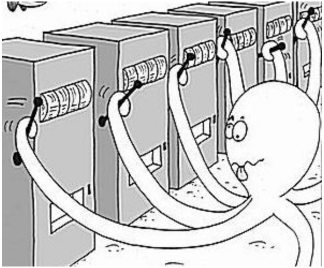
Stochastic bandit : a simple MDP

A stochastic multi-armed bandit model is 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

Typical applications

Clinical trials

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

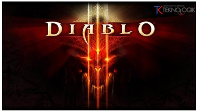





- What treatment should be allocated to the next patient based on responses observed on previous patients ?

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 (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

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 (for now !) : 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. $R_t \in \{1, \dots, 5\}$)

Goal : maximize the sum of ratings

Regret of a bandit algorithm

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

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

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

The greedy strategy

Select each arm once, then exploit the current knowledge :

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

where

- $N_a(t) = \sum_{s=1}^{t} \mathbb{1}(A_s = a)$ is the number of selections of arm a
- $\hat{\mu}_a(t) = \frac{1}{N_a(t)} \sum_{s=1}^{t} X_s \mathbb{1}(A_s = a)$ is the empirical mean of the rewards collected from arm a

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Thre greedy strategy can fail ! $\nu_1 = \mathcal{B}(\mu_1), \nu_2 = \mathcal{B}(\mu_2)$, $\mu_1 > \mu_2$

$$\mathbb{E}[N_2(T)] \geq (1-\mu_1)\mu_2 \times (T-1)$$

➜ **Exploitation** is not enough, we need to add some **exploration**

Outline

1. Fixing the greedy strategy
2. Optimistic Exploration
   - A simple UCB algorithm
   - Towards optimal algorithms
3. Randomized Exploration : Thompson Sampling
4. Contextual Bandits
   - Lin-UCB
   - Linear Thompson Sampling
5. Bandits beyond Regret

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

A Concentration Inequality

Sub-Gaussian random variables : $Z - \mu$ 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 $s \geq 1$

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

- 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. $\mu_1 > \mu_2$, $\Delta := \mu_1 - \mu_2$.

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

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

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$+$ logarithmic regret !

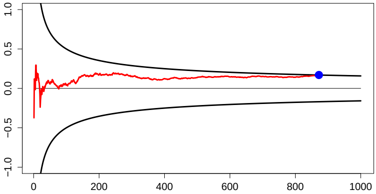
$-$ requires the knowledge of T and Δ

Sequential Explore-Then-Commit

- explore uniformly until a random time of the form

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

- $\hat{a}_\tau = \mathrm{argmax}_{\,a}\ \hat{\mu}_a(\tau)$ 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

... but larger regret as that of the best fully sequential strategy

Another possible fix : ϵ-greedy

The ϵ-greedy rule [Sutton and Barto, 1998] is a simple randomized 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 $1 - \epsilon$

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

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

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

Another possible fix : ϵ-greedy

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 $1 - \epsilon_t$

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

Theorem [Auer et al., 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 :

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

$$\mathrm{LCB} = \text{Lower Confidence Bound}$$
$$\mathrm{UCB} = \text{Upper Confidence Bound}$$

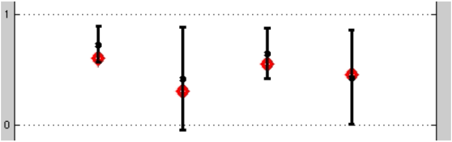

FIGURE – Confidence intervals on the means after t rounds

The optimism principle

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

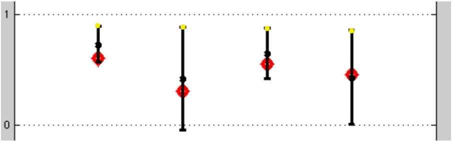

FIGURE – Confidence intervals on the means after t rounds

- That is, select

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

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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

Reminder : Hoeffding inequality

Z_i i.i.d. with mean μ s.t. $\mathbb{E}[e^{\lambda(Z_1-\mu)}] \leq e^{\frac{\lambda^2\sigma^2}{2}}$. For all $s \geq 1$

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

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Z_i i.i.d. with mean μ s.t. $\mathbb{E}[e^{\lambda(Z_1-\mu)}] \leq e^{\frac{\lambda^2\sigma^2}{2}}$. For all $s \geq 1$

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

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

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

$$\mathbb{P}\left(\mu_a \leq \hat{\mu}_a(t) + \sqrt{\frac{6\sigma^2 \log(t)}{N_a(t)}}\right) \geq 1 - \frac{1}{t^2}$$

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Proof.

$$\mathbb{P}\left(\mu_a > \hat{\mu}_a(t) + \sqrt{\frac{6\sigma^2\log(t)}{N_a(t)}}\right) \leq \mathbb{P}\left(\exists s \leq t : \mu_a > \hat{\mu}_{a,s} + \sqrt{\frac{6\sigma^2\log(t)}{s}}\right)$$

$$\leq \sum_{s=1}^{t}\mathbb{P}\left(\hat{\mu}_{a,s} < \mu_a - \sqrt{\frac{6\sigma^2\log(t)}{s}}\right) \leq \sum_{s=1}^{t}\frac{1}{t^3} = \frac{1}{t^2}.$$

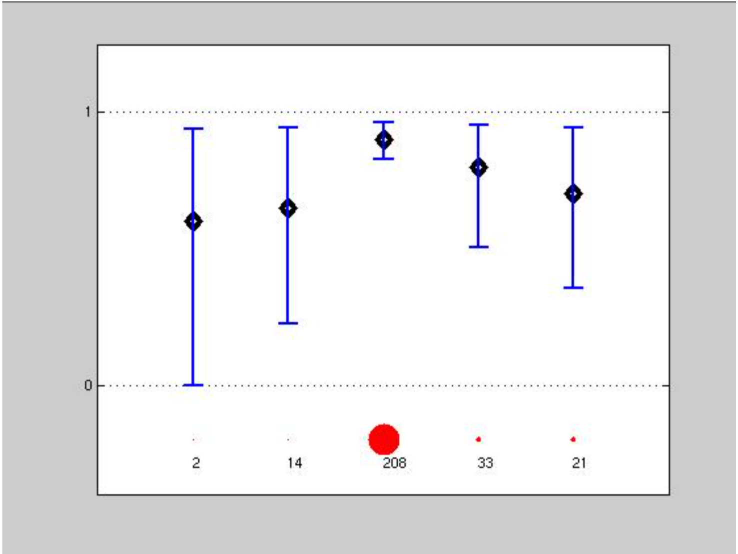
A first UCB algorithm

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

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

- this form of UCB was first proposed for Gaussian rewards [Katehakis and Robbins, 1995]
- 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



A regret bound for UCB(α)

Theorem

For σ^2-subGaussian rewards, the UCB algorithm with parameter $\alpha = 6\sigma^2$ satisfies, for any sub-optimal arm a,

$$\mathbb{E}_{\boldsymbol{\mu}}[N_a(T)] \leq \frac{24\sigma^2}{\Delta_a^2} \log(T) + 1 + \frac{\pi^2}{3}$$

where $\Delta_a = \mu_\star - \mu_a$.

Consequence :

$$\mathcal{R}_\nu(\mathrm{UCB}(6\sigma^2), T) \leq \left(\sum_{a : \mu_a < \mu_\star} \frac{24\sigma^2}{\Delta_a} \right) \log(T) + \left(1 + \frac{\pi^2}{3}\right) \sum_{a=1}^{K} \Delta_a$$

Proof (1/2)

For each arm $i \in \{1, a\}$, define the two ends of the confidence interval :

$$\begin{aligned}
\mathrm{UCB}_i(t) &= \hat{\mu}_i(t) + \sqrt{\frac{6\sigma^2 \log(t)}{N_i(t)}} \\
\mathrm{LCB}_i(t) &= \hat{\mu}_i(t) - \sqrt{\frac{6\sigma^2 \log(t)}{N_i(t)}}
\end{aligned}$$

and the *good event*

$$\mathcal{E}_t = (\mu_1 < \mathrm{UCB}_1(t)) \cap (\mu_a > \mathrm{LCB}_a(t))$$

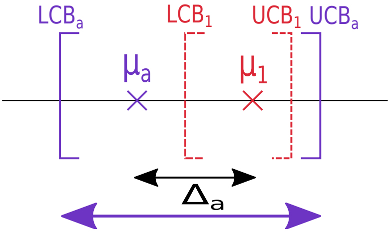
- **Step 1** : Hoeffding inequality + union bound :

$$\mathbb{P}\left(\mathcal{E}_t^c\right) \leq \mathbb{P}\left(\mu_1 > \hat{\mu}_1(t) + \sqrt{\frac{6\sigma^2 \log(t)}{N_1(t)}}\right) + \mathbb{P}\left(\mu_a < \hat{\mu}_a(t) - \sqrt{\frac{6\sigma^2 \log(t)}{N_a(t)}}\right) \leq \frac{2}{t^2}$$

Proof (2/2)

- **Step 2 :** What happens on the good event ?

$$(A_{t+1} = a) \cap (\mu_1 < \mathrm{UCB}_1(t)) \cap (\mu_a > \mathrm{LCB}_a(t))$$



$$\Rightarrow \quad N_a(t) \leq \frac{24\sigma^2 \log(t)}{\Delta_a^2}$$

Proof (2/2)

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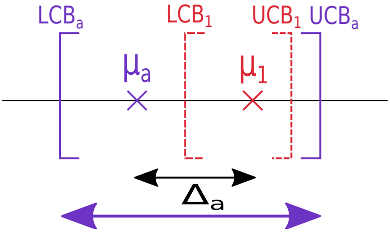


$$\Rightarrow \quad N_a(t) \leq \frac{24\sigma^2 \log(t)}{\Delta_a^2}$$

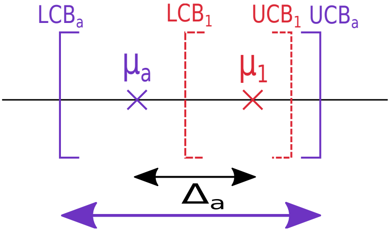
- **Step 3 :** Putting everything together

$$\begin{aligned}
\mathbb{E}[N_a(T)] &\leq 1 + \sum_{t=K}^{T-1} \mathbb{P}\left(\mathcal{E}_t^c\right) + \sum_{t=K}^{T-1} \mathbb{P}\left(A_{t+1} = a, \mathcal{E}_t\right) \\
&\leq 1 + \frac{\pi^2}{3} + \sum_{t=K}^{T-1} \mathbb{P}\left(A_{t+1} = a, N_a(t) \leq \frac{24\sigma^2 \log(T)}{\Delta_a^2}\right)
\end{aligned}$$

Proof (2/2)

- **Step 2 :** What happens on the good event ?

$$(A_{t+1} = a) \cap (\mu_1 < \mathrm{UCB}_1(t)) \cap (\mu_a > \mathrm{LCB}_a(t))$$



$$\Rightarrow \quad N_a(t) \leq \frac{24\sigma^2 \log(t)}{\Delta_a^2}$$

- **Step 3 :** Putting everything together

$$\begin{aligned}\mathbb{E}[N_a(T)] &\leq 1 + \sum_{t=K}^{T-1} \mathbb{P}\left(\mathcal{E}_t^c\right) + \sum_{t=K}^{T-1} \mathbb{P}\left(A_{t+1} = a, \mathcal{E}_t\right) \\ &\leq 1 + \frac{\pi^2}{3} + \frac{24\sigma^2 \log(T)}{\Delta_a^2}\end{aligned}$$

A worse-case regret bound

Corollary

$$\mathcal{R}_\nu(\mathrm{UCB}(6\sigma^2), T) \leq 10\sqrt{KT\log(T)} + \left(1 + \frac{\pi^2}{3}\right)\left(\sum_{a=1}^{K} \Delta_a\right)$$

Proof. For any algorithm satisfying $\mathbb{E}[N_a(T)] \leq C\frac{\log(T)}{\Delta_a} + D$ for all sub-optimal arm a, for any $\Delta > 0$,

$$\begin{aligned}
\mathcal{R}_\nu(T) &= \sum_{a:\Delta_a \leq \Delta} \Delta_a \mathbb{E}[N_a(T)] + \sum_{a:\Delta_a \geq \Delta} \Delta_a \mathbb{E}[N_a(T)] \\
&\leq \Delta T + \sum_{a:\Delta_a \geq \Delta} \left(C\frac{\log(T)}{\Delta_a} + D\Delta_a\right) \\
&\leq \Delta T + \frac{CK\log(T)}{\Delta} + D\left(\sum_{a=1}^{K} \Delta_a\right) \\
&= 2\sqrt{CKT\log(T)} + D\left(\sum_{a=1}^{K} \Delta_a\right) \quad \text{for } \Delta = \sqrt{\frac{CK\log(T)}{T}}
\end{aligned}$$

Best known problem-dependent bound

Context : σ^2 sub-Gaussian rewards

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

($c = 0$ corresponds to $\mathrm{UCB}(\alpha)$ *with* $\alpha = 2\sigma^2$*)*

Theorem [Cappé et al.'13]

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

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

Summary

For UCB(α) applied to σ^2-subGaussian reward, setting $\alpha = 2\sigma^2$ yields

- a problem-dependent regret bound of

$$\left(\sum_{a=1}^{K} \frac{2\sigma^2}{\Delta_a}\right) \log(T) + o(\log(T))$$

- a worse-case regret of order

$$O\left(\sqrt{KT\log(T)}\right)$$

➜ how good are these regret rates ?

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A worse-case lower bound

Theorem [Cesa-Bianchi and Lugosi, 2006]

Fix $T \in \mathbb{N}$. For every bandit algorithm $\mathcal{A}$, there exists a stochastic bandit model ν with rewards supported in $[0,1]$ such that

$$\mathcal{R}_\nu(\mathcal{A}, T) \geq \frac{1}{20}\sqrt{KT}$$

- worse-case model :

$$\begin{cases} \nu_a & = & \mathcal{B}(1/2) \text{ for all } a \neq i \\ \nu_i & = & \mathcal{B}(1/2 + \Delta) \end{cases}$$

with $\Delta \simeq \sqrt{K/T}$.

Remark. UCB achieves $\mathcal{O}(\sqrt{KT \log(T)})$ (near-optimal)
There exists worse-case optimal algorithms, e.g., MOSS or Tsallis-Inf [Audibert and Bubeck, 2010, Zimmert and Seldin, 2021]

The Lai and Robbins lower bound

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

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

Key tool : Kullback-Leibler divergence.

Kullback-Leibler divergence

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

Theorem

For *uniformly good* algorithm,

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

[Lai and Robbins, 1985]

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Kullback-Leibler divergence

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

Theorem

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

[Lai and Robbins, 1985]

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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,

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

[Lai and Robbins, 1985]

UCB compared to the lower bound

Gaussian distributions with variance σ^2

- **Lower bound** : $\mathbb{E}[N_a(T)] \gtrsim \frac{2\sigma^2}{(\mu_\star - \mu_a)^2} \log(T)$
- **Upper bound** : for UCB(α) with $\alpha = 2\sigma^2$

$$\mathbb{E}[N_a(T)] \lesssim \frac{2\sigma^2}{(\mu_\star - \mu_a)^2} \log(T)$$

➜ UCB is asymptotically optimal for Gaussian rewards !

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Bernoulli distributions (bounded, $\sigma^2 = 1/4$)

- **Lower bound** : $\mathbb{E}[N_a(T)] \gtrsim \frac{1}{\mathrm{kl}(\mu_a, \mu_\star)} \log(T)$
- **Upper bound** : for UCB(α) with $\alpha = 1/2$

$$\mathbb{E}[N_a(T)] \lesssim \frac{1}{2(\mu_\star - \mu_a)^2} \log(T)$$

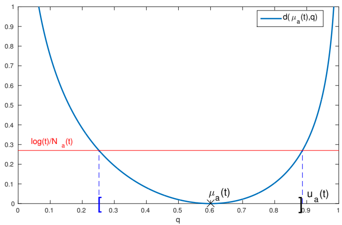
Pinsker's inequality : $\mathrm{kl}(\mu_a, \mu_\star) > 2(\mu_\star - \mu_a)^2$

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

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 rewards in a one-dimensional exponential family [a],

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

a. e.g., Bernoulli, Gaussian with known variances, Poisson, Exponential

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 $\mu_a < \mu_\star$,

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

- asymptotically optimal for Bernoulli rewards (and one-dimenionsal exponential families) :

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

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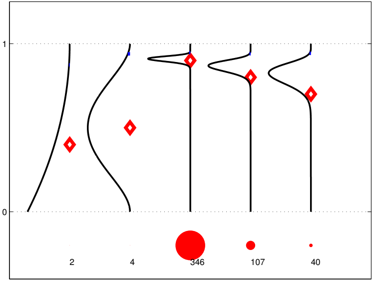
A Bayesian algorithm

$\pi_a(0)$: prior distribution on μ_a
$\pi_a(t) = \mathcal{L}(\mu_a | Y_{a,1}, \dots, Y_{a,N_a(t)})$: posterior distribution on μ_a



Two equivalent interpretations :

- [Thompson, 1933] : "randomize the arms according to their posterior probability being optimal"
- modern view : "draw a possible bandit model from the posterior distribution and act optimally in this sampled model"

Russo et al. 2018, *A Tutorial on Thompson Sampling*

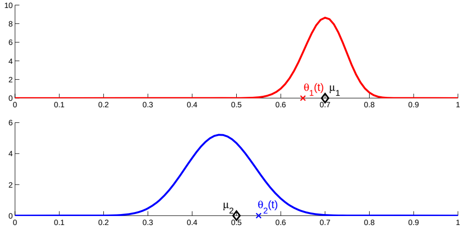
Thompson Sampling

Input : a prior distribution $\pi(0)$

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

Thompson Sampling for Bernoulli distributions $\nu_a = \mathcal{B}(\mu_a)$

- $\pi_a(0) = \mathcal{U}([0,1])$
- $\pi_a(t) = \mathrm{Beta}\left(S_a(t) + 1; N_a(t) - S_a(t) + 1\right)$



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Thompson Sampling for Gaussian distributions $\nu_a = \mathcal{N}(\mu_a, \sigma^2)$

- $\pi_a(0) \propto 1$
- $\pi_a(t) = \mathcal{N}\left(\hat{\mu}_a(t); \frac{\sigma^2}{N_a(t)}\right)$

Regret bounds

Upper bound on sub-optimal selections

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

where $\mathrm{kl}(\mu_a, \mu_\star)$ is the KL divergence between ν_a and $\nu_{a_\star}$

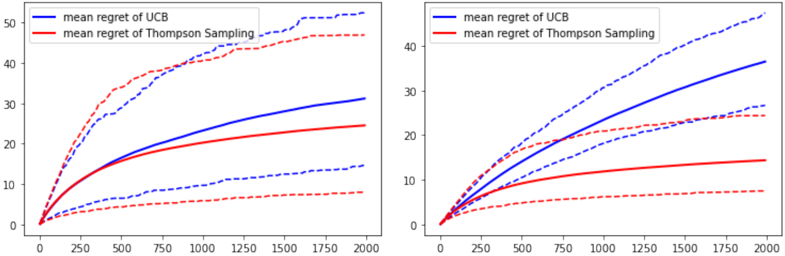
- proved for Bernoulli bandits, with a uniform prior [Kaufmann et al., 2012, Agrawal and Goyal, 2013a]
- for 1-dimensional exponential families, with a conjuguate prior [Agrawal and Goyal, 2017, Korda et al., 2013]

→ Thompson Sampling is **asymptotically optimal** in these cases

- beyond 1-parameter models, the prior has to be well chosen... [Honda and Takemura, 2014]

Practical performance

Regret curves for UCB ($\alpha = 1/2$) and Thompson Sampling on two Bernoulli bandit problems, averaged over 500 runs.



Who is who ? Try it out !

$\boldsymbol{\mu_A} = [0.45\ 0.5\ 0.6] \qquad \boldsymbol{\mu_B} = [0.1\ 0.05\ 0.02\ 0.01]$

Summary so far

Several important ideas to tackle the exploration/exploitation challenge in a simple multi-armed bandit model with independent arms :

- Explore then Commit
- ε-greedy
- Optimistic algorithms : Upper Confidence Bounds strategies
- Randomized (Bayesian) exploration : Thompson Sampling

Can these ideas be extended to more **structured** models that are better suited for applications ?

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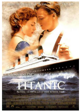
Motivation



Which movie should Netflix recommend to a particular user, given the ratings provided by previous users ?

➜ to make good recommendation, we should take into account the characteristics of the movies / users

Arm in $\{1, 2, \ldots, K\} \leftrightarrow$ Context vector in some space $\mathcal{X}$

A **contextual bandit model** incorporates two components :

- a sequential interaction protocol :
  pick an arm, receive a reward
- a regression model for the dependency between context and reward

Generic Contextual Bandit Model

In each round t, the agent

- is given a set of *arms* $\mathcal{X}_t \subseteq \mathcal{X}$ *(can be different in each round)*
- selects an *arm* $x_t \in \mathcal{X}_t$
- receives a reward

$$r_t = f_\star(x_t) + \varepsilon_t$$

where

- $f_\star : \mathcal{X} \to \mathbb{R}$ is an unknown regression function
- ε_t is a centered noise, independent from previous data

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Example

- user t : descriptor $c_t \in \mathbb{R}^p$
- item a : descriptor $x_a \in \mathbb{R}^{p'}$

➜ build a user-item feature vector for (t, a) : $x_{t,a} \in \mathbb{R}^d$

$$\mathcal{X}_t = \{x_{t,a}, a \in \mathcal{K}_t\}$$

Contextual linear bandits

In each round t, the agent

- receives a (finite) set of arms $\mathcal{X}_t \subseteq \mathbb{R}^d$
- chooses an arm $x_t \in \mathcal{X}_t$
- gets a reward $r_t = \theta_\star^\top x_t + \varepsilon_t$

where

- $\theta_\star \in \mathbb{R}^d$ is an unknown regression vector
- ε_t is a centered noise, independent from past data

Assumption : σ^2- sub-Gaussian noise

$$\forall \lambda \in \mathbb{R}, \; \mathbb{E}\left[e^{\lambda \varepsilon_t} | \mathcal{F}_{t-1}, x_t\right] \leq e^{\frac{\lambda^2 \sigma^2}{2}}$$

e.g., Gaussian noise, bounded noise.

Contextual linear bandits

In each round t, the agent

- receives a (finite) set of arms $\mathcal{X}_t \subseteq \mathbb{R}^d$
- chooses an arm $x_t \in \mathcal{X}_t$
- gets a reward $r_t = \theta_\star^\top x_t + \varepsilon_t$

where

- $\theta_\star \in \mathbb{R}^d$ is an unknown regression vector
- ε_t is a centered noise, independent from past data

(Pseudo)-regret for contextual bandit

maximizing expected total reward $\leftrightarrow$ minimizing the (expectation of)

$$R_T(\mathcal{A}) = \sum_{t=1}^{T} \left(\max_{x \in \mathcal{X}_t} \theta_\star^\top x - \theta_\star^\top x_t \right)$$

➜ in each round, comparison to a possibly different optimal action !

Tools

Algorithms will rely on estimates / confidence regions / posterior distributions for $\theta_\star \in \mathbb{R}^d$.

- design matrix (with regularization parameter $\lambda > 0$)

$$B_t^\lambda = \lambda I_d + \sum_{s=1}^{t} x_s x_s^\top$$

- regularized least-square estimate

$$\hat{\theta}_t^\lambda = \left(B_t^\lambda\right)^{-1} \left(\sum_{s=1}^{t} r_t x_t\right)$$

- estimate of the expected reward of an arm $x \in \mathbb{R}^d$: $x^\top \hat{\theta}_t^\lambda$

➜ sufficient for ε-greedy or ETC, but not for smarter algorithms...

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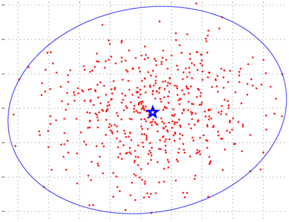
How to build (tight) confidence interval on the mean rewards ?

Idea : rely on a confidence ellispoid around $\hat{\theta}_t^\lambda$



$$\theta_\star \in \left\{ \theta \in \mathbb{R}^d : \|\theta - \hat{\theta}_t^\lambda\|_A \leq \beta_t \right\}$$

Why ? For all invertible matrix positive semi-definite matrix A,

$$\forall x \in \mathbb{R}^d, \quad \left| x^\top \theta_\star - x^\top \hat{\theta}_t^\lambda \right| \leq \|x\|_{A^{-1}} \left\| \theta_\star - \hat{\theta}_t^\lambda \right\|_A$$

$\|x\|_A = \sqrt{x^\top A x}$

How to build (tight) confidence interval on the mean rewards ?

Wanted : $\theta_\star \in \left\{\theta \in \mathbb{R}^d : \|\theta - \hat{\theta}_t^\lambda\|_A \leq \beta_t\right\}$

Example of threshold [Abbasi-Yadkori et al., 2011]

Assuming that the noise ε_t is σ^2-sub-Gaussian, and that for all t and $x \in \mathcal{X}_t$, $\|x\| \leq L$, we have

$$\mathbb{P}\left(\exists t \in \mathbb{N}^\star : \|\theta_\star - \hat{\theta}_t^\lambda\|_{B_t^\lambda} > \beta(t,\delta)\right) \leq \delta$$

with $\beta(t,\delta) = \sigma\sqrt{2\log\left(1/\delta\right) + d\log\left(1 + t\frac{L}{d\lambda}\right)} + \sqrt{\lambda}\|\theta_\star\|$.

➜ Letting

$$C_t(\delta) = \left\{\theta \in \mathbb{R}^d : \|\theta - \hat{\theta}_t^\lambda\|_{B_t^\lambda} \leq \beta(t,\delta)\right\},$$

one has $\mathbb{P}\left(\forall t \in \mathbb{N}, \theta_\star \in C_t(\delta)\right) \geq 1 - \delta$.

A Lin-UCB algorithm

Consequence :

$$\mathbb{P}\left(\forall t \in \mathbb{N}^*, \forall x \in \mathcal{X}_{t+1}, \quad \underbrace{x^\top \theta_\star}_{\substack{\text{unknown mean} \\ \text{of arm } x}} \leq \underbrace{x^\top \hat{\theta}_t^\lambda + \|x\|_{(B_t^\lambda)^{-1}} \beta(t,\delta)}_{\text{Upper Confidence Bound}}\right) \geq 1 - \delta.$$

One can assign to each arm $x \in \mathcal{X}_{t+1}$

$$\mathrm{UCB}_x(t) = \underbrace{x^\top \hat{\theta}_t^\lambda}_{\substack{\text{empirical mean} \\ \text{(exploitation term)}}} + \underbrace{\|x\|_{(B_t^\lambda)^{-1}} \beta(t,\delta)}_{\text{exploration bonus}}$$

Lin-UCB

In each round $t+1$, the algorithm selects

$$x_{t+1} = \underset{x \in \mathcal{X}_{t+1}}{\mathrm{argmax}} \left[x^\top \hat{\theta}_t^\lambda + \|x\|_{(B_t^\lambda)^{-1}} \beta(t,\delta)\right]$$

(many algorithms of this style, with different choices of $\beta(t,\delta)$)

Theoretical guarantees

We want to bound the pseudo-regret

$$R_T(\text{Lin-UCB}) = \sum_{t=1}^{T} \left(\max_{x \in \mathcal{X}_t} \theta_\star^\top x - \theta_\star^\top x_t \right)$$

or its expectation, the regret $\mathcal{R}_T(\text{Lin-UCB}) = \mathbb{E}[R_T(\text{Lin-UCB})]$.

Lemma

One can prove that, with probability larger than $1 - \delta$,

$$\forall T \in \mathbb{N}^*, R_T(\text{Lin-UCB}) \leq C\beta(T, \delta)\sqrt{dT \log(T)}$$

- with the choice of $\beta(t, \delta)$ presented before, with high probability

$$R_T(\text{Lin-UCB}) = \mathcal{O}(d\sqrt{T}\log(T) + \sqrt{dT \log(T)\log(1/\delta)})$$

- choosing $\delta = 1/T$, $\mathcal{R}_T(\text{Lin-UCB}) = \mathcal{O}(d\sqrt{T}\log(T))$

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A Bayesian view on Linear Regression

Bayesian model :

- likelihood : $r_t = \theta_\star^\top x_t + \varepsilon_t$
- prior : $\theta_\star \sim \mathcal{N}(0, \kappa^2 \mathrm{I}_d)$

Assuming further that the noise is Gaussian : $\varepsilon_t \sim \mathcal{N}(0, \sigma^2)$, the posterior distribution of $\theta_\star$ has a closed form :

$$\theta_\star | x_1, r_1, \dots, x_t, r_t \;\sim\; \mathcal{N}\left(\hat{\theta}_t^\lambda, \sigma^2 \left(B_t^\lambda\right)^{-1}\right)$$

with

- $B_t^\lambda = \lambda \mathrm{I}_d + \sum_{s=1}^t x_s x_s^\top$
- $\hat{\theta}_t^\lambda = \left(B_t^\lambda\right)^{-1} \left(\sum_{s=1}^t r_s x_s\right)$ is the regularized least square estimate

with a regularization parameter $\lambda = \frac{\sigma^2}{\kappa^2}$.

Thompson Sampling for Linear Bandits

Recall the Thompson Sampling principle :

> "draw a possible model from the posterior distribution and act optimally in this sampled model"

Thompson Sampling in linear bandits

In each round $t+1$,

$$\begin{aligned} \widetilde{\theta}_t &\sim \mathcal{N}\left(\hat{\theta}_t^\lambda, \sigma^2 \left(B_t^\lambda\right)^{-1}\right) \\ x_{t+1} &= \underset{x \in \mathcal{X}_{t+1}}{\operatorname{argmax}} \; x^\top \widetilde{\theta}_t \end{aligned}$$

Numerical complexity : one need to draw a sample from a multivariate Gaussian distribution, e.g.

$$\widetilde{\theta}_t = \hat{\theta}_t^\lambda + \sigma \left(B_t^\lambda\right)^{-1/2} X$$

where X is a vector with d independent $\mathcal{N}(0,1)$ entries.

Theoretical guarantees

[Agrawal and Goyal, 2013b] analyze a *variant* of Thompson Sampling using some "posterior inflation" :

$$\begin{aligned} \widetilde{\theta}_t & \sim \mathcal{N}\left(\hat{\theta}_t^1, v^2 \left(B_t^1\right)^{-1}\right) \\ x_{t+1} & = \underset{x \in \mathcal{X}_{t+1}}{\operatorname{argmax}} \ x^\top \widetilde{\theta}_t \end{aligned}$$

where $v = \sigma\sqrt{9d \ln(T/\delta)}$.

Theorem

If the noise is σ^2-sub-Gaussian, the above algorithm satisfies

$$\mathbb{P}\left(R_T(\mathrm{TS}) = \mathcal{O}\left(d^{3/2}\sqrt{T}\left[\ln(T) + \sqrt{\ln(T)\ln(1/\delta)}\right]\right)\right) \geq 1 - \delta.$$

- slightly worse than Lin-UCB... in theory
- do we need the posterior inflation ?

Beyond linear bandits

Depending on the application, other parametric models may be better suited than the simple linear model, for example the logistic model.

$$\begin{aligned} \mathbb{P}\left(r_t = 1 | x_t\right) &= \frac{1}{1 + e^{-\theta_\star^\top x_t}} \\ \mathbb{P}\left(r_t = 0 | x_t\right) &= \frac{e^{-\theta_\star^\top x_t}}{1 + e^{-\theta_\star^\top x_t}} \end{aligned}$$

e.g., clic / no-clic on an add depending on a user/add feature $x_t \in \mathbb{R}^d$

- [Filippi et al., 2010] : first UCB style algorithm for Generalized Linear Bandit models
- Thompson Sampling for logistic bandits [Dumitrascu et al., 2018]
- going further : UCB/TS for neural bandits !

Outline

1. Fixing the greedy strategy
2. Optimistic Exploration
   - A simple UCB algorithm
   - Towards optimal algorithms
3. Randomized Exploration : Thompson Sampling
4. Contextual Bandits
   - Lin-UCB
   - Linear Thompson Sampling
5. Bandits beyond Regret

Bandits without rewards ?

$\mathcal{B}(\mu_1)$ $\mathcal{B}(\mu_2)$ $\mathcal{B}(\mu_3)$ $\mathcal{B}(\mu_4)$ $\mathcal{B}(\mu_5)$

For the t-th patient in a clinical study,

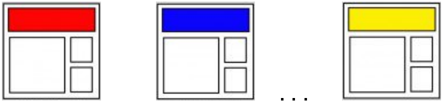
- chooses a treatment A_t
- observes a response $X_t \in \{0, 1\} : \mathbb{P}(X_t = 1) = \mu_{A_t}$

Maximize rewards $\leftrightarrow$ cure as many patients as possible

Alternative goal : identify as quickly as possible the best treatment (without trying to cure patients during the study)

Bandits without rewards ?

Probability that some version of a website generates a conversion :



μ_1 μ_2 μ_K

Best version : $a_\star = \underset{a=1,\dots,K}{\text{argmax}}\ \mu_a$

Sequential protocol : for the t-th visitor :

- display version A_t
- observe conversion indicator $X_t \sim \mathcal{B}(\mu_{A_t})$.

Maximize rewards $\leftrightarrow$ maximize the number of conversions

Alternative goal : identify the best version
(without trying to maximize conversions during the test)

A Pure Exploration Problem

Goal : identify an arm with mean close to $\mu_\star$ as quickly and accurately as possible $\simeq$ identify

$$a_\star = \underset{a=1,\dots,K}{\operatorname{argmax}} \ \mu_a.$$

Algorithm : made of three components :

- ➜ sampling rule : A_t (arm to explore)
- ➜ recommendation rule : B_t (current guess for the best arm)
- ➜ stopping rule τ (when do we stop exploring ?)

Probability of error

The probability of error after T rounds is

$$p_\nu(T) = \mathbb{P}_\nu\left(B_T \neq a_\star\right).$$

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Simple regret [Bubeck et al., 2011]

The simple regret after n rounds is

$$r_\nu(n) = \mu_\star - \mu_{B_n}.$$

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Simple regret [Bubeck et al., 2011]

The simple regret after n rounds is

$$r_\nu(n) = \mu_\star - \mu_{B_n}.$$

$$\Delta_{\min} p_\nu(T) \leq \mathbb{E}_\nu[r_\nu(T)] \leq \Delta_{\max} p_\nu(T)$$

Several objectives

Algorithm : made of three components :

➜ sampling rule : A_t (arm to explore)

➜ recommendation rule : B_t (current guess for the best arm)

➜ stopping rule τ (when do we stop exploring ?)

- **Objectives studied in the literature :**

Fixed-budget setting	Fixed-confidence setting
input : budget T	input : risk parameter δ (tolerance parameter ϵ)
$\tau = T$ minimize $\mathbb{P}(B_T \neq a_\star)$ or $\mathbb{E}[r_T(\nu)]$	minimize $\mathbb{E}[\tau]$ $\mathbb{P}(B_\tau \neq a_\star) \leq \delta$ or $\mathbb{P}(r_\nu(\tau) > \epsilon) \leq \delta$
[Bubeck et al., 2011] [Audibert et al., 2010]	[Even-Dar et al., 2006]

Can we use UCB ?

Context : bounded rewards (ν_a supported in $[0,1]$)

We know good algorithms to maximize rewards, for example $\mathrm{UCB}(\alpha)$

$$A_{t+1} = \underset{a=1,\dots,K}{\operatorname{argmax}} \ \hat{\mu}_a(t) + \sqrt{\frac{\alpha \ln(t)}{N_a(t)}}$$

- How good is it for best arm identification ?

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- How good is it for best arm identification ?

Possible recommendation rules :

Empirical Best Arm (EBA)	$B_t = \text{argmax}_a \ \hat{\mu}_a(t)$
Most Played Arm (MPA)	$B_t = \text{argmax}_a \ N_a(t)$
Empirical Distribution of Plays (EDP)	$B_t \sim p_t$, where $p_t = \left(\frac{N_1(t)}{t}, \dots, \frac{N_K(t)}{t}\right)$

[Bubeck et al., 2011]

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[Bubeck et al., 2011]

Can we use UCB ?

- **UCB + Empirical Distribution of Plays**

$$
\begin{aligned}
\mathbb{E}\left[r_\nu(T)\right] &= \mathbb{E}\left[\mu_\star - \mu_{B_T}\right] = \mathbb{E}\left[\sum_{b=1}^{K}(\mu_\star - \mu_b)\mathbb{1}_{(B_T=b)}\right] \\
&= \mathbb{E}\left[\sum_{b=1}^{K}(\mu_\star - \mu_b)\mathbb{P}(B_T = b|\mathcal{F}_T)\right] \\
&= \mathbb{E}\left[\sum_{b=1}^{K}(\mu_\star - \mu_b)\frac{N_b(T)}{T}\right] \\
&= \frac{1}{T}\sum_{b=1}^{K}(\mu_\star - \mu_b)\mathbb{E}[N_b(T)] \\
&= \frac{\mathcal{R}_\nu(T)}{T}.
\end{aligned}
$$

➜ a conversion from cumulative regret to simple regret !

Can we use UCB ?

- **UCB + Empirical Distribution of Plays**

$$\mathbb{E}\left[r_\nu\left(\texttt{UCB}(\alpha), T\right)\right] \leq \frac{\mathcal{R}_\nu(\texttt{UCB}(\alpha), T)}{T} \leq \frac{C(\nu)\ln(T)}{T}$$

Can we use UCB ?

- **UCB + Empirical Distribution of Plays**

$$\mathbb{E}\left[r_\nu\left(\texttt{UCB}(\alpha), T\right)\right] \leq \frac{\mathcal{R}_\nu(\texttt{UCB}(\alpha), T)}{T} \leq C\sqrt{\frac{K\ln(T)}{T}}$$

Can we use UCB ?

- **UCB + Empirical Distribution of Plays**

$$\mathbb{E}\left[r_\nu\left(\mathtt{UCB}(\alpha), T\right)\right] \leq \frac{\mathcal{R}_\nu(\mathtt{UCB}(\alpha), T)}{T} \leq C\sqrt{\frac{K\ln(T)}{T}}$$

- Almost optimal in the **worse case**

Lower bound [Bubeck et al., 2011]

For every algorithm $\mathcal{A}$, there exists a bandit instance ν in which

$$\mathbb{E}[r_\nu(\mathcal{A}, T)] \geq \frac{1}{20}\sqrt{\frac{K}{T}}$$

Can we use UCB ?

- **UCB + Empirical Distribution of Plays**

$$\mathbb{E}\left[r_\nu\left(\texttt{UCB}(\alpha), T\right)\right] \leq \frac{\mathcal{R}_\nu(\texttt{UCB}(\alpha), T)}{T} \leq C\sqrt{\frac{K\ln(T)}{T}}$$

- ... but potentially bad in the **problem-dependent** regime

The simple regret or the uniform sampling strategy decays exponentially :

$$\mathbb{E}_\nu\left[r_\nu\left(\texttt{Unif}, T\right)\right] \leq (K-1)\Delta_{\max}\exp\left(-\frac{1}{2}\frac{T}{K}\Delta_{\min}^2\right)$$

➜ UCB does not always provably outperform uniform sampling...

(Problem-dependent) sample complexity

With Uniform Sampling, the number of sample needed to get an error probability smaller than δ is of order

$$T \simeq \frac{K}{\Delta_{\min}^2} \log\left(\frac{1}{\delta}\right)$$

(assuming, e.g. rewards in [0,1])

- Can be improved for smarter algorithms to

$$T \simeq \mathcal{O}\left(H(\nu) \log\left(\frac{1}{\delta}\right)\right)$$

where

$$H(\nu) = \sum_{a=1}^{K} \frac{1}{\Delta_a^2} \quad \text{with} \quad \Delta_{a_\star} = \min_{a \neq a_\star} \Delta_a \ .$$

(and more precise complexity measures for parametric distributions [Garivier and Kaufmann, 2016])

Fixed Budget : Sequential Halving

Input : total number of plays T

Idea : split the budget in $\log_2(K)$ phases of equal length, eliminate the worst half of the remaining arms after each phase.

Initialisation : $S_0 = \{1, \dots, K\}$;
For $r = 0$ **to** $\lceil \ln_2(K) \rceil - 1$, **do**

sample each arm $a \in S_r$ $t_r = \left\lfloor \frac{T}{|S_r| \lceil \log_2(K) \rceil} \right\rfloor$ times ;

let $\hat{\mu}_a^r$ be the empirical mean of arm a ;

let S_{r+1} be the set of $\lceil |S_r|/2 \rceil$ arms with largest $\hat{\mu}_a^r$

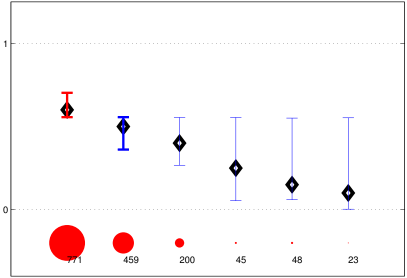
Output : B_T the unique arm in $S_{\lceil \log_2(K) \rceil}$

Theorem [Karnin et al., 2013]

$$\mathbb{P}_\nu \left(B_T \neq a_\star \right) \leq 3 \log_2(K) \exp\left(- \frac{T}{8 \log_2(K) H(\nu)} \right).$$

Fixed Confidence : LUCB

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



- At round t, draw

$$\begin{aligned} B_t &= \underset{b}{\mathrm{argmax}} \ \hat{\mu}_b(t) \\ C_t &= \underset{c \neq B_t}{\mathrm{argmax}} \ \mathrm{UCB}_c(t) \end{aligned}$$

- Stop at round t if

$$\mathrm{LCB}_{B_t}(t) > \mathrm{UCB}_{C_t}(t) - \epsilon$$

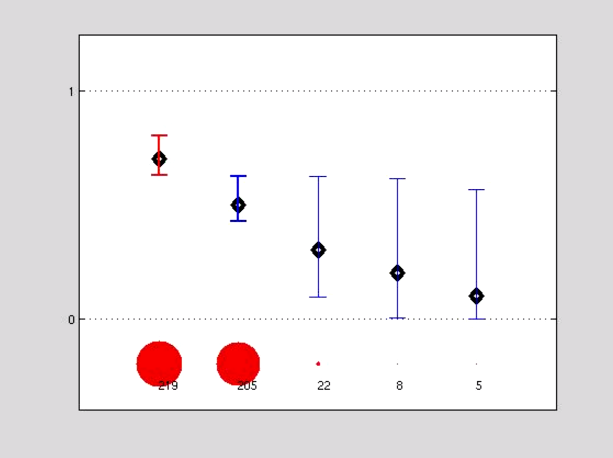
Theorem [Kalyanakrishnan et al., 2012]

For well-chosen confidence intervals, $\mathbb{P}_\nu(\mu_{B_\tau} > \mu_\star - \epsilon) \geq 1 - \delta$ and

$$\mathbb{E}[\tau_\delta] = \mathcal{O}\left(\left[\sum_{a=1}^{K} \frac{1}{\Delta_a^2 \vee \epsilon^2}\right] \ln\left(\frac{1}{\delta}\right)\right)$$

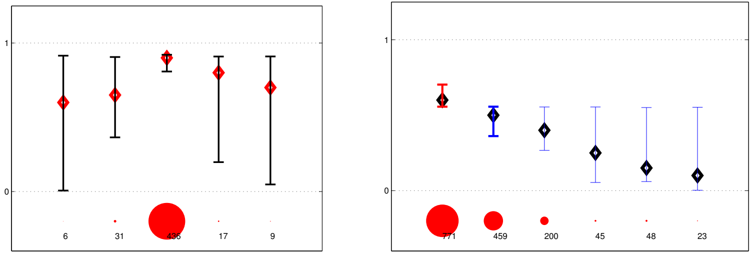
(kl)-LUCB in action

$$\begin{aligned} \mathrm{UCB}_a(t) &= \max\left\{q \in [0,1] : N_a(t)\mathrm{kl}(\hat{\mu}_a(t), q) \leq \log(Ct^2/\delta)\right\} \\ \mathrm{LCB}_a(t) &= \min\left\{q \in [0,1] : N_a(t)\mathrm{kl}(\hat{\mu}_a(t), q) \leq \log(Ct^2/\delta)\right\} \end{aligned}$$



A comparison with UCB

Regret minimizing algorithms and Best Arm Identification algorithms behave quite differently



Number of selections and confidence intervals for KL-UCB (left) and KL-LUCB (right)

Conclusion

In bandits, ε-greedy can be replaced by smarter algorithms

- both for learning while maximizing rewards *(regret)*
- and for fast identification of the best action *(sample complexity)*

Two important tools :

- confidence intervals
- posterior distributions

to better take into account the uncertainty and perform more efficient ("directed") exploration.

Those tools can also be used in contextual bandit models.
How about general Markov Decision Processes ?

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