

Sequential Learning

Lecture 8 : Bandit Identification

Rémy Degenne
(remy.degenne@inria.fr)



Université
de Lille



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Finding the best policy

Reinforcement Learning

- ▶ Interact with an unknown MDP
- ▶ Goal : Maximize the expected cumulative reward

Observations :

- ▶ There exists an optimal policy π^* independent of the starting state
- ▶ If an algorithm samples according to $\pi_t \approx \pi^*$, then it gets high expected cumulative reward

Results in reinforcement learning

For small MDPs with known dynamics :

Theorem

Value iteration converges in at most $\log \left(\frac{\|T^*(V_0) - V_0\|_\infty}{\epsilon} \right) / \log(1/\gamma)$ iterations and outputs a policy π satisfying $\|V^\pi - V^*\| \leq \frac{\gamma\epsilon}{1-\gamma}$.

Theorem

Policy iteration terminates after a **finite number of steps** and outputs the **optimal policy π^*** .

- ▶ No result on the actual sum of rewards obtained during learning.
- ▶ Only guaranty that we eventually approach π^* .
- ▶ Results only get worse for larger and unknown MDPs.

Regret minimization in bandits

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

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

Results :

- ▶ Lower bounds on the regret of consistent algorithms
- ▶ Algorithms with $O(\log T)$ regret upper bounds

Finding the best policy in bandits ?



$\mathcal{B}(\mu_1)$

$\mathcal{B}(\mu_2)$

$\mathcal{B}(\mu_3)$

$\mathcal{B}(\mu_4)$

$\mathcal{B}(\mu_5)$

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)

Finding the best policy in bandits ?



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Maximize rewards \leftrightarrow cure as many patients as possible

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(without trying to cure patients during the study)

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

Best arm identification

Bandit interaction

At time t ,

- ▶ choose an arm A_t
- ▶ observe a response $X_t \in \mathbb{R}$, sampled from distribution ν_{A_t} , with mean μ_{A_t}

Best arm identification goal : interact with the bandit for a while, then return the arm with highest mean.

Best arm identification

Bandit interaction

At time t ,

- ▶ choose an arm A_t
- ▶ observe a response $X_t \in \mathbb{R}$, sampled from distribution ν_{A_t} , with mean μ_{A_t}

Best arm identification goal : interact with the bandit for a while, then return the arm with highest mean.

That is, find the best policy.

Goals : multiple objectives

Bandit interaction

At time t ,

- ▶ choose an arm A_t
- ▶ observe a response $X_t \in \mathbb{R}$, sampled from distribution ν_{A_t} , with mean μ_{A_t}

Best arm identification goal : interact with the bandit for a while, then return the arm with highest mean.

Two goals

- ▶ Find the best arm with high probability
- ▶ Stop quickly

Let's formalize the problem

K arms with distributions (ν_1, \dots, ν_K) , with means (μ_1, \dots, μ_K)

At each time t , until the algorithm stops,

- ▶ choose an arm A_t
- ▶ observe a response $X_t \in \mathbb{R}$, sampled from distribution ν_{A_t}
- ▶ decide whether to stop or not

Let τ be the stopping time.

At τ , return $\hat{A}_\tau \in [K]$.

The algorithm makes a mistake if $\hat{A}_\tau \neq a^* := \operatorname{argmax}_a \mu_a$.

Let's formalize the problem

K arms with distributions (ν_1, \dots, ν_K) , with means (μ_1, \dots, μ_K)

At each time t , until the algorithm stops,

- ▶ choose an arm $A_t \rightarrow$ **sampling rule**
- ▶ observe a response $X_t \in \mathbb{R}$, sampled from distribution ν_{A_t}
- ▶ decide whether to stop or not

Let τ be the stopping time. \rightarrow **stopping rule**

At τ , return $\hat{A}_\tau \in [K]$. \rightarrow **recommendation rule**

The algorithm makes a **mistake** if $\hat{A}_\tau \neq a^* := \operatorname{argmax}_a \mu_a$.

Two problems

Two goals

- ▶ Find the best arm with high probability
- ▶ Stop quickly

Multiple objectives are hard to optimize simultaneously.

Solution : optimize one objective, under a constraint on the other.

- ▶ **Fixed confidence identification** :
Optimize the stopping time of an algorithm, under a constraint on the probability of mistake
- ▶ **Fixed budget identification** :
Optimize the probability of mistake after a given time

Outline

1 Fixed Budget Identification

2 Fixed Confidence Identification

Fixed budget identification

Fixed budget identification : minimize the probability of mistake after a given time.

Fixed Budget

Horizon T is known in advance, and the algorithm stops at $\tau = T$.

Goal : find an algorithm such that the probability of mistake $\mathbb{P}_\nu(\hat{A}_T \neq a^*)$ is as small as possible.

Simple algorithm : uniform sampling

Uniform sampling algorithm :

- ▶ sample all arms $\lfloor T/K \rfloor$ times \rightarrow [sampling rule](#)
- ▶ return the best arm of the empirical mean vector $\hat{\mu}_T$
 \rightarrow [recommendation rule](#)

What is the probability of mistake ?

$$\begin{aligned}\mathbb{P}_\nu(\hat{A}_T \neq a^*) &= \mathbb{P}_\nu(\operatorname{argmax}_a \hat{\mu}_{T,a} \neq \operatorname{argmax}_a \mu_a) \\ &= \mathbb{P}_\nu(\exists a \neq a^*, \hat{\mu}_{T,a} > \hat{\mu}_{T,a^*}) \\ &\leq \sum_{a \neq a^*} \mathbb{P}_\nu(\hat{\mu}_{T,a} > \hat{\mu}_{T,a^*}).\end{aligned}$$

Concentration again

We need to bound $\mathbb{P}_\nu(\hat{\mu}_{T,a} > \hat{\mu}_{T,a^*})$. Use a **concentration inequality**.

Hoeffding inequality

Z_i i.i.d. σ -sub-Gaussian random variables. For all $s \geq 1$

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

Both $\hat{\mu}_{T,a}$ and $\hat{\mu}_{T,a^*}$ are averages of T/K i.i.d. random variables, with respective means μ_a and μ^* .

$$\begin{aligned} & \mathbb{P}_\nu(\hat{\mu}_{T,a} > \hat{\mu}_{T,a^*}) \\ &= \mathbb{P}_\nu(\hat{\mu}_{T,a} > \hat{\mu}_{T,a^*}, \hat{\mu}_{T,a^*} \leq \mu^* - \frac{\Delta_a}{2}) + \mathbb{P}_\nu(\hat{\mu}_{T,a} > \hat{\mu}_{T,a^*}, \hat{\mu}_{T,a^*} > \mu^* - \frac{\Delta_a}{2}) \\ &\leq \mathbb{P}_\nu(\hat{\mu}_{T,a^*} \leq \mu^* - \frac{\Delta_a}{2}) + \mathbb{P}_\nu(\hat{\mu}_{T,a} > \mu^* - \frac{\Delta_a}{2}) \\ &= \mathbb{P}_\nu(\hat{\mu}_{T,a^*} \leq \mu^* - \frac{\Delta_a}{2}) + \mathbb{P}_\nu(\hat{\mu}_{T,a} > \mu_a + \frac{\Delta_a}{2}) \leq 2 \exp\left(-\lfloor T/K \rfloor \frac{\Delta_a^2}{8\sigma^2}\right). \end{aligned}$$

Error probability of uniform sampling

Theorem

On the fixed budget best arm identification problem with budget T , uniform sampling has error probability

$$\mathbb{P}_\nu(\hat{A}_T \neq a^*) \leq 2 \sum_{a \neq a^*} \exp\left(-\lfloor T/K \rfloor \frac{\Delta_a^2}{8\sigma^2}\right)$$

This error probability is of order $\exp(-T\Delta_{\min}^2/(8K\sigma^2))$.

- ▶ Exponentially decreasing with T
- ▶ Rate of decrease of order Δ_{\min}^2/K .

Oracle

Suppose we sample each arm n_a times, fixed in advance, not random, with $\sum_{a \in [K]} n_a = T$.

Return the best arm of the empirical mean vector $\hat{\mu}_T$.

Theorem

On the fixed budget best arm identification problem with budget T , that sampling scheme has error probability

$$\mathbb{P}_\nu(\hat{A}_T \neq a^*) \leq K \sum_{a \neq a^*} \exp\left(-n_{a^*} \frac{\Delta_a^2}{8\sigma^2}\right) + \sum_{a \neq a^*} \exp\left(-n_a \frac{\Delta_a^2}{8\sigma^2}\right)$$

We call **static sampling oracle** at μ the allocation $(n_a^*)_{a \in [K]}$ which minimizes the probability of error.

It **depends on** μ (hence the name oracle) and verifies

$$\mathbb{P}_\nu(\hat{A}_T \neq a^*) \leq K \exp\left(-\frac{T}{8\sigma^2 \sum_a \frac{1}{\Delta_a^2}}\right).$$

where $\Delta_{a^*} = \min_{a \neq a^*} \Delta_a$.
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Can we match the oracle ?

The static sampling oracle depends on the unknown μ , with

$$n_a^* \approx \frac{1/\Delta_a^2}{\sum_b 1/\Delta_b^2}.$$

Can we reach the same error probability without knowing μ ?

No, we can't [Carpentier and Locatelli, 2016]

Let $H(\mu) = \sum_a \frac{1}{\Delta_a^2}$. For any fixed budget identification algorithm, there exists a bandit problem with Gaussian arms with variance 1 such that

$$\mathbb{P}_\mu(\hat{A}_T \neq a^*) \geq C_{K,T} \exp\left(-\frac{T}{H(\mu) \log K}\right).$$

No algorithm can match the oracle rate of $\frac{T}{H(\mu)}$ everywhere.

But can we do almost as well ? Can we get $H(\mu) \log K$, since $H(\mu)$ is impossible ?

UCB-E

UCB for Exploration (UCB-E) [Audibert et al., 2010].

- ▶ Sample $A_t = \operatorname{argmax}_a \hat{\mu}_{t,a} + \sqrt{\frac{a}{N_{t,a}}}$.
- ▶ Recommend $\hat{A}_T = \operatorname{argmax}_a \hat{\mu}_{T,a}$.

Theorem

If UCB-E is run with parameter $0 < a \leq \frac{25}{36} \frac{T-K}{H(\mu)}$, then it satisfies

$$\mathbb{P}_\mu(\hat{A}_T \neq a^*) \leq 2TK \exp\left(-\frac{2a}{25}\right).$$

In particular for $a = \frac{25}{36} \frac{T-K}{H(\mu)}$, we have $\mathbb{P}_\mu(\hat{A}_T \neq a^*) \leq 2TK \exp\left(-\frac{T-K}{18H(\mu)}\right)$.

Can match $T/H(\mu)$... if we know $H(\mu)$!

Successive Rejects

Idea : sample uniformly for a while, then reject the lowest arm. Sample the remaining arms uniformly, then reject the lowest, etc.

Successive Rejects [Audibert et al., 2010]

Let $\mathcal{A}_1 = [K]$, $\overline{\log}(K) = \frac{1}{2} + \sum_{k=2}^K \frac{1}{k}$, $n_0 = 0$ and for $k \in \{1, \dots, K-1\}$,

$$n_k = \left\lceil \frac{T - K}{\overline{\log}(K)(K + 1 - k)} \right\rceil.$$

For each phase $k = 1, 2, \dots, K_1$,

- 1 For each $a \in \mathcal{A}_k$, pull arm a for $n_k - n_{k-1}$ rounds.
- 2 Let $\mathcal{A}_{k+1} = \mathcal{A}_k \setminus \{\operatorname{argmin}_{a \in \mathcal{A}_k} \hat{\mu}_{n_k, a}\}$.

Return the unique element of \mathcal{A}_K as \hat{A}_T

Error probability of Successive Rejects

Theorem

The probability of error of successive rejects satisfies

$$\mathbb{P}_{\mu}(\hat{A}_T \neq a^*) \leq K^2 \exp \left(-\frac{T - K}{\log(K) H_2(\mu)} \right),$$

where $H_2(\mu) = \max_{k \in [K]} \frac{k}{\Delta_k^2}$.

$$H_2(\mu) \leq H(\mu) \leq \log(K) H_2(\mu).$$

► Successive Rejects attains $T / (H(\mu) \log K)$ everywhere.

Open questions in fixed budget identification

- ▶ What is the complexity of parametric best arm identification? (with Kullback-Leibler divergences and not gaps)
- ▶ What if the question is not to find the best arm, but something else about the distributions? Lower bound, algorithms?
- ▶ Can we have an algorithm that stops early if the problem is easy?

Outline

1 Fixed Budget Identification

2 Fixed Confidence Identification

Fixed confidence identification

Fixed confidence identification : Optimize the stopping time of an algorithm, under a constraint on the probability of mistake

δ -correct algorithm

An algorithm is said to be δ -correct on a set of bandit problems \mathcal{D} if for all distribution tuples $\nu \in \mathcal{D}$,

$$\mathbb{P}_{\nu}(\hat{A}_{\tau} \neq a^*) \leq \delta .$$

Goal : find a δ -correct algorithm such that the expected stopping time $\mathbb{E}_{\nu}[\tau]$ is as small as possible.

Variant : minimize $T_{\nu,\delta}$ such that with probability $1 - \delta$, the algorithm stops before $T_{\nu,\delta}$ and is correct.

Simple algorithm : uniform sampling

Idea : sample all arms in turn, until we can stop.

When is that ?

In addition to the **sampling rule** and the **recommendation rule** we need a **stopping rule** .

Stopping rule : confidence intervals

Concentration-based stopping rule :

- ▶ Maintain confidence intervals for the means of all arms
- ▶ Once the confidence interval of the best arm does not overlap with any other, stop

Recommendation rule : empirical best arm.

Suppose that with probability $1 - \delta$, the confidence intervals hold for all times.

Then with that probability : if the algorithm stops then the answer is correct.

- ▶ This is independent of the sampling rule !

Stopping rule : confidence intervals

Suppose that the arm distributions are σ^2 -sub-Gaussian. Then

$$\mathbb{P} \left(\exists a, \exists t \in \mathbb{N}, \hat{\mu}_{t,a} \notin \left[\mu_a - \sqrt{\frac{2\sigma^2 \log(\frac{2Kt^2}{\delta})}{N_{t,a}}}, \mu_a + \sqrt{\frac{2\sigma^2 \log(\frac{2Kt^2}{\delta})}{N_{t,a}}} \right] \right) \leq \delta$$

Proof : Hoeffding's inequality, union bounds.

Uniform sampling

- ▶ Sample uniformly.
- ▶ Stop when the interval of the best arm does not overlap any other interval.
- ▶ Recommend that arm.

Theorem

With probability $1 - \delta$, that algorithm is correct and stops before

$$T_{\mu,\delta} := \inf \left\{ t \mid \sqrt{\frac{2\sigma^2 \log(Kt^2/\delta)}{t/K}} \leq \frac{\Delta_{\min}}{2} \right\}.$$

That is, $T_{\mu,\delta} \approx \frac{K}{\Delta_{\min}^2} 8\sigma^2 \log(K/\delta)$

Faster than uniform sampling ?

- ▶ Stop sampling arms that can be eliminated by another arm :

Successive Elimination [Even-Dar et al., 2006]

$$T_{\mu,\delta} \approx \left(\sum_a \frac{1}{\Delta_a^2}\right) 8\sigma^2 \log(K/\delta)$$

But what about the bad event of probability δ ?

If the best arm is eliminated, the algorithm might run for a very long time (see board).

- ▶ Sample the best arm and a well chosen challenger (LUCB [Kalyanakrishnan et al., 2012], Top Two algorithms [Russo, 2016, Jourdan et al., 2022])

We can get bounds on the **expected** stopping time $\mathbb{E}[\tau]$, also of order $\left(\sum_a \frac{1}{\Delta_a^2}\right) \sigma^2 \log(1/\delta)$.

Towards optimality : lower bound

Our goal : get $\mathbb{E}[\tau]$ which is exactly as low as possible.

Lower bound

Any δ -correct algorithm on \mathcal{D} verifies

$$\mathbb{E}_{\nu}[\tau] \max_{w \in \Delta_K} \inf_{\lambda \in \mathcal{D}: a^*(\lambda) \neq a^*(\nu)} \sum_a w_a \text{KL}(\nu_a, \lambda_a) \geq \log \frac{1}{2.4\delta} .$$

Proof based on the chain rule and data processing inequality for the Kullback Leibler divergence.



GLRT stopping rule

\mathcal{D} is a family of parametric distributions, parametrized by their means (technically we need a one-parameter exponential family).

$\text{KL}(\mu_a, \lambda_a)$ for $\mu_a, \lambda_a \in \mathbb{R}$, denotes the KL between the corresponding distributions.

let $\hat{\mu}_t$ be the maximum likelihood estimator for the means at time t .

Lemma : LLR concentration

Under μ , with probability $1 - \delta$, for all $t \in \mathbb{N}$,

$$\sum_{s=1}^t \log \frac{d\mathbb{P}_{\hat{\mu}_t, A_s}}{d\mathbb{P}_{\mu, A_s}}(X_{s, A_s}) \leq \log\left(\frac{t^2}{\delta}\right).$$

Like we did with confidence intervals, we can get a stopping rule from this.

GLRT stopping rule

Lemma : LLR concentration

Under μ , with probability $1 - \delta$, for all $t \in \mathbb{N}$,

$$\sum_{s=1}^t \log \frac{d\mathbb{P}_{\hat{\mu}_t, A_s}}{d\mathbb{P}_{\mu_{A_s}}}(X_{s, A_s}) \leq \log\left(\frac{t^2}{\delta}\right).$$

Stop if

$$\inf_{\lambda \in \text{alt}(\hat{\mu}_t)} \sum_{s=1}^t \log \frac{d\mathbb{P}_{\hat{\mu}_t, A_s}}{d\mathbb{P}_{\lambda_{A_s}}}(X_{s, A_s}) > \log\left(\frac{t^2}{\delta}\right),$$

where $\text{alt}(\hat{\mu}_t) = \{\lambda \in \mathcal{D} \mid a^*(\lambda) \neq a^*(\hat{\mu}_t)\}$.

Return $\hat{A}_\tau = a^*(\hat{\mu}_\tau)$.

→ ensures δ -correct.

Why that likelihood ratio test ?

The expectation of a likelihood ratio is a KL :

$$\mathbb{E}_{X \sim \mu_a} \left[\log \frac{d\mathbb{P}_{\mu_a}}{d\mathbb{P}_{\lambda_a}}(X_a) \right] = \text{KL}(\mu_a, \lambda_a) .$$

$$\mathbb{E}_{\mu} \left[\sum_{s=1}^t \log \frac{d\mathbb{P}_{\mu_{A_s}}}{d\mathbb{P}_{\lambda_{A_s}}}(X_{s,A_s}) \right] = \mathbb{E}_{\mu} \left[\sum_{s=1}^t \text{KL}(\mu_{A_s}, \lambda_{A_s}) \right] = \sum_a \mathbb{E}[N_{t,a}] \text{KL}(\mu_a, \lambda_a)$$

Suppose that we sampled each arm “ tw_a times” and did not stop at t .
Then

$$\begin{aligned} \log\left(\frac{t^2}{\delta}\right) &\geq \inf_{\lambda \in \text{alt}(\hat{\mu}_t)} \sum_{s=1}^t \log \frac{d\mathbb{P}_{\hat{\mu}_{t,A_s}}}{d\mathbb{P}_{\lambda_{A_s}}}(X_{s,A_s}) \\ &= t \inf_{\lambda \in \text{alt}(\hat{\mu}_t)} \sum_a w_a \log \frac{d\mathbb{P}_{\hat{\mu}_{t,a}}}{d\mathbb{P}_{\lambda_a}}(\hat{\mu}_{t,a}) \\ &\approx t \inf_{\lambda \in \text{alt}(\mu)} \sum_a w_a \text{KL}(\mu_a, \lambda_a) . \end{aligned}$$

Static proportions oracle

Suppose that we sampled each arm “ tw_a times” (big enough for all a) and did not stop at t .

$$\log\left(\frac{t^2}{\delta}\right) \gtrsim t \inf_{\lambda \in \text{alt}(\mu)} \sum_a w_a \text{KL}(\mu_a, \lambda_a).$$

Optimizing over w_a , we get something very close to the lower bound : for that optimal sampling (which depends on μ),

$$t \max_{w \in \Delta_K} \inf_{\lambda \in \text{alt}(\mu)} \sum_a w_a \text{KL}(\mu_a, \lambda_a) \lesssim \log\left(\frac{t^2}{\delta}\right)$$

Track and Stop

Track and Stop

Sample every arm once, then at each time t until the algorithm stops,

- 1 Compute $\hat{w}_t^* = \operatorname{argmax}_w \inf_{\lambda \in \text{alt}(\hat{\mu}_t)} \sum_a w_a \log \frac{d\mathbb{P}_{\hat{\mu}_{t,a}}}{d\mathbb{P}_{\lambda_a}}(\hat{\mu}_{t,a})$
- 2 If there exists one arm with $N_{t,a} < \sqrt{t}$, pull it, (forced exploration)
otherwise pull $A_t = \operatorname{argmin}_a N_{t,a} - t\hat{w}_{t,a}^*$ (tracking)
- 3 Check the GLRT stopping rule

Recommend the empirical best arm

Theorem

Track-and-Stop is asymptotically optimal, that is

$$\lim_{\delta \rightarrow 0} \frac{\mathbb{E}_\mu[\tau]}{\log(1/\delta)} \leq \frac{1}{\max_{w \in \Delta_K} \inf_{\lambda \in \text{alt}(\mu)} \sum_a w_a \text{KL}(\mu_a, \lambda_a)}.$$

Asymptotically optimal : upper bound identical to lower bound.

Limitations and improvements of TnS

Computing the argmax can be hard

- ▶ We can use an iterative method and do only one step at each time.

The forced exploration is harmful in practice

- ▶ We can introduce optimism to avoid it

Computing the argmin over the alternative could be hard in general identification problems.

Open problems in fixed confidence

- ▶ What is the complexity for δ not close to 0? Lower bounds and matching algorithms?
- ▶ Can we have fixed confidence algorithms that we can choose to stop early, and still get error bounds?

Reinforcement Learning

Ongoing research work :

- ▶ Can we get lower bounds on the time needed to find the best policy in RL ?
- ▶ Can we use the notion of alternative and apply methods like TnS ? (efficiently, preferably)



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