Sequential Learning

Lecture 7 : Bandit Identification

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

Theorem

Policy iteration terminates after a finite number of steps and outputs the optimal policy $\pi^\star$.

- 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

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

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

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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(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

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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

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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 $(\nu_1, \ldots, \nu_K)$, with means $(\mu_1, \ldots, \mu_K)$
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 $\hat{A}_\tau \neq a^\star := \mathrm{argmax}_a \mu_a$.

Let's formalize the problem

K arms with distributions $(\nu_1, \dots, \nu_K)$, with means $(\mu_1, \dots, \mu_K)$
At each time t, until the algorithm stops,

- choose an arm A_t $\to$ 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. $\to$ stopping rule
At τ, return $\hat{A}_\tau \in [K]$. $\to$ recommendation rule

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

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

Fixed budget identification

Fixed budgete 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 $\mathbb{P}_\nu(\hat{A}_T \neq a^\star)$is as small as possible.

Simple algorithm : uniform sampling

Uniform sampling algorithm :

- sample all arms $\lfloor T/K \rfloor$ times $\to$ sampling rule
- return the best arm of the empirical mean vector $\hat{\mu}_T$
  $\to$ recommendation rule

What is the probability of mistake ?

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

Concentration again

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

Hoeffding inequality

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

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

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

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

Error probability of uniform sampling

Theorem

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

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

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

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

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

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

We call static sampling oracle at μ the allocation $(n_a^\star)_{a \in [K]}$ which minimizes the probability of error.
It depends on μ (hence the name oracle) and verifies

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

where $\Delta_{a^\star} = \min_{a \neq a^*} \Delta_a$.

Can we match the oracle ?

The static sampling oracle depends on the unknown μ, with
$n_a^\star \approx \frac{1/\Delta_a^2}{\sum_b 1/\Delta_b^2}$.
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

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

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

Theorem

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

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

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

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 $k \in \{1, \ldots, K-1\}$,

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

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

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

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

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

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

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 $\nu \in \mathcal{D}$,

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

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

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

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

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 $(\sum_a \frac{1}{\Delta_a^2}) \sigma^2 \log(1/\delta)$.

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

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

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 distirbutions, parametrized by their means (technically we need a one-parameter exponential family).
$\mathrm{KL}(\mu_a, \lambda_a)$ 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 $t \in \mathbb{N}$,

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

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 $t \in \mathbb{N}$,

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

Stop if

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

where $\mathrm{alt}(\hat{\mu}_t) = \{\lambda \in \mathcal{D} \mid a^\star(\lambda) \neq a^\star(\hat{\mu}_t)\}$.
Return $\hat{A}_\tau = a^\star(\hat{\mu}_\tau)$.

$\rightarrow$ ensures δ-correct.

Why that likelihood ratio test ?

The expectation of a likelihood ratio is a KL :

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

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

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

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

$$= t \inf_{\lambda\in \mathrm{alt}(\hat{\mu}_t)} \sum_a w_a \log \frac{d\mathbb{P}_{\hat{\mu}_{t,a}}}{d\mathbb{P}_{\lambda_a}}(\hat{\mu}_{t,a})$$

$$\approx t \inf_{\lambda\in \mathrm{alt}(\mu)} \sum_a w_a \mathrm{KL}(\mu_a, \lambda_a) \, .$$

Static proportions oracle

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

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

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

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

Track and Stop

Track and Stop

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

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

Recommend the empirical best arm

Theorem

Track-and-Stop is asymptotically optimal, that is

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

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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