Dynamic resource allocation as an estimation problem

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5ème journée de rencontre LPT-IMT, le 24 mai 2013

Roadmap

1. The Model
2. Lower Bound for the Regret
3. Optimistic Algorithms
4. An Optimistic Algorithm based on Kullback-Leibler Divergence
5. Parametric setting: the kl-UCB Algorithm
6. Non-parametric setting and Empirical Likelihood
7. Conclusion

Dynamic resource allocation

Imagine you are a doctor:

- patients visit you *one after another* for a given disease
- you prescribe one of the (say) *5 treatments* available
- the treatments are *not equally efficient*
- you do not know which one is the best, you *observe the effect* of the prescribed treatment on each patient

⇒ What do you do?

- You must choose each prescription using only the *previous observations*
- Your goal is not to estimate each treatment's efficiency precisely, but to *heal as many patients as possible*

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. Examples: 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, Regret

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

Our goal Choose π so as to maximize

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

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

Regret Minimization equivalent to minimizing

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

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

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Asymptotically Optimal Strategies

- A strategy π is said to be consistent if, for any $(\nu_a)_a \in \mathcal{F}^K$,

$$\frac{1}{T}\mathbb{E}[S_T] \to \mu^*$$

- The strategy is efficient if for all $\theta \in [0,1]^K$ and all $\alpha > 0$,

$$R_T = o(T^\alpha)$$

- There are efficient strategies and we consider the best achievable asymptotic performance among efficient strategies

The Bound of Lai and Robbins

One-parameter reward distribution $\nu_a = \nu_{\theta_a}, \theta_a \in \Theta \subset \mathbb{R}$.

Theorem [Lai and Robbins, '85]

If π is an efficient strategy, then, for any $\theta \in \Theta^K$,

$$\liminf_{T\to\infty} \frac{R_T}{\log(T)} \geq \sum_{a:\mu_a<\mu^*} \frac{\mu^* - \mu_a}{\mathrm{KL}(\nu_a, \nu^*)}$$

where $\mathrm{KL}(\nu, \nu')$ denotes the Kullback-Leibler divergence

For example, in the Bernoulli case:

$$KL\big(\mathcal{B}(p), \mathcal{B}(q)\big) = d_{\text{BER}}(p, q) = p \log \frac{p}{q} + (1-p) \log \frac{1-p}{1-q}$$

The Bound of Burnetas and Katehakis

More general reward distributions $\nu_a \in \mathcal{F}_a$

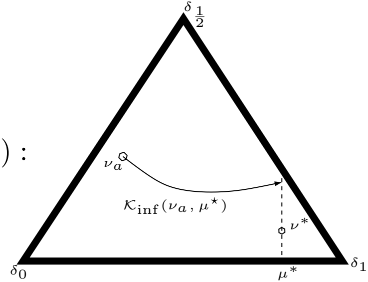
Theorem [Burnetas and Katehakis, '96]

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

$$\liminf_{T\to\infty} \frac{R_T}{\log(T)} \geq \sum_{a:\mu_a<\mu^*} \frac{\mu^* - \mu_a}{K_{inf}(\nu_a, \mu^*)}$$

where

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



Intuition

- First assume that μ^* is known and that T is fixed
- How many draws n_a of ν_a are necessary to know that $\mu_a < \mu^*$ with probability at least $1 - 1/T$?
- Test: $H_0 : \mu_a = \mu^*$ against $H_1 : \nu = \nu_a$
- Stein's Lemma: if the first type error $\alpha_{n_a} \leq 1/T$, then

$$\beta_{n_a} \gtrsim \exp\big(-n_a K_{inf}(\nu_a, \mu^*)\big)$$

$\Longrightarrow$ it can be smaller than $1/T$ if

$$n_a \geq \frac{\log(T)}{K_{inf}(\nu_a, \mu^*)}$$

- How to do as well without knowing μ^* and T in advance? Not asymptotically?

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Optimism in the Face of Uncertainty

Optimism in an heuristic principle popularized by [Lai&Robins '85; Agrawal '95] which consists in letting the agent

> play as if the environment was the most favorable
> among all environments that are sufficiently likely
> given the observations accumulated so far

Surprisingly, this simple heuristic principle can be instantiated into algorithms that are robust, efficient and easy to implement in many scenarios pertaining to reinforcement learning

Upper Confidence Bound Strategies

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

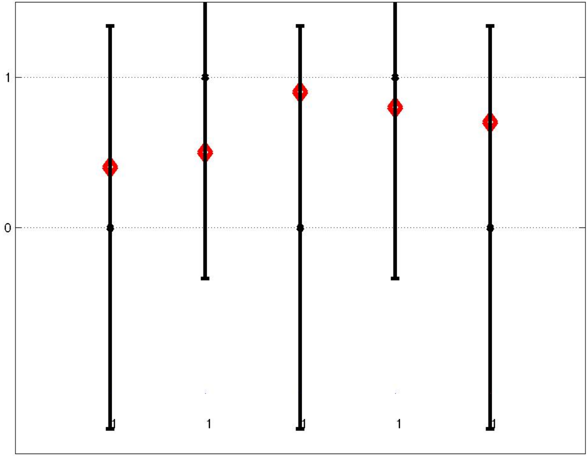
- Construct an upper confidence bound for the expected reward of each arm:

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

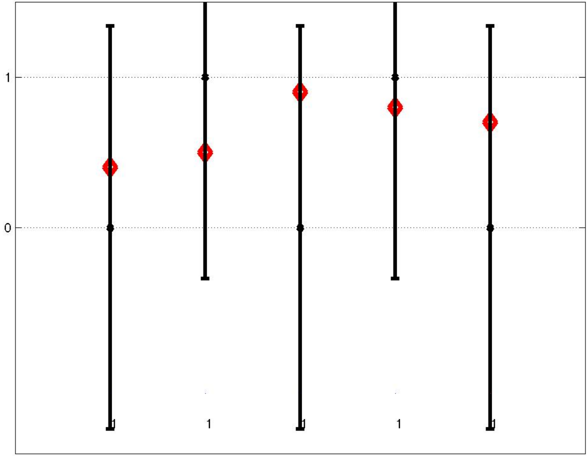
- Choose the arm with the highest UCB

- It is an *index strategy* [Gittins '79]
- Its behavior is easily interpretable and intuitively appealing

UCB in Action



UCB in Action



Performance of UCB

For rewards in $[0,1]$, the regret of UCB is upper-bounded as

$$E[R_T] = O(\log(T))$$

(finite-time regret bound) and

$$\limsup_{T\to\infty} \frac{\mathbb{E}[R_T]}{\log(T)} \leq \sum_{a:\mu_a<\mu^*} \frac{1}{2(\mu^* - \mu_a)}$$

Yet, in the case of Bernoulli variables, the rhs. is greater than suggested by the bound by Lai & Robbins

Many variants have been suggested to incorporate an estimate of the variance in the exploration bonus (e.g., [Audibert&al '07])

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The KL-UCB algorithm

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

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

```
for $t = K$ to $T - 1$ do
    compute for each arm $a$ the quantity
        $U_a(t) = \sup\left\{ E(\nu) : \quad \nu \in \mathcal{F} \quad \text{and} \quad KL\Big(\Pi_{\mathcal{F}}\big(\hat{\nu}_a(t)\big),\, \nu\Big) \leq \frac{f(t)}{N_a(t)} \right\}$
    pick an arm    $A_{t+1} \in \operatorname*{arg\,max}_{a \in \{1,\dots,K\}} U_a(t)$
end for
```

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Exponential Family Rewards

- Assume that $\mathcal{F}_a = \mathcal{F} =$ *canonical exponential family*, i.e. such that the pdf of the rewards is given by

$$p_{\theta_a}(x) = \exp\big(x\theta_a - b(\theta_a) + c(x)\big), \quad 1 \le a \le K$$

for a parameter $\theta \in \mathbb{R}^K$, expectation $\mu_a = \dot{b}(\theta_a)$

- The KL-UCB si simply:

$$U_a(t) = \sup\left\{\mu \in \overline{I} : \quad d\big(\hat{\mu}_a(t), \mu\big) \le \frac{f(t)}{N_a(t)}\right\}$$

- For instance,
  - for Bernoulli rewards:

$$d_{\text{BER}}(p, q) = p \log \frac{p}{q} + (1-p) \log \frac{1-p}{1-q}$$

  - for exponential rewards $p_{\theta_a}(x) = \theta_a \mathrm{e}^{-\theta_a x}$:

$$d_{\exp}(u, v) = u - v + u \log \frac{u}{v}$$

- The analysis is generic and yields a non-asymptotic regret bound optimal in the sense of Lai and Robbins.

Parametric version: the kl-UCB algorithm

Parameters: $\mathcal{F}$ parameterized by the expectation $\mu \in I \subset \mathbb{R}$ with divergence d, a non-decreasing function $f : \mathbb{N} \to \mathbb{R}$

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

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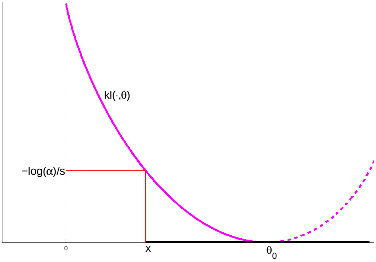
for $t = K$ to $T - 1$ do
    compute for each arm $a$ the quantity
        $U_a(t) = \sup\left\{\mu \in \overline{I} : \quad d\big(\hat{\mu}_a(t), \, \mu\big) \leq \frac{f(t)}{N_a(t)}\right\}$
    pick an arm    $A_{t+1} \in \operatorname*{arg\,max}_{a \in \{1,\ldots,K\}} U_a(t)$
end for
```

The kl Upper Confidence Bound in Picture

If $Z_1, \dots, Z_s \overset{iid}{\sim} \mathcal{B}(\theta_0)$, $x < \theta_0$ and if $\hat{p}_s = (Z_1 + \dots + Z_s)/s$, then

$$\mathbb{P}_{\theta_0}\left(\hat{p}_s \leq x\right) \leq \exp\left(-s\,\mathrm{kl}(x, \theta_0)\right)$$



In other words, if $\alpha = \exp\left(-s\,\mathrm{kl}(x, \theta_0)\right)$:

$$\mathbb{P}_{\theta_0}\left(\hat{p}_s \leq x\right) = \mathbb{P}_{\theta_0}\left(\mathrm{kl}(\hat{p}_s, \theta_0) \leq -\frac{\log(\alpha)}{s},\ \hat{p}_s < \theta_0\right) \leq \alpha$$

$\Longrightarrow$ upper confidence bound for p at risk α :

$$u_s = \sup\left\{\theta > \hat{p}_s : \mathrm{kl}(\hat{p}_s, \theta) \leq -\frac{\log(\alpha)}{s}\right\}$$

The kl Upper Confidence Bound in Picture

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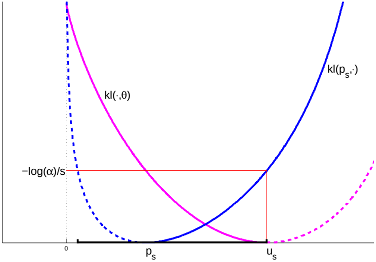

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Key Tool: Deviation Inequality for Self-Normalized Sums

- Problem: random number of summands
- Solution: peeling trick (as in the proof of the LIL)

Theorem For all $\epsilon > 1$,

$$\mathbb{P}\Big(\mu_a > \hat{\mu}_a(t) \quad \text{and} \quad N_a(t)\, d\big(\hat{\mu}_a(t),\, \mu_a\big) \geq \epsilon\Big) \leq e\big\lceil \epsilon \log(t) \big\rceil\, e^{-\epsilon}\,.$$

Thus,

$$P\big(U_a(t) < \mu_a\big) \leq e\big\lceil f(t) \log(t) \big\rceil\, e^{-f(t)}$$

Regret bound

Theorem: Assume that all arms belong to a canonical, regular, exponential family $\mathcal{F} = \{\nu_\theta : \theta \in \Theta\}$ of probability distributions indexed by its natural parameter space $\Theta \subseteq \mathbb{R}$. Then, with the choice $f(t) = \log(t) + 3\log\log(t)$ for $t \geq 3$, the number of draws of any suboptimal arm a is upper bounded for any horizon $T \geq 3$ as

$$\mathbb{E}\left[N_a(T)\right] \leq \frac{\log(T)}{d\left(\mu_a, \mu^\star\right)} + 2\sqrt{\frac{2\pi\sigma_{a,\star}^2 \left(d'(\mu_a, \mu^\star)\right)^2}{\left(d(\mu_a, \mu^\star)\right)^3}}\sqrt{\log(T) + 3\log(\log(T))}$$
$$+ \left(4e + \frac{3}{d(\mu_a, \mu^\star)}\right)\log(\log(T)) + 8\sigma_{a,\star}^2\left(\frac{d'(\mu_a, \mu^\star)}{d(\mu_a, \mu^\star)}\right)^2 + 6\,,$$

where $\sigma_{a,\star}^2 = \max\left\{\mathrm{Var}(\nu_\theta) :\ \mu_a \leq E(\nu_\theta) \leq \mu^\star\right\}$ and where $d'(\,\cdot\,, \mu^\star)$ denotes the derivative of $d(\,\cdot\,, \mu^\star)$.

Results: Two-Arm Scenario

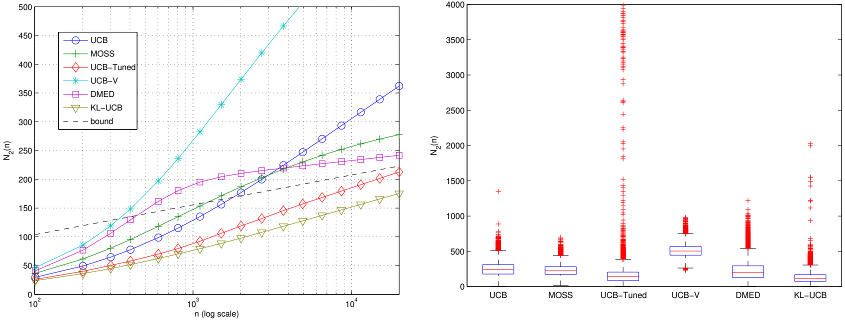

Figure: Performance of various algorithms when $\theta = (0.9, 0.8)$. Left: average number of draws of the sub-optimal arm as a function of time. Right: box-and-whiskers plot for the number of draws of the sub-optimal arm at time $T = 5,000$. Results based on $50,000$ independent replications

Results: Ten-Arm Scenario with Low Rewards

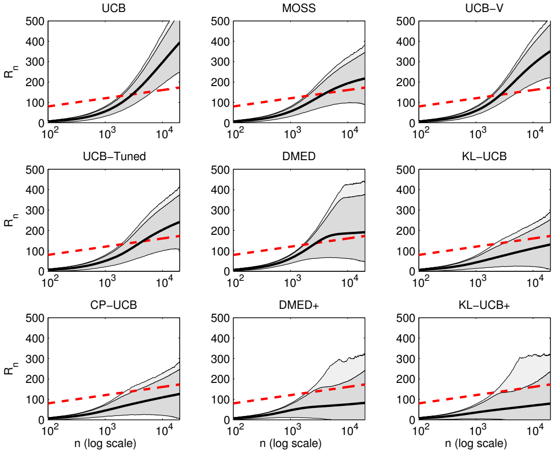

Figure: Average regret as a function of time when $\theta = (0.1, 0.05, 0.05, 0.05, 0.02, 0.02, 0.02, 0.01, 0.01, 0.01)$. Red line: Lai & Robbins lower bound; thick line: average regret; shaded regions: central 99% region an upper 99.95% quantile

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Non-parametric setting

- Rewards are only assumed to be bounded (say in $[0,1]$)
- Need for an estimation procedure
  - with non-asymptotic guarantees
  - efficient in the sense of Stein / Bahadur

$\Longrightarrow$ Idea 1: use d_{BER} (Hoeffding)

$\Longrightarrow$ Idea 2: Empirical Likelihood [Owen '01]

- Bad idea: use Bernstein / Bennett

First idea: use d_{BER}

Idea: rescale to $[0,1]$, and take the divergence d_{BER}.

$\longrightarrow$ because Bernoulli distributions maximize deviations among bounded variables with given expectation:

Lemma (Hoeffding '63)

Let X denote a random variable such that $0 \leq X \leq 1$ and denote by $\mu = \mathbb{E}[X]$ its mean. Then, for any $\lambda \in \mathbb{R}$,

$$E\left[\exp(\lambda X)\right] \leq 1 - \mu + \mu \exp(\lambda) \ .$$

This fact is well-known for the variance, but also true for all exponential moments and thus for Cramer-type deviation bounds

Regret Bound for kl-UCB

Theorem

With the divergence d_{BER}, for all $T > 3$,

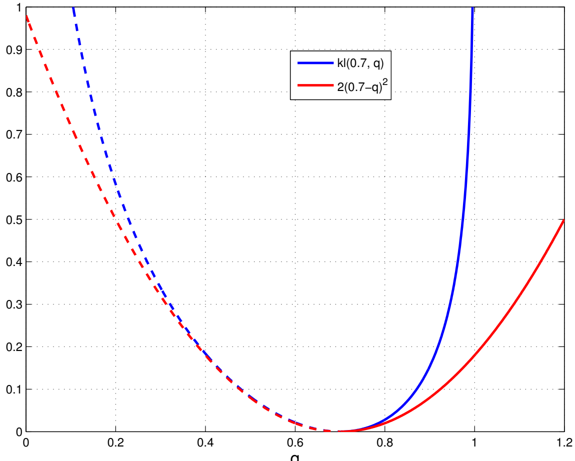
$$\mathbb{E}\big[N_a(T)\big] \le \frac{\log(T)}{d_{\mathrm{BER}}(\mu_a,\mu^\star)} + \frac{\sqrt{2\pi}\log\left(\frac{\mu^\star(1-\mu_a)}{\mu_a(1-\mu^\star)}\right)}{\big(d_{\mathrm{BER}}(\mu_a,\mu^\star)\big)^{3/2}}\sqrt{\log(T)+3\log\big(\log(T)\big)} + \left(4e+\frac{3}{d_{\mathrm{BER}}(\mu_a,\mu^\star)}\right)\log\big(\log(T)\big) + \frac{2\left(\log\left(\frac{\mu^\star(1-\mu_a)}{\mu_a(1-\mu^\star)}\right)\right)^2}{\big(d_{\mathrm{BER}}(\mu_a,\mu^\star)\big)^2} + 6\,.$$

- kl-UCB satisfies an improved logarithmic finite-time regret bound
- Besides, it is asymptotically optimal in the Bernoulli case

Comparison to UCB

KL-UCB addresses exactly the same problem as UCB, with the same generality, but it has always a smaller regret as can be seen from Pinsker's inequality

$$d_{\text{BER}}(\mu_1, \mu_2) \geq 2(\mu_1 - \mu_2)^2$$

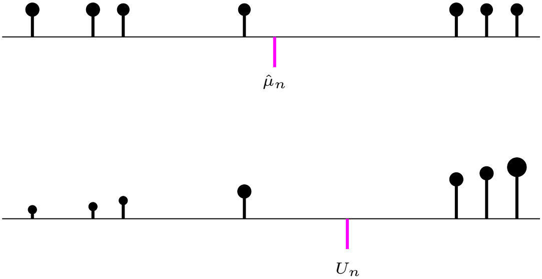


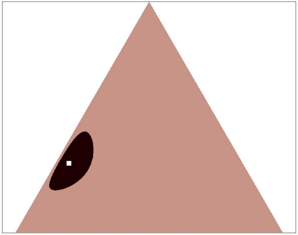
Idea 2: Empirical Likelihood

$$U(\hat{\nu}_n, \epsilon) = \sup\Big\{E(\nu') : \nu' \in \mathfrak{M}_1\big(\mathrm{Supp}(\hat{\nu}_n)\big) \text{ and } \mathrm{KL}(\hat{\nu}_n,\, \nu') \leq \epsilon\Big\}$$

or, rather, *modified Empirical Likelihood*:

$$U(\hat{\nu}_n, \epsilon) = \sup\Big\{E(\nu') : \nu' \in \mathfrak{M}_1\big(\mathrm{Supp}(\hat{\nu}_n) \cup \{1\}\big) \text{ and } \mathrm{KL}(\hat{\nu}_n,\, \nu') \leq \epsilon\Big\}$$





Coverage properties of the modified EL confidence bound

Proposition: Let $\nu_0 \in \mathfrak{M}_1([0,1])$ with $E(\nu_0) \in (0,1)$ and let $X_1, \ldots, X_n$ be independent random variables with common distribution $\nu_0 \in \mathfrak{M}_1\big([0,1]\big)$, not necessarily with finite support. Then, for all $\epsilon > 0$,

$$\begin{aligned}\mathbb{P}\big\{U(\hat{\nu}_n, \epsilon) \leq E(\nu_0)\big\} &\leq \mathbb{P}\Big\{K_{inf}\big(\hat{\nu}_n,\, E(\nu_0)\big) \geq \epsilon\Big\} \\ &\leq e(n+2)\exp(-n\epsilon)\ .\end{aligned}$$

Remark: For $\{0,1\}$–valued observations, it is readily seen that $U(\hat{\nu}_n, \epsilon)$ boils down to the upper-confidence bound above.
$\implies$ This proposition is at least not always optimal: the presence of the factor n in front of the exponential $\exp(-n\epsilon)$ term is questionable.

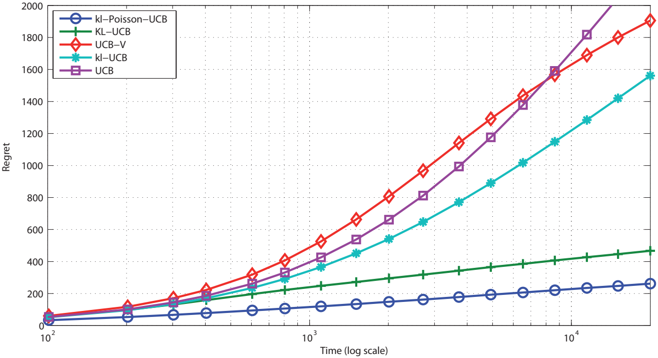
Regret bound

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 $\mu^\star < 1$. There exists a constant $M(\nu_a, \mu^\star) > 0$ only depending on ν_a and $\mu^\star$ such that, with the choice $f(t) = \log(t) + \log\big(\log(t)\big)$ for $t \geq 2$, for all $T \geq 3$:

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

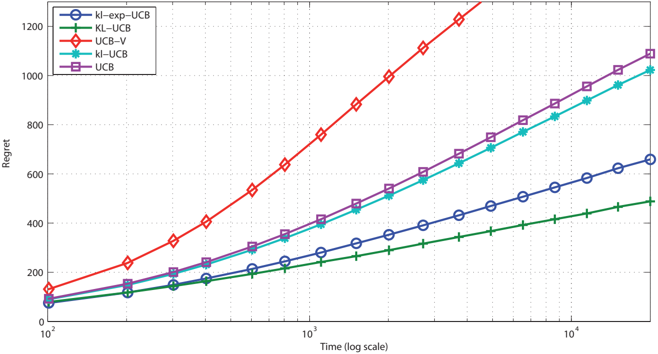
Example: truncated Poisson rewards

- for each arm $1 \leq a \leq 6$ is associated with ν_a, a Poisson distribution with expectation $(2+a)/4$, truncated at 10.
- $N = 10,000$ Monte-Carlo replications on an horizon of $T = 20,000$ steps.



Example: truncated Exponential rewards

- exponential rewards with respective parameters $1/5$, $1/4$, $1/3$, $1/2$ and 1, truncated at $x_{\max} = 10$;
- kl-UCB uses the divergence $d(x, y) = x/y - 1 - \log(x/y)$ prescribed for genuine exponential distributions, but it ignores the fact that the rewards are truncated.



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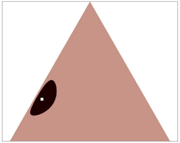
1. Use kl-UCB rather than UCB-1 or UCB-2
2. Use KL-UCB if speed is not a problem
3. todo: improve on the deviation bounds, address general non-parametric families of distributions

For model-based Reinforcement Learning in Markov Decision Processes, see Filippi *et al.*, *Optimism in Reinforcement Learning and Kullback-Leibler Divergence*, Allerton Conference, 2010



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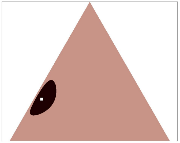

Thank you for your attention!