Reinforcement Learning Some Insights from the Bandit Literature

Emilie Kaufmann









M2 MVA, 2023/2024

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

RL ↔ Learn a good policy in an unknown Markov Decision Process

Good policy: according to some notion of value

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

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

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Learn: with what constraints?

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

RL \(\ldot \) Learn a good policy in an unknown Markov Decision Process

Good policy: according to some notion of value

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Learn: with what constraints?

to minimize

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

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







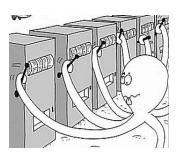


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Stochastic bandit : a simple MDP

A stochastic multi-armed bandit model is an MDP with a single state so

- ▶ unknown reward distribution $v_{s_0,a}$ with mean $r(s_0,a)$
- ightharpoonup 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 :

- \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 $\sum_{t=1}^{T} R_t$. cumulative reward but not discounted

The Stochastic Multi-Armed Bandit Setup

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











 ν_5

At round t, an agent :

- chooses an arm A_t
- lacktriangleright receives a reward $R_t = X_{A_t,t} \sim
 u_{A_t}$ independently from past rewards

Sequential sampling strategy (bandit algorithm) :

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

Goal (for now!): Maximize $\mathbb{E}\left[\sum_{t=1}^{T} R_{t}\right]$ finite horizon T here but in general don't know how much we will interact with env

→ a particular reinforcement learning problem

Clinical trials

Historical motivation [Thompson, 1933]



For the *t*-th patient in a clinical study, time t <=> patient t, independent of previous patient

- ightharpoonup 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

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]

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

What regret rate can we achieve?

- ightharpoonup consistency : $\frac{\mathcal{R}_{\nu}(\mathcal{A}, T)}{T}
 ightarrow 0$
- → 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. R_t=E[R_t|H_{t-1}] and R_t \sim \nu_{A_t}. Thus E[R_t|H_{t-1}]=\mu_{A_t}. Then \mu_{A_t}=\sum_{k=1}^K \mu_a 1_{A_t=a}



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 :

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

⇒ Exploration / Exploitation trade-off

The greedy strategy

Select each arm once, then exploit the current knowledge :

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

where

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

The greedy strategy

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Thre greedy strategy can fail!
$$\nu_1 = \mathcal{B}(\mu_1), \nu_2 = \mathcal{B}(\mu_2), \ \mu_1 > \mu_2$$
 pas compris
$$\mathbb{E}[\mathcal{N}_2(T)] \geq (1 - \mu_1)\mu_2 \times (T - 1)$$

→ Exploitation is not enough, we need to add some exploration

Outline

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

- draw each arm m times
- ightharpoonup compute the empirical best arm $\hat{a} = \operatorname{argmax}_a \hat{\mu}_a(Km)$
- \triangleright 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
- \triangleright 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. $\mu_1 > \mu_2$, $\Delta := \mu_1 - \mu_2$.

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

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

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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 $a \to \text{requires a concentration inequality}$

A Concentration Inequality

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 $s \ge 1$

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

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

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 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].

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

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

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

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

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

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

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

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

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

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ight) + 1
ight].$$

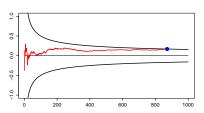
- + logarithmic regret!
- requires the knowledge of T and Δ

Sequential Explore-Then-Commit

explore uniformly until a random time of the form

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

lacksquare $\hat{a}_{ au} = \operatorname{argmax}_{a} \hat{\mu}_{a}(au)$ and $(A_{t+1} = \hat{a}_{ au})$ for $t \in \{ au + 1, \dots, T\}$



- \Rightarrow [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,

ightharpoonup with probability ϵ

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

ightharpoonup with probability $1-\epsilon$

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

→ <u>Linear regret</u> : \mathcal{R}_{ν} (ϵ -greedy, T) $\geq \epsilon \frac{\kappa-1}{\kappa} \Delta_{\min} T$. Regret is at least linear $\Delta_{\min} = \min_{a:U_a < U_a} \Delta_a$

Another possible fix : ϵ -greedy

ϵ_t -greedy strategy

At round t.

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

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

ightharpoonup with probability $1 - \epsilon_t$

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

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}

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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 :

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

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

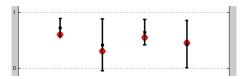


FIGURE - Confidence intervals on the means after t rounds

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

▶ That is, select

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

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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

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 $s\geq 1$

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

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

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

$$\mathbb{P}\left(\mu_{\mathsf{a}} \leq \hat{\mu}_{\mathsf{a}}(t) + \sqrt{\frac{6\sigma^2 \log(t)}{\mathsf{N}_{\mathsf{a}}(t)}}\right) \geq 1 - \frac{1}{t^2}$$

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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

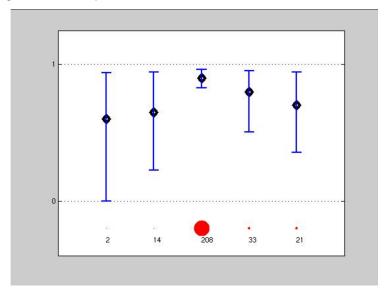
$$UCB(\alpha)$$
 selects $A_{t+1} = \underset{a}{\operatorname{argmax}} UCB_a(t)$ where

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

if a not chosen for long time, log(t) increases so UCB increases until it becomes the biggest one, which makes us choose a.

- ▶ 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 vidéo: algorithm kind of equalizes the UBS of each arm



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A regret bound for $UCB(\alpha)$

Theorem

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

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

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

Consequence:

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

Proof (1/2)

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

$$UCB_{i}(t) = \hat{\mu}_{i}(t) + \sqrt{\frac{6\sigma^{2}\log(t)}{N_{i}(t)}}$$

$$LCB_{i}(t) = \hat{\mu}_{i}(t) - \sqrt{\frac{6\sigma^{2}\log(t)}{N_{i}(t)}}$$

and the good event

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

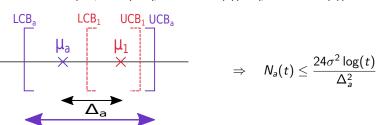
▶ **Step 1** : Hoeffding inequality + union bound :

$$\mathbb{P}\left(\mathcal{E}^c_t\right) \leq \mathbb{P}\left(\mu_1 > \hat{\mu}_1(t) + \sqrt{\frac{6\sigma^2\log(t)}{N_1(t)}}\right) + \mathbb{P}\left(\mu_{\boldsymbol{s}} < \hat{\mu}_{\boldsymbol{s}}(t) - \sqrt{\frac{6\sigma^2\log(t)}{N_{\boldsymbol{s}}(t)}}\right) \leq \frac{2}{t^2}$$

Proof (2/2)

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

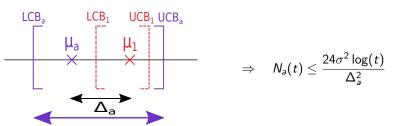
$$(A_{t+1} = a) \cap (\mu_1 < \mathrm{UCB}_1(t)) \cap (\mu_a > \mathrm{LCB}_a(t))$$



Proof (2/2)

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

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



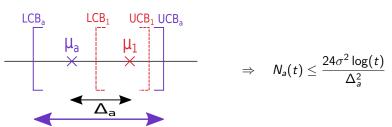
▶ **Step 3**: Putting everything together

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

Proof (2/2)

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

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



▶ **Step 3**: Putting everything together

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

A worse-case regret bound

Corollary

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

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 $\Delta > 0$,

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

Best known problem-dependent bound

previous slide was simplest UCB calibration but there are more sophisticated ones. Here is the best SOTA:

Context: σ^2 sub-Gaussian rewards

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

(c = 0 corresponds to $UCB(\alpha)$ with $\alpha = 2\sigma^2$)

Theorem [Cappé et al.'13]

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

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

Summary

For UCB(lpha) applied to σ^2 -subGaussian reward, setting $lpha=2\sigma^2$ 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 $\Delta \simeq \sqrt{K/T}$. in this case, we have \sqrt{KTlog(T)} regret

Remark. UCB achieves $\mathcal{O}(\sqrt{\mathsf{KT}\log(\mathcal{T})})$ (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 $\nu = (\nu_{\mu_1}, \dots, \nu_{\mu_K}), \ \mu_a \in \mathcal{I}.$

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

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]

The Lai and Robbins lower bound

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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]

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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,

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

[Lai and Robbins, 1985]

UCB compared to the lower bound

Gaussian distributions with variance σ^{2}

- ▶ Lower bound : $\mathbb{E}[N_a(T)] \gtrsim \frac{2\sigma^2}{(\mu_* \mu_a)^2} \log(T)$
- ▶ **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!

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 $\alpha = 2\sigma^2$

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

→ UCB is asymptotically optimal for Gaussian rewards!

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

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

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

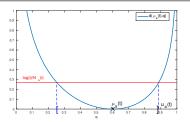
Pinsker's inequality : $kl(\mu_a, \mu_\star) > 2(\mu_\star - \mu_a)^2$

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

The kl-UCB algorithm

Exploits the KL-divergence in the lower bound!

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



A tighter concentration inequality [Garivier and Cappé, 2011]

For rewards in a one-dimensional exponential family a,

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

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

An asymptotically optimal algorithm

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

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

Theorem [Cappé et al., 2013]

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

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

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

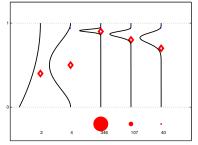
$$\mathcal{R}_{m{\mu}}(ext{kl-UCB}, T) \simeq \left(\sum_{eta: \mu_{\star} < \mu_{\star}} rac{\Delta_{m{artheta}}}{ ext{kl}(\mu_{m{artheta}}, \mu_{\star})}
ight) \log(T).$$

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A Bayesian algorithm

 $\pi_a(0)$: prior distribution on μ_a $\pi_{a}(t) = \mathcal{L}(\mu_{a}|Y_{a,1},\ldots,Y_{a,N_{a}(t)})$: 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"

Thompson Sampling

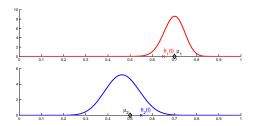
Input: a prior distribution $\pi(0)$

$$\left\{egin{array}{l} orall a \in \{1..K\}, & heta_a(t) \sim \pi_a(t) \ A_{t+1} = \mathop{\mathrm{argmax}}_{a=1...K} heta_a(t). \end{array}
ight.$$

Thompson Sampling for Bernoulli distributions

$$u_{\mathsf{a}} = \mathcal{B}(\mu_{\mathsf{a}})$$

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



Thompson Sampling

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

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

Thompson Sampling for Bernoulli distributions

$$u_{\mathsf{a}} = \mathcal{B}(\mu_{\mathsf{a}})$$

$$\pi_a(0) = \mathcal{U}([0,1])$$

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

Thompson Sampling for Gaussian distributions

$$u_{\mathsf{a}} = \mathcal{N}(\mu_{\mathsf{a}}, \sigma^2)$$

$$ightharpoonup \pi_a(0) \propto 1$$

$$ightarrow \pi_{\mathsf{a}}(t) = \mathcal{N}\left(\hat{\mu}_{\mathsf{a}}(t); rac{\sigma^2}{N_{\mathsf{a}}(t)}
ight)$$

Regret bounds

Upper bound on sub-optimal selections

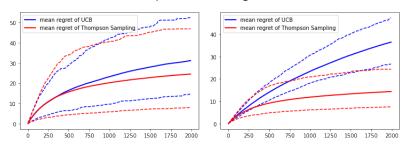
$$\forall a \neq a_{\star}, \ \mathbb{E}_{\mu}[N_a(T)] \leq \frac{\log(T)}{\mathrm{kl}(\mu_a, \mu_{\star})} + o_{\mu}(\log(T)).$$

where $kl(\mu_a, \mu_{\star})$ 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!

$$\mu_{A} = [0.45 \ 0.5 \ 0.6]$$
 $\mu_{B} = [0.1 \ 0.05 \ 0.02 \ 0.01]$

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
- \triangleright 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 $\{1,2,\ldots,K\} \leftrightarrow \mathsf{Context}$ 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

- lacktriangleright is given a set of arms $\mathcal{X}_t \subseteq \mathcal{X}$ (can be different in each round)
- ightharpoonup 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 $x_a \in \mathbb{R}^{p'}$
- \rightarrow 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

it is an extension of classical bandits, which would be the case \theta^*= \mu_1,\dots,\mu_K) and X=(e_1,\dots,e_K) so \theta^*e_a=\mu_a

In each round t, the agent

- ightharpoonup 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 $r_t = \theta_{\star}^{\top} x_t + \varepsilon_t$ linearity lies here

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

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

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 ↔ minimizing the (expectation of)

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

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

Tools

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

- **b** design matrix (with regularization parameter $\lambda > 0$)
- estimate of covariance (among dimensions) matrix of chosen arms x_s ? Or estimator in least squares? $B_t^\lambda = \lambda I_d + \sum_{s=1}^t x_s x_s^\top$
 - regularized least-square estimate

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

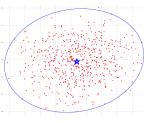
- ▶ estimate of the expected reward of an arm $x \in \mathbb{R}^d : x^\top \hat{\theta}_{\lambda}^{\lambda}$
- \Rightarrow sufficient for ε -greedy or ETC, but not for smarter algorithms...

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

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



here d=2 example

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

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

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

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

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 $x \in \mathcal{X}_t$, $\|x\| \le L$, we have borne en probabilité sur distance de notre estimée

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

→ 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 $\mathbb{P}(\forall t \in \mathbb{N}, \theta_{\star} \in C_{t}(\delta)) > 1 - \delta$.

A Lin-UCB algorithm

family of algorithms

Consequence:

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

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

$$\text{UCB}_{\mathsf{x}}(t) = \underbrace{\mathbf{x}^{\mathsf{T}} \hat{\boldsymbol{\theta}}_{t}^{\lambda}}_{\text{empirical mean}} + \underbrace{\|\mathbf{x}\|_{(\mathcal{B}_{t}^{\lambda})^{-1}} \beta(t, \delta)}_{\text{exploration bonus}}$$

Lin-UCB

In each round t+1, the algorithm selects

$$\mathbf{x}_{t+1} = \operatorname*{argmax}_{\mathbf{x} \in \mathcal{X}_{t+1}} \left[\mathbf{x}^{\top} \hat{\theta}_{\underline{t}}^{\lambda} + \|\mathbf{x}\|_{(B_{\underline{t}}^{\lambda})^{-1}} \beta(t, \delta) \right]$$

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

Theoretical guarantees

We want to bound the pseudo-regret

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

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 $1 - \delta$,

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

 \blacktriangleright 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 : $\theta_{\star} \sim \mathcal{N}(0, \kappa^2 I_d)$

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

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

with

- $B_t^{\lambda} = \lambda I_d + \sum_{s=1}^t x_s x_s^{\top}$
- $\hat{ heta}_t^\lambda = \left(B_t^\lambda
 ight)^{-1}\left(\sum_{s=1}^t r_s x_s
 ight)$ 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.

$$\widetilde{\theta}_{t} = \widehat{\theta}_{t}^{\lambda} + \sigma \left(B_{t}^{\lambda} \right)^{-1/2} X$$

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 parameteric models may be better suited than the simple linear model, for example the logistic model.

$$\mathbb{P}(r_t = 1|x_t) = \frac{1}{1 + e^{-\theta_{\star}^{\top} x_t}}$$

$$\mathbb{P}(r_t = 0|x_t) = \frac{e^{-\theta_{\star}^{\top} x_t}}{1 + e^{-\theta_{\star}^{\top} x_t}}$$

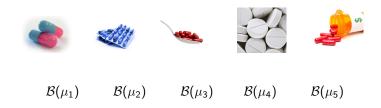
e.g., clic / no-clic on an add depending on a user/add feature $x_t \in \mathbb{R}^d$

- ► [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?



For the t-th patient in a clinical study,

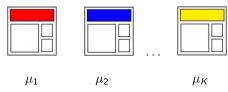
- chooses a treatment A_t
- $lackbox{ observes a response } X_t \in \{0,1\}: \mathbb{P}(X_t=1) = \mu_{A_t}$

 $\textbf{Maximize rewards} \leftrightarrow \text{cure as many patients as possible}$

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 :



Best version :
$$a_{\star} = \underset{a=1,...,K}{\operatorname{argmax}} \mu_{a}$$

Sequential protocol: for the *t*-th visitor:

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

Maximize rewards ↔ 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 μ_{\star} as quickly and accurately as possible \simeq identify

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

Algorithm: made of three components:

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

Probability of error

The probability of error after T rounds is

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

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if best and second best arm too close, it takes too much time to discriminate btn them, so:

Simple regret [Bubeck et al., 2011]

The simple regret after n rounds is

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

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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:

- \rightarrow sampling rule : A_t (arm to explore)
- \rightarrow recommendation rule : B_t (current guess for the best arm)
- \rightarrow 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 $\mathbb{E}[au]$
minimize $\mathbb{P}(B_T \neq a_\star)$	$\mathbb{P}(B_ au eq a_\star) \leq \delta$
or $\mathbb{E}[r_T(u)]$	or $\mathbb{P}(r_{\nu}(\tau) > \epsilon) \leq \delta$
[Bubeck et al., 2011]	[Even-Dar et al., 2006]
[Audibert et al., 2010]	

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

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

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

▶ 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	$B_t = \operatorname{argmax}_a \hat{\mu}_a(t)$
(EBA)	
Most Played Arm	$B_t = \operatorname{argmax}_a N_a(t)$
(MPA)	
Empirical Distribution of Plays	$B_t \sim p_t$, where
(EDP)	$ ho_t = \left(rac{ extstyle N_1(t)}{t}, \dots, rac{ extstyle N_K(t)}{t} ight)$

[Bubeck et al., 2011]

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[Bubeck et al., 2011]

▶ UCB + Empirical Distribution of Plays

$$\mathbb{E}\left[r_{\nu}(T)\right] = \mathbb{E}\left[\mu_{\star} - \mu_{B_{T}}\right] = \mathbb{E}\left[\sum_{b=1}^{K} (\mu_{\star} - \mu_{b}) \mathbb{1}_{(B_{T} = b)}\right]$$

$$= \mathbb{E}\left[\sum_{b=1}^{K} (\mu_{\star} - \mu_{b}) \mathbb{P}(B_{T} = b | \mathcal{F}_{T})\right]$$

$$= \mathbb{E}\left[\sum_{b=1}^{K} (\mu_{\star} - \mu_{b}) \frac{N_{b}(T)}{T}\right]$$

$$= \frac{1}{T} \sum_{b=1}^{K} (\mu_{\star} - \mu_{b}) \mathbb{E}[N_{b}(T)]$$

$$= \frac{\mathcal{R}_{\nu}(T)}{T}.$$

→ a conversion from cumulative regret to simple regret!

▶ UCB + Empirical Distribution of Plays

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

▶ UCB + Empirical Distribution of Plays

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

► UCB + Empirical Distribution of Plays

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

vs. Uniform Sampling

The simple regret or the uniform strategy decays exponentially :

$$\mathbb{E}_{
u}\left[r_{
u}\left(\mathtt{Unif},T
ight)
ight] \leq (\mathcal{K}-1)\Delta_{\mathsf{max}}\exp\left(-rac{1}{2}rac{\mathcal{T}}{\mathcal{K}}\Delta_{\mathsf{min}}^{2}
ight)$$

→ UCB does not provably outperform uniform sampling...

Sample complexity

With Uniform Sampling, the number of sample needed to get an error probability (or simple regret) smaller than δ is of order

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

(assuming, e.g. bounded rewards)

► Can be improved for smarter algorithms to

$$\mathcal{T} \simeq \mathcal{O}\left(\mathcal{H}(
u)\log\left(rac{1}{\delta}
ight)
ight)$$

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.

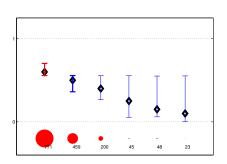
```
Initialisation : S_0 = \{1, \dots, K\}; For r = 0 to \lceil \ln_2(K) \rceil - 1, do sample each arm a \in S_r t_r = \left\lfloor \frac{T}{|S_r| \lceil \log_2(K) \rceil} \right\rfloor times; let \hat{\mu}_a^r be the empirical mean of arm a; let S_{r+1} be the set of \lceil |S_r|/2 \rceil arms with 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

$$\mathcal{I}_a(t) = [LCB_a(t), UCB_a(t)].$$



► At round t, draw

$$B_t = \underset{b}{\operatorname{argmax}} \hat{\mu}_b(t)$$
 $C_t = \underset{c \neq B_t}{\operatorname{argmax}} \operatorname{UCB}_c(t)$

Stop at round t if

$$LCB_{B_t}(t) > UCB_{C_t}(t) - \epsilon$$

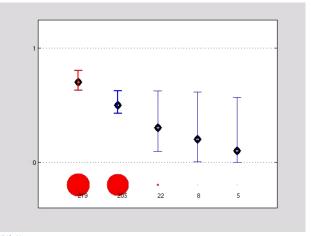
Theorem [Kalyanakrishnan et al., 2012]

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

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

(kl)-LUCB in action

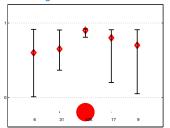
$$\begin{aligned} \mathrm{UCB}_{\boldsymbol{a}}(t) &=& \max \left\{ q \in [0,1] : N_{\boldsymbol{a}}(t) \mathrm{kl}(\hat{\mu}_{\boldsymbol{a}}(t),q) \leq \log(Ct^2/\delta) \right\} \\ \mathrm{LCB}_{\boldsymbol{a}}(t) &=& \min \left\{ q \in [0,1] : N_{\boldsymbol{a}}(t) \mathrm{kl}(\hat{\mu}_{\boldsymbol{a}}(t),q)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



A comparison with UCB

Regret minimizing algorithms and Best Arm Identification algorithms behave quite differently

regret minimization algo: most mass on best arm



lot of mass on the 2-3 best arms because hard to discriminate

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

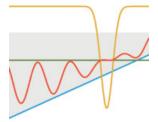
to better take into account the uncertainty and perform more efficient ("directed") exploration.

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

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