

On the Complexity of Best Arm Identification in Multi-Armed Bandit Models

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Roadmap

1 Simple Multi-Armed Bandit Model

2 Complexity of Best Arm Identification

- Lower bounds on the complexities
- Gaussian Feedback
- Binary Feedback

The (stochastic) Multi-Armed Bandit Model

Environment K arms with parameters $\theta = (\theta_1, \dots, \theta_K)$ such that for any possible choice of arm $a_t \in \{1, \dots, K\}$ at time t , one receives the reward

$$X_t = X_{a_t, t}$$

where, for any $1 \leq a \leq K$ and $s \geq 1$, $X_{a, s} \sim \nu_a$, and the $(X_{a, s})_{a, s}$ are independent.

Reward distributions $\nu_a \in \mathcal{F}_a$ parametric family, or not:
 canonical exponential family, general bounded rewards

Example Bernoulli rewards: $\theta \in [0, 1]^K$, $\nu_a = \mathcal{B}(\theta_a)$

Strategy The agent's actions follow a dynamical strategy $\pi = (\pi_1, \pi_2, \dots)$ such that

$$A_t = \pi_t(X_1, \dots, X_{t-1})$$

Real challenges

- Randomized clinical trials
 - original motivation since the 1930's
 - dynamic strategies can save resources
- Recommender systems:

- advertisement
- website optimization
- news, blog posts, . . .



- Computer experiments
 - large systems can be simulated in order to optimize some criterion over a set of parameters
 - but the simulation cost may be high, so that only few choices are possible for the parameters
- Games and planning (tree-structured options)

Performance Evaluation: Cumulated Regret

Cumulated Reward: $S_T = \sum_{t=1}^T X_t$

Goal: Choose π so as to maximize

$$\begin{aligned}\mathbb{E}[S_T] &= \sum_{t=1}^T \sum_{a=1}^K \mathbb{E}[\mathbb{E}[X_t \mathbb{1}\{A_t = a\} | X_1, \dots, X_{t-1}]] \\ &= \sum_{a=1}^K \mu_a \mathbb{E}[N_a^\pi(T)]\end{aligned}$$

where $N_a^\pi(T) = \sum_{t \leq T} \mathbb{1}\{A_t = a\}$ is the number of draws of arm a up to time T , and $\mu_a = E(\nu_a)$.

Regret Minimization: maximizing $\mathbb{E}[S_T] \iff$ minimizing

$$R_T = T\mu^* - \mathbb{E}[S_T] = \sum_{a: \mu_a < \mu^*} (\mu^* - \mu_a) \mathbb{E}[N_a^\pi(T)]$$

where $\mu^* \in \max\{\mu_a : 1 \leq a \leq K\}$

Upper Confidence Bound Strategies

UCB [Lai&Robins '85; Agrawal '95; Auer&al '02]

- Construct an upper confidence bound for the expected reward of each arm:

$$\underbrace{\frac{S_a(t)}{N_a(t)}}_{\text{estimated reward}} + \underbrace{\sqrt{\frac{\log(t)}{2N_a(t)}}}_{\text{exploration bonus}}$$

- Choose the arm with the highest UCB
- It is an *index strategy* [Gittins '79]
- Its behavior is easily interpretable and intuitively appealing
- Listen to Robert Nowak's talk tomorrow!

Optimality?

Generalization of [Lai&Robbins '85]

Theorem [Burnetas and Katehakis, '96]

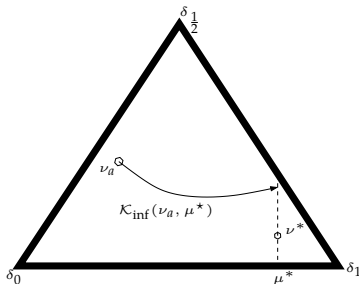
If π is a **uniformly** efficient strategy, then for any $\theta \in [0, 1]^K$,

$$\liminf_{T \rightarrow \infty} \frac{\mathbb{E}[N_a(T)]}{\log(T)} \geq \frac{1}{K_{\text{inf}}(\nu_a, \mu^*)}$$

where

$$K_{\text{inf}}(\nu_a, \mu^*) = \inf \left\{ K(\nu_a, \nu') : \nu' \in \mathcal{F}_a, E(\nu') \geq \mu^* \right\}$$

Idea: change of distribution



Reaching Optimality: Empirical Likelihood

The KL-UCB Algorithm, AoS 2013

joint work with O. Cappé, O-A. Maillard, R. Munos, G. Stoltz

Parameters: An operator $\Pi_{\mathcal{F}} : \mathcal{M}_1(\mathcal{S}) \rightarrow \mathcal{F}$; a non-decreasing function $f : \mathbb{N} \rightarrow \mathbb{R}$

Initialization: Pull each arm of $\{1, \dots, K\}$ once

for $t = K$ to $T - 1$ **do**

 compute for each arm a the quantity

$$U_a(t) = \sup \left\{ E(\nu) : \nu \in \mathcal{F} \text{ and } KL\left(\Pi_{\mathcal{F}}(\hat{\nu}_a(t)), \nu\right) \leq \frac{f(t)}{N_a(t)} \right\}$$

 pick an arm $A_{t+1} \in \arg \max_{a \in \{1, \dots, K\}} U_a(t)$

end for

Regret bound

Theorem: Assume that \mathcal{F} is the set of finitely supported probability distributions over $\mathcal{S} = [0, 1]$, that $\mu_a > 0$ for all arms a and that $\mu^* < 1$. There exists a constant $M(\nu_a, \mu^*) > 0$ only depending on ν_a and μ^* such that, with the choice $f(t) = \log(t) + \log(\log(t))$ for $t \geq 2$, for all $T \geq 3$:

$$\begin{aligned} \mathbb{E}[N_a(T)] &\leq \frac{\log(T)}{K_{\inf}(\nu_a, \mu^*)} + \frac{36}{(\mu^*)^4} (\log(T))^{4/5} \log(\log(T)) \\ &\quad + \left(\frac{72}{(\mu^*)^4} + \frac{2\mu^*}{(1 - \mu^*) K_{\inf}(\nu_a, \mu^*)^2} \right) (\log(T))^{4/5} \\ &\quad + \frac{(1 - \mu^*)^2 M(\nu_a, \mu^*)}{2(\mu^*)^2} (\log(T))^{2/5} \\ &\quad + \frac{\log(\log(T))}{K_{\inf}(\nu_a, \mu^*)} + \frac{2\mu^*}{(1 - \mu^*) K_{\inf}(\nu_a, \mu^*)^2} + 4. \end{aligned}$$

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Best Arm Identification Strategies

A two-armed bandit model is

- a pair $\nu = (\nu_1, \nu_2)$ of probability distributions ('arms') with respective means μ_1 and μ_2
- $a^* = \operatorname{argmax}_a \mu_a$ is the (unknown) best arm

Strategy =

- a *sampling rule* $(A_t)_{t \in \mathbb{N}}$ where $A_t \in \{1, 2\}$ is the arm chosen at time t (based on past observations) a sample $Z_t \sim \nu_{A_t}$ is observed
- a *stopping rule* τ indicating when he stops sampling the arms
- a *recommendation rule* $\hat{a}_\tau \in \{1, 2\}$ indicating which arm he thinks is best (at the end of the interaction)

In classical A/B Testing, the sampling rule A_t is uniform on $\{1, 2\}$ and the stopping rule $\tau = t$ is fixed in advance.

Best Arm Identification

Joint work with Emilie Kaufmann and Olivier Cappé (Telecom ParisTech)

Goal: design a strategy $\mathcal{A} = ((A_t), \tau, \hat{a}_\tau)$ such that:

Fixed-budget setting	Fixed-confidence setting
$\tau = t$ $p_t(\nu) := \mathbb{P}_\nu(\hat{a}_t \neq a^*)$ as small as possible	$\mathbb{P}_\nu(\hat{a}_\tau \neq a^*) \leq \delta$ $\mathbb{E}_\nu[\tau]$ as small as possible

See also: [Mannor&Tsitsiklis '04], [Even-Dar&al. '06], [Audibert&al.'10], [Bubeck&al. '11,'13], [Kalyanakrishnan&al. '12], [Karnin&al. '13], [Jamieson&al. '14]...

Two possible goals

Goal: design a strategy $\mathcal{A} = ((A_t), \tau, \hat{a}_\tau)$ such that:

Fixed-budget setting	Fixed-confidence setting
$\tau = t$ $p_t(\nu) := \mathbb{P}_\nu(\hat{a}_t \neq a^*)$ as small as possible	$\mathbb{P}_\nu(\hat{a}_\tau \neq a^*) \leq \delta$ $\mathbb{E}_\nu[\tau]$ as small as possible

In the particular case of **uniform sampling** :

Fixed-budget setting	Fixed-confidence setting
classical test of $(\mu_1 > \mu_2)$ against $(\mu_1 < \mu_2)$ based on t samples	sequential test of $(\mu_1 > \mu_2)$ against $(\mu_1 < \mu_2)$ with probability of error uniformly bounded by δ

[Siegmund 85]: sequential tests can save samples !

The complexities of best-arm identification

For a class \mathcal{M} bandit models, algorithm $\mathcal{A} = ((A_t), \tau, \hat{a}_\tau)$ is...

Fixed-budget setting	Fixed-confidence setting
<p>consistent on \mathcal{M} if</p> $\forall \nu \in \mathcal{M}, p_t(\nu) = \mathbb{P}_\nu(\hat{a}_t \neq a^*) \xrightarrow[t \rightarrow \infty]{} 0$	<p>δ-PAC on \mathcal{M} if</p> $\forall \nu \in \mathcal{M}, \mathbb{P}_\nu(\hat{a}_\tau \neq a^*) \leq \delta$

From the literature

$p_t(\nu) \simeq \exp\left(-\frac{t}{cH(\nu)}\right)$ <p>[Audibert&al.'10],[Bubeck&al'11] [Bubeck&al'13],...</p>	$\mathbb{E}_\nu[\tau] \simeq C'H'(\nu) \log(1/\delta)$ <p>[Mannor&Tsitsiklis '04],[Even-Dar&al. '06] [Kalanakrishnan&al'12],...</p>
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\implies **two complexities**

$\kappa_B(\nu) = \inf_{\mathcal{A} \text{ cons.}} \left(\limsup_{t \rightarrow \infty} -\frac{1}{t} \log p_t(\nu) \right)^{-1}$ <p>for a probability of error $\leq \delta$, budget $t \simeq \kappa_B(\nu) \log(1/\delta)$</p>	$\kappa_C(\nu) = \inf_{\mathcal{A} \delta\text{-PAC}} \limsup_{\delta \rightarrow 0} \frac{\mathbb{E}_\nu[\tau]}{\log(1/\delta)}$ <p>for a probability of error $\leq \delta$, $\mathbb{E}_\nu[\tau] \simeq \kappa_C(\nu) \log(1/\delta)$</p>
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Changes of distribution

Theorem: *how to use (and hide) the change of distribution*

Let ν and ν' be two bandit models with K arms such that for all a , the distributions ν_a and ν'_a are mutually absolutely continuous. For any almost-surely finite stopping time σ with respect to (\mathcal{F}_t) ,

$$\sum_{a=1}^K \mathbb{E}_{\nu} [N_a(\sigma)] \text{KL}(\nu_a, \nu'_a) \geq \sup_{\mathcal{E} \in \mathcal{F}_{\sigma}} \text{kl}(\mathbb{P}_{\nu}(\mathcal{E}), \mathbb{P}_{\nu'}(\mathcal{E})),$$

where $\text{kl}(x, y) = x \log(x/y) + (1-x) \log((1-x)/(1-y))$.

Useful remark:

$$\forall \delta \in [0, 1], \quad \text{kl}(\delta, 1 - \delta) \geq \log \frac{1}{2.4 \delta},$$

General lower bounds

Theorem 1

Let \mathcal{M} be a class of two armed bandit models that are continuously parametrized by their means. Let

$$\nu = (\nu_1, \nu_2) \in \mathcal{M}.$$

Fixed-budget setting	Fixed-confidence setting
any consistent algorithm satisfies	any δ -PAC algorithm satisfies
$\limsup_{t \rightarrow \infty} -\frac{1}{t} \log p_t(\nu) \leq K^*(\nu_1, \nu_2)$	$\mathbb{E}_\nu[\tau] \geq \frac{1}{K_*(\nu_1, \nu_2)} \log\left(\frac{1}{2.4\delta}\right)$
<p>with $K^*(\nu_1, \nu_2)$ $= \text{KL}(\nu^*, \nu_1) = \text{KL}(\nu^*, \nu_2)$</p>	<p>with $K_*(\nu_1, \nu_2)$ $= \text{KL}(\nu_1, \nu_*) = \text{KL}(\nu_2, \nu_*)$</p>
Thus, $\kappa_B(\nu) \geq \frac{1}{K^*(\nu_1, \nu_2)}$	Thus, $\kappa_C(\nu) \geq \frac{1}{K_*(\nu_1, \nu_2)}$

Gaussian Rewards: Fixed-Budget Setting

For fixed (known) values σ_1, σ_2 , we consider Gaussian bandit models

$$\mathcal{M} = \{ \nu = (\mathcal{N}(\mu_1, \sigma_1^2), \mathcal{N}(\mu_2, \sigma_2^2)) : (\mu_1, \mu_2) \in \mathbb{R}^2, \mu_1 \neq \mu_2 \}$$

■ Theorem 1:

$$\kappa_B(\nu) \geq \frac{2(\sigma_1 + \sigma_2)^2}{(\mu_1 - \mu_2)^2}$$

- A strategy allocating $t_1 = \left\lceil \frac{\sigma_1}{\sigma_1 + \sigma_2} t \right\rceil$ samples to arm 1 and $t_2 = t - t_1$ samples to arm 2, and recommending the empirical best satisfies

$$\liminf_{t \rightarrow \infty} -\frac{1}{t} \log p_t(\nu) \geq \frac{(\mu_1 - \mu_2)^2}{2(\sigma_1 + \sigma_2)^2}$$

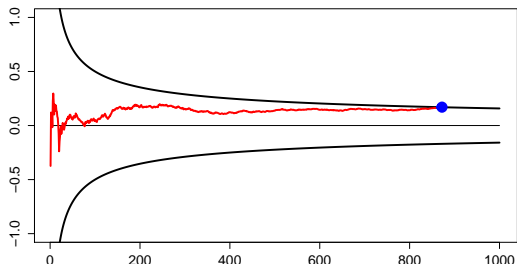
$$\kappa_B(\nu) = \frac{2(\sigma_1 + \sigma_2)^2}{(\mu_1 - \mu_2)^2}$$

Gaussian Rewards: Fixed-confidence setting

The α -Elimination algorithm with exploration rate $\beta(t, \delta)$

- chooses A_t in order to keep a proportion $N_1(t)/t \simeq \alpha$
- if $\hat{\mu}_a(t)$ is the empirical mean of rewards obtained from a up to time t , $\sigma_t^2(\alpha) = \sigma_1^2/\lceil \alpha t \rceil + \sigma_2^2/(t - \lceil \alpha t \rceil)$,

$$\tau = \inf \left\{ t \in \mathbb{N} : |\hat{\mu}_1(t) - \hat{\mu}_2(t)| > \sqrt{2\sigma_t^2(\alpha)\beta(t, \delta)} \right\}$$



- recommends the empirical best arm $\hat{a}_\tau = \operatorname{argmax}_a \hat{\mu}_a(\tau)$

Gaussian Rewards: Fixed-confidence setting

- From Theorem 1:

$$\mathbb{E}_\nu[\tau] \geq \frac{2(\sigma_1 + \sigma_2)^2}{(\mu_1 - \mu_2)^2} \log \left(\frac{1}{2.4\delta} \right)$$

- $\frac{\sigma_1}{\sigma_1 + \sigma_2}$ -Elimination with $\beta(t, \delta) = \log \frac{t}{\delta} + 2 \log \log(6t)$ is δ -PAC and

$$\forall \epsilon > 0, \quad \mathbb{E}_\nu[\tau] \leq (1 + \epsilon) \frac{2(\sigma_1 + \sigma_2)^2}{(\mu_1 - \mu_2)^2} \log \left(\frac{1}{2.4\delta} \right) + \frac{o_\epsilon}{\delta \rightarrow 0} \left(\log \frac{1}{\delta} \right)$$

$$\kappa_C(\nu) = \frac{2(\sigma_1 + \sigma_2)^2}{(\mu_1 - \mu_2)^2}$$

Gaussian Rewards: Conclusion

For any two fixed values of σ_1 and σ_2 ,

$$\kappa_B(\nu) = \kappa_C(\nu) = \frac{2(\sigma_1 + \sigma_2)^2}{(\mu_1 - \mu_2)^2}$$

If the variances are equal, $\sigma_1 = \sigma_2 = \sigma$,

$$\kappa_B(\nu) = \kappa_C(\nu) = \frac{8\sigma^2}{(\mu_1 - \mu_2)^2}$$

- **uniform sampling** is optimal only when $\sigma_1 = \sigma_2$
- 1/2-Elimination is δ -PAC for a smaller exploration rate
 $\beta(t, \delta) \simeq \log(\log(t)/\delta)$

Binary Rewards: Lower Bounds

$$\mathcal{M} = \{\nu = (\mathcal{B}(\mu_1), \mathcal{B}(\mu_2)) : (\mu_1, \mu_2) \in]0; 1[^2, \mu_1 \neq \mu_2\},$$

shorthand: $K(\mu, \mu') = \text{KL}(\mathcal{B}(\mu), \mathcal{B}(\mu'))$.

Fixed-budget setting	Fixed-confidence setting
any consistent algorithm satisfies	any δ -PAC algorithm satisfies
$\limsup_{t \rightarrow \infty} -\frac{1}{t} \log p_t(\nu) \leq K^*(\mu_1, \mu_2)$ <p>(Chernoff information)</p>	$\mathbb{E}_\nu[\tau] \geq \frac{1}{K_*(\mu_1, \mu_2)} \log\left(\frac{1}{2\delta}\right)$

$$K^*(\mu_1, \mu_2) > K_*(\mu_1, \mu_2)$$

Binary Rewards: Uniform Sampling

	For any consistent...	For any δ -PAC...
... algorithm	$p_t(\nu) \gtrsim e^{-K^*(\mu_1, \mu_2)t}$	$\frac{\mathbb{E}_\nu[\tau]}{\log(1/\delta)} \gtrsim \frac{1}{K_*(\mu_1, \mu_2)}$
... algorithm using uniform sampling	$p_t(\nu) \gtrsim e^{-\frac{K(\bar{\mu}, \mu_1) + K(\bar{\mu}, \mu_2)}{2}t}$ with $\bar{\mu} = f(\mu_1, \mu_2)$	$\frac{\mathbb{E}_\nu[\tau]}{\log(1/\delta)} \gtrsim \frac{2}{K(\mu_1, \underline{\mu}) + K(\mu_2, \underline{\mu})}$ with $\underline{\mu} = \frac{\mu_1 + \mu_2}{2}$

Remark: Quantities in the same column appear to be close from one another

\Rightarrow **Binary rewards: uniform sampling close to optimal**

Binary Rewards: Uniform Sampling

	For any consistent...	For any δ -PAC...
... algorithm	$p_t(\nu) \simeq e^{-K^*(\mu_1, \mu_2)t}$	$\frac{\mathbb{E}_\nu[\tau]}{\log(1/\delta)} \gtrsim \frac{1}{K_*(\mu_1, \mu_2)}$
... algorithm using uniform sampling	$p_t(\nu) \simeq e^{-\frac{K(\bar{\mu}, \mu_1) + K(\bar{\mu}, \mu_2)}{2}t}$ with $\bar{\mu} = f(\mu_1, \mu_2)$	$\frac{\mathbb{E}_\nu[\tau]}{\log(1/\delta)} \gtrsim \frac{2}{K(\mu_1, \underline{\mu}) + K(\mu_2, \underline{\mu})}$ with $\underline{\mu} = \frac{\mu_1 + \mu_2}{2}$

Remark: Quantities in the same column appear to be close from one another

\Rightarrow **Binary rewards: uniform sampling close to optimal**

Binary Rewards: Fixed-Budget Setting

In fact,

$$\kappa_B(\nu) = \frac{1}{\mathbf{K}^*(\mu_1, \mu_2)}$$

The algorithm using **uniform sampling** and recommending the empirical best arm **is very close to optimal**

Binary Rewards: Fixed-Confidence Setting

δ -PAC algorithms using uniform sampling satisfy

$$\frac{\mathbb{E}_\nu[\tau]}{\log(1/\delta)} \geq \frac{1}{I_*(\nu)} \quad \text{with} \quad I_*(\nu) = \frac{\mathsf{K}\left(\mu_1, \frac{\mu_1 + \mu_2}{2}\right) + \mathsf{K}\left(\mu_2, \frac{\mu_1 + \mu_2}{2}\right)}{2}.$$

The algorithm using uniform sampling and

$$\tau = \inf \left\{ t \in 2\mathbb{N}^* : |\hat{\mu}_1(t) - \hat{\mu}_2(t)| > \log \frac{\log(t) + 1}{\delta} \right\}$$

is δ -PAC but not optimal: $\frac{\mathbb{E}[\tau]}{\log(1/\delta)} \simeq \frac{2}{(\mu_1 - \mu_2)^2} > \frac{1}{I_*(\nu)}$.

A better stopping rule NOT based on the difference of empirical means

$$\tau = \inf \left\{ t \in 2\mathbb{N}^* : t I_*(\hat{\mu}_1(t), \hat{\mu}_2(t)) > \log \frac{\log(t) + 1}{\delta} \right\}$$

Binary Rewards: Conclusion

Regarding the complexities:

- $\kappa_B(\nu) = \frac{1}{K^*(\mu_1, \mu_2)}$
- $\kappa_C(\nu) \geq \frac{1}{K_*(\mu_1, \mu_2)} > \frac{1}{K^*(\mu_1, \mu_2)}$

Thus

$$\kappa_C(\nu) > \kappa_B(\nu)$$

Regarding the algorithms

- There is not much to gain by departing from uniform sampling
- In the fixed-confidence setting, a sequential test based on the difference of the empirical means is no longer optimal

Conclusion

- the complexities $\kappa_B(\nu)$ and $\kappa_C(\nu)$ are not always equal (and feature some different informational quantities)
- strategies using random stopping do not necessarily lead to a saving in terms of the number of sample used
- for Bernoulli distributions and Gaussian with similar variances, strategies using uniform sampling are (almost) optimal
- Generalization to m best arms identification among K arms

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