

huge Reinforcement Learning

Lecture 3 : Structured bandits

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Centrale Lille, 2022/2023

Recap from last class

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
- ▶ Bayesian algorithms : Thompson Sampling

Some of these can be extended to more realistic **structured** models that are suited for different applications.

More about UCB : worst case bound

Context : σ^2 sub-Gaussian rewards

$$\text{UCB}_a(t) = \hat{\mu}_a(t) + \sqrt{\frac{8\sigma^2 \log(t)}{N_a(t)}}$$

Theorem

The UCB algorithm associated to the above index satisfies

$$\mathbb{E}[N_a(T)] \leq \frac{32\sigma^2}{(\mu_\star - \mu_a)^2} \log(T) + 2.$$

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

Regret bounds :

- ▶ Distribution-dependent : $\mathbb{E}[R_T] \leq \sum_{a: \Delta_a > 0} \frac{32\sigma^2}{\Delta_a} \log(T) + 2\Delta_a.$
- ▶ Worst-case : $\mathbb{E}[R_T] \leq C\sqrt{KT \log T}.$

Outline

1 Contextual Bandits

2 Solving Linear Bandits

- Lin-UCB
- Linear Thompson Sampling

3 Other variants of the classical MAB

Contextual Bandits

Example : movie recommendation



What 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**

Contextual bandit problem : at time t

- ▶ a context c_t is observed
- ▶ an arm A_t is chosen
- ▶ a reward R_t that depends on c_t, A_t is received.

RL as a contextual bandit

RL can be cast as a contextual bandit

- ▶ a context c_t is observed $\rightarrow c_t = s_t$, the state
- ▶ an arm A_t is chosen
- ▶ a reward R_t that depends on c_t, A_t is received. reward depends on state and action

RL as a contextual bandit

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But you should not do that

- ▶ All information about transitions is lost !
- ▶ No link between successive contexts

Independent bandits

Contextual bandit problem : at time t

- ▶ a context c_t is observed
- ▶ an arm A_t is chosen
- ▶ a reward R_t that depends on c_t, A_t is received.

Idea : 1 context = 1 bandit

- ▶ Run many bandit algorithms, one per context
- ▶ Regret depends on the number of context \rightarrow not practical

We have to **link different context together**, to avoid the independent bandits situation.

Mixing bandits and regression models

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

Mixing bandits and regression models

A (stochastic) **contextual bandit model** incorporates two components :

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

Mixing bandits and regression models

A **(stochastic) contextual bandit model** incorporates two components :

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

General stochastic contextual bandit model

In each round t , the agent

- ▶ observes a context $c_t \in \mathcal{C}$ *(user characteristics)*
- ▶ selects an arm $A_t \in \mathcal{A}_t$ *(an item out of a possibly changing pool)*
- ▶ the agent receives a reward

$$r_t = f_{A_t}(c_t) + \varepsilon_t$$

where ε_t is an independent noise : $\mathbb{E}[\varepsilon_t] = 0$.

$f_a : \mathcal{C} \rightarrow \mathbb{R}$ maps a context c to the average reward of arm a , $f_a(c)$

Examples

Example 1

- user t : descriptor $c_t \in \mathbb{R}^p$
- item a : descriptor $\theta_a \in \mathbb{R}^p$

$$r_t = \theta_{A_t}^\top c_t + \varepsilon_t$$

Linear function $f_a(c) = \theta_a^\top c$

Observation : if $\mathcal{A}_t = \{1, \dots, K\}$ is a fixed set of items

- ▶ the model is parameterized by $\theta_1, \theta_2, \dots, \theta_K \in (\mathbb{R}^p)^K$
- ▶ it can also be rewritten $r_t = \theta_\star^\top (x_{t,A_t}) + \varepsilon_t$ with

$$\theta_\star = \begin{pmatrix} \theta_1 \\ \dots \\ \theta_a \\ \dots \\ \theta_K \end{pmatrix} \in \mathbb{R}^{p \times K}, \quad x_{t,a} = \begin{pmatrix} 0 \\ \dots \\ c_t \\ \dots \\ 0 \end{pmatrix} \in \mathbb{R}^{p \times K}$$

$x_{t,a}$: feature vector for the user-item pair (t, a)

Examples

Example 2

- 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 $(t, a) : x_{t,a} \in \mathbb{R}^d$
(feature engineering)

$$r_t = \theta_\star^\top x_{t,A_t} + \varepsilon_t$$

Observation :

- ▶ the model is parameterized by $\theta_\star \in \mathbb{R}^d$
- ▶ in each round t , the user-item feature vectors belong to the set

$$\mathcal{X}_t = \{x_{t,a}, a \in \mathcal{A}_t\} \subseteq \mathbb{R}^d$$

- ▶ picking an arm $a \leftrightarrow$ picking a feature vector $x_t \in \mathcal{X}_t$

$$r_t = \theta_\star^\top x_t + \varepsilon_t$$

Examples

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

Two formulations

Contextual MAB, version 1

In each round t , the agent

- ▶ observes a context $c_t \in \mathcal{C}$
- ▶ selects an arm $A_t \in \mathcal{A}_t$ *(set of arm can vary in each round)*
- ▶ the agent receives a reward $r_t = f_{A_t}(c_t) + \varepsilon_t$

Unknown : regression functions (f_a) for all possible arm a

Contextual MAB (more general)

In each round t , the agent

- ▶ is given a set of arms \mathcal{X}_t *(can be different in each round)*
- ▶ selects an arm $x_t \in \mathcal{X}_t$
- ▶ the agent receives a reward $r_t = f_*(x_t) + \varepsilon_t$

Unknown : regression function f_*

Two formulations

Contextual MAB, version 1

In each round t , the agent

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Contextual MAB (more general)

In each round t , the agent

- ▶ is given a set of arms \mathcal{X}_t *(can be different in each round)*
- ▶ selects an arm $x_t \in \mathcal{X}_t$
- ▶ the agent receives a reward $r_t = f_*(x_t) + \varepsilon_t$

Unknown : regression function f_*

→ **Goal** : learn the unknown function f_* ... while maximizing rewards !

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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

$$\forall \lambda \in \mathbb{R}, \mathbb{E} [e^{\lambda X}] \leq e^{\frac{\lambda^2 \sigma^2}{2}}$$

e.g., Gaussian noise, bounded noise.

Contextual linear bandits

In each round t , the agent

- ▶ receives a (finite) set of arms $\mathcal{X}_t \subseteq \mathbb{R}^d$
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(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 !

Linear Regression

Goal : find estimate $\hat{\theta}_t$ of θ_* , given observations $(x_1, y_1), \dots, (x_t, y_t)$, where $y_s = \theta_*^\top x_s + \varepsilon_s$.

Loss function : squared loss + regularization

Goal : find $\operatorname{argmin}_{\theta} \sum_{s=1}^t (y_s - \theta^\top x_s)^2 + \lambda \|\theta\|^2$.



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

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

Remark : easy online update ! use the Sherman-Morrison formula.

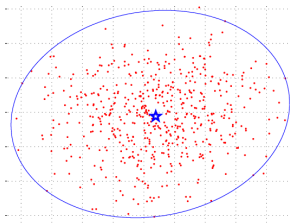
- ▶ estimate of the expected reward of an arm $x \in \mathbb{R}^d$: $x^\top \hat{\theta}_t^\lambda$
- sufficient for Follow the Leader, but not for smarter algorithms !

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

Idea : rely on a **confidence ellipsoid** 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

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

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

A Lin-UCB algorithm

Consequence :

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

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

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

Lin-UCB

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

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

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

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 :

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

with

- $B_t^\lambda = \lambda I_d + \sum_{s=1}^t x_s x_s^\top$
- $\hat{\theta}_t^\lambda = (B_t^\lambda)^{-1} (\sum_{s=1}^t r_s x_s)$ 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 $t + 1$,

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

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

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

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

Theoretical guarantees

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

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

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

Theorem

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

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

- ▶ slightly worse than Lin-UCB... how about in practice ?
- ▶ 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**.

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

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 [Dumitrescu et al., 2018]
- ▶ going further : UCB/TS for neural bandits !

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Many possible structures

\mathcal{X} -armed bandits : $\mathcal{X}_t = \mathcal{X}$ arbitrary metric space

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

with non-parametric assumption on f_\star .

Examples :

- ▶ f_\star is a Lipschitz function :

$$|f_\star(x) - f_\star(y)| \leq Ld(x, y)$$

where d is a metric on \mathcal{X} .

[Bubeck et al., 2008]

- ▶ f_\star is a unimodal function
- ▶ f_\star is drawn from a Gaussian process prior

[Srinivas et al., 2009]

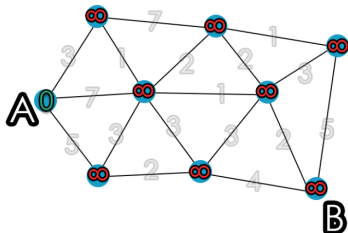
- ▶ ...

Beyond one arm : Combinatorial bandits

classical bandit : **one arm** is selected in each round

combinatorial bandit : possibility to select a **group of arms** (action)

e.g., [Chen et al., 2013]



Example :

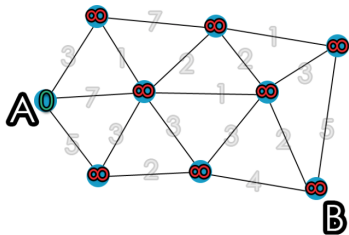
- ▶ arms : edges in a graph
- ▶ actions : paths from A to B
- ▶ reward : some function of the edges's rewards in the chosen path
(e.g. - (total travelling distance))

Beyond one arm : Combinatorial bandits

classical bandit : **one arm** is selected in each round

combinatorial bandit : possibility to select a **group of arms** (action)

e.g., [Chen et al., 2013]



Combinatorial bandit : $\text{Actions} \subseteq \mathcal{P}(\{1, \dots, K\})$.

In round t , the agent

- ▶ selects an action $\text{Act}_t \in \text{Actions}$
- ▶ a reward $r_{a,t}$ is generated for every arm $a \in \text{Act}_t$
- ▶ the agent receives as a reward $\sum_{a \in \text{Act}_t} r_{a,t}$ (or some other function)

Beyond one agent : Multi-Player bandits

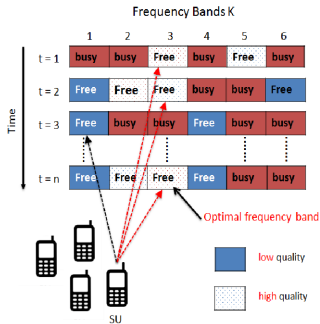
classical bandit : **one agent** select and arm in each round

multi-player bandit : **several agents** play on the same bandit

e.g., [Besson and Kaufmann, 2018]

Example : (cognitive radio system)

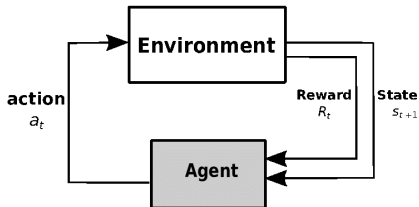
- ▶ arm : availability of a radio channel
- ▶ agent : a radio device, picking a channel in each round
- ▶ reward : quality of the communication
- if two agents select the same arm, the reward is reduced...



Beyond one state : Reinforcement Learning

In most bandit models, the agent repeatedly faces the **same set of actions** (or at least the set of available actions in round does not depend on the past decisions).

- no longer true in **reinforcement learning**, in which an action also triggers a transition to a new **state**



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 ?



$\mathcal{B}(\mu_1)$

$\mathcal{B}(\mu_2)$

$\mathcal{B}(\mu_3)$

$\mathcal{B}(\mu_4)$

$\mathcal{B}(\mu_5)$

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→ Pure exploration, Best arm identification [Bubeck et al., 2011]



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