Algorithms and Uncertainty, Summer 2021

Lecture 18 (5 pages)

Stochastic Multi-Armed Bandits

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So far, we have seen examples of online algorithms, in which we know nothing about the future; it can be arbitrary. We have also seen examples of Markov Decision processes, in which we have precise knowledge of the underlying stochastic process and its involved probabilities. Today, we will move to the space in between. There is an underlying stochastic process but we do not know it. In contrast to online algorithms, we can try to "learn" the involved probability distributions.

1 Model

Again we will have a version of a multi-armed bandit but there are no states. That is, whenever pulling arm i, the reward is an independent draw from some probability distribution. The crux is that we do not know these distributions. The only thing we can do is repeatedly pull arms, observe the reward, and make our decision which arms to pull based on the observed rewards up to this point.

In more detail, there are n arms with initially unknown reward probability distributions $\mathcal{D}_1, \ldots, \mathcal{D}_n$ with means μ_1, \ldots, μ_n . In step t, the algorithm chooses an arm I_t and experiences reward $R_t \in [0,1]$ drawn from \mathcal{D}_{I_t} . So, the overall expected reward is $\mathbf{E}\left[\sum_{t=1}^T R_t\right]$. We assume that $T \geq n$.

If we had perfect knowledge of $\mathcal{D}_1, \ldots, \mathcal{D}_n$, the expected reward would be maximized by always choosing arm i^* defined by $\mu_{i^*} = \max_i \mu_i$. The expected regret of an algorithm is the difference between this expected reward and the one experienced by the algorithm

Regret =
$$T \cdot \max_{i} \mu_{i} - \mathbf{E} \left[\sum_{t=1}^{T} R_{t} \right]$$
.

2 A Simple Explore-Exploit Algorithm

A very simple algorithm works as follows. There are two phases. In the *exploration* phase, we try out each arm exactly k times, so the length of this phase is kn steps. Afterwards, we have k samples from each distribution. From this, we can compute an empirical average $\hat{\mu}_i$ for each arm. If k is large enough, then $\hat{\mu}_i$ should be close to the actual mean μ_i . Therefore, in the *exploitation* phase (of length T - kn), we always play the arm that maximizes $\hat{\mu}_i$.

There is a clear trade-off between the exploration and the exploitation. If we set k too small, then $\hat{\mu}_i$ is computed only based on a few samples and can be far from μ_i . If k is too large, the exploration phase takes too long, during which we also play very bad arms.

Theorem 18.1. Setting $k = \left(\frac{T}{n}\right)^{\frac{2}{3}}$, the expected regret of the simple algorithm is upper-bounded by $O(n^{\frac{1}{3}}T^{\frac{2}{3}}\ln(nT))$.

To prove this theorem, we will use two standard inequalities without proofs. Hoeffding's inequality is a quantitative version of the law of large numbers. It states that we get close to the expectation if we take the average of sufficiently many independent draws from a distribution.

¹For simplicity we assume that this arm is unique.

Lemma 18.2 (Hoeffding's inequality). Let Z_1, \ldots, Z_N be independent random variables such that $a_i \leq Z_i \leq b_i$ with probability 1. Let $\bar{Z} = \frac{1}{N} \sum_{i=1}^N Z_i$ be their average. Then for all $\gamma \geq 0$

$$\mathbf{Pr}\left[|\bar{Z} - \mathbf{E}\left[\bar{Z}\right]| \ge \gamma\right] \le 2 \exp\left(-\frac{2N^2 \gamma^2}{\sum_{i=1}^{N} (b_i - a_i)^2}\right) .$$

The union bound gives an easy upper bound on the probability of a union of events.

Lemma 18.3 (Union Bound). For any sequence of not necessarily disjoint events $\mathcal{E}_1, \mathcal{E}_2 \dots$, we have

$$\mathbf{Pr}\left[\mathcal{E}_1 \cup \mathcal{E}_2 \cup \ldots\right] \leq \mathbf{Pr}\left[\mathcal{E}_1\right] + \mathbf{Pr}\left[\mathcal{E}_2\right] + \ldots .$$

Proof of Theorem 18.1. By Hoeffding's inequality, we get that for all arms i and all $\gamma > 0$

$$\Pr[|\hat{\mu}_i - \mu_i| \ge \gamma] \le 2 \exp\left(-\frac{2k^2\gamma^2}{k(1-0)^2}\right) = 2 \exp(-2k\gamma^2)$$
.

In combination with the union bound, we get

$$\mathbf{Pr}\left[\exists i: |\hat{\mu}_i - \mu_i| \ge \gamma\right] \le \sum_{i=1}^n \mathbf{Pr}\left[|\hat{\mu}_i - \mu_i| \ge \gamma\right] \le 2n \exp(-2k\gamma^2) .$$

If $|\hat{\mu}_i - \mu_i| < \gamma$ for all i, this means the following. Consider the arm i that is played during the exploitation phase. We have

$$\mu_i \ge \hat{\mu}_i - \gamma \ge \hat{\mu}_{i^*} - \gamma \ge \mu_{i^*} - 2\gamma$$
.

Every reward is always non-negative. So, we can lower-bound the overall expected reward by taking into consideration only the rewards from the exploitation phase in the case that $|\hat{\mu}_i - \mu_i| < \gamma$ for all i. Writing ϵ for $2n \exp(-2k\gamma^2)$, we get in combination

$$\mathbf{E}\left[\sum_{t=1}^{T} R_{t}\right] \geq \mathbf{Pr}\left[\forall i : |\hat{\mu}_{i} - \mu_{i}| < \gamma\right] (T - nk)(\mu_{i^{*}} - 2\gamma)$$

$$\geq (1 - \epsilon) (T - nk)(\mu_{i^{*}} - 2\gamma)$$

$$\geq T\mu_{i^{*}} - \epsilon T - nk - T2\gamma ,$$

where we also used that $\mu_{i^*} \leq 1$ and $\epsilon \leq 1$.

Therefore, the expected regret will be at most

$$T\mu_{i^*} - \mathbf{E}\left[\sum_{t=1}^T R_t\right] \le \epsilon T + nk + 2\gamma T$$
.

This bound holds for all k and all γ . Observe that $\gamma = \sqrt{\frac{1}{2k} \ln \frac{2n}{\epsilon}}$. If we now choose $k = \left(\frac{T}{n}\right)^{\frac{2}{3}}$, $\epsilon = \left(\frac{n}{T}\right)^{\frac{1}{3}}$ and the γ that is implied by this choice, the bound holds.

3 UCB1 Algorithm

One of the major weaknesses of the simple algorithm is that it does not adapt the exploration to its observations: If an arm turns out to be very bad, intuitively it should be clear that it can be ignored after only a few samples.

The UCB1 algorithm is smarter. UCB stands for upper confidence bound. This almost explains the entire algorithm. We make no further distinction between exploration and exploitation. In each step, we use the empirical averages $\hat{\mu}_i^{(t)}$ of the arms observed so far. The actual means μ_i are close. They are closer, the more often we pulled the respective arm. Out of the empirical average and the number of times we pulled the arm so far, Q_i , we can compute confidence bounds, in which we expect the μ_i values to lie. We are optimistic and choose the arm with the highest upper bound on μ_i .

In more detail, in the first n steps, we pull each arm once. In any step t > n, we let $\hat{\mu}_i^{(t)}$ be the empirical average of arm i seen in steps before t. Furthermore, we let $Q_i^{(t)}$ denote the number of times that we pulled arm before step t.

From this, compute $\operatorname{Index}_i^{(t)} = \hat{\mu}_i^{(t)} + \sqrt{\frac{\ln T}{Q_i^{(t)}}}$ and play the arm i with highest $\operatorname{Index}_i^{(t)}$.

Theorem 18.4. The expected regret of UCB1 is at most $8\sqrt{nT \ln n} + 4n$.

Below, we will prove the following lemma.

Lemma 18.5. For any arm i, let $Q_i = Q_i^{(T+1)}$ denote the number of times that arm i is pulled overall. Then $\mathbf{Pr}\left[Q_i > s_i\right] \leq \frac{4}{T}$, where $s_i = \frac{4 \ln T}{\Delta_i^2}$, where $\Delta_i = \mu_{i^*} - \mu_i$.

This lemma shows that it is unlikely that a bad arm (for which Δ_i is large) is pulled often. It is actually all the work we have to do; the rest follows in a pretty straightforward way.

Proof of Theorem 18.4. Let $X_{i,t} = 1$ if the algorithm chooses to play i in step t, 0 otherwise. Furthermore, for each i, we define a potential reward $Y_{i,t}$, which the algorithm would get from pulling arm i in step t (irrespective of whether the algorithm will actually pull this arm). Importantly, these two random variables are independent. Therefore $\mathbf{E}[X_{i,t}Y_{i,t}] = \mathbf{E}[X_{i,t}]\mathbf{E}[Y_{i,t}] = \mathbf{E}[X_{i,t}]\mu_i$.

As $\mathbf{E}[R_t] = \mathbf{E}[\sum_{i=1}^n X_{i,t}Y_{i,t}]$, by linearity of expectation, the algorithm's expected reward is

$$\mathbf{E}\left[\sum_{t=1}^{T} R_{t}\right] = \mathbf{E}\left[\sum_{i=1}^{n} \sum_{t=1}^{T} X_{i,t} Y_{i,t}\right] = \sum_{i=1}^{n} \sum_{t=1}^{T} \mathbf{E}\left[X_{i,t}\right] \mu_{i} = \sum_{i=1}^{n} \mathbf{E}\left[\sum_{t=1}^{T} X_{i,t}\right] \mu_{i} = \sum_{i=1}^{n} \mathbf{E}\left[Q_{i}\right] \mu_{i}.$$

So, as always $\sum_{i=1}^{n} Q_i = T$, the expected regret is

Regret =
$$T\mu_{i^*} - \mathbf{E}\left[\sum_{t=1}^{T} R_t\right] = \sum_{i=1}^{n} \mathbf{E}\left[Q_i\right] (\mu_{i^*} - \mu_i) = \sum_{i=1}^{n} \mathbf{E}\left[Q_i\right] \Delta_i$$
.

Using Lemma 18.5, we can upper-bound $\mathbf{E}[Q_i]$ by

$$\mathbf{E}[Q_i] \le \mathbf{Pr}[Q_i \le s_i] \, s_i + \mathbf{Pr}[Q_i > s_i] \, T \le s_i + \mathbf{Pr}[Q_i > s_i] \, T \le s_i + 4$$
.

Now we make a case distinction. Call an arm i bad if $\Delta_i \geq \delta := \sqrt{\frac{n \ln T}{T}}$. For such a bad arm, we have

$$\mathbf{E}\left[Q_{i}\right]\Delta_{i} \leq \frac{4\ln T}{\Delta_{i}} + 4\Delta_{i} \leq \frac{4\ln T}{\delta} + 4 = 4\sqrt{\frac{T\ln T}{n}} + 4$$

This lets us bound the expected regret by

Regret
$$\leq T\delta + \sum_{i:i \text{ is bad}} \mathbf{E} [Q_i] \Delta_i \leq 4\sqrt{nT \ln n} + 4\sqrt{nT \ln n} + 4n$$
.

4 Proof of Lemma 18.5

So, it only remains to prove Lemma 18.5. Interestingly, this only has to be a statement about one single arm i. We will have to show that the larger Δ_i the earlier the algorithm stops pulling the arm.

We do a major part of the work by proving the following lemma. It finally quantifies the frequently mentioned intuition that $\hat{\mu}_i^{(t)}$ is close to μ_i if arm i has been pulled often.

Lemma 18.6. For all i, we have

$$\mathbf{Pr}\left[\exists t: |\hat{\mu}_i^{(t)} - \mu_i| \ge \sqrt{\frac{\ln T}{Q_i^{(t)}}}\right] \le \frac{2}{T} .$$

Proof. The difficulty is that we cannot apply Hoeffding's inequality on a fixed $\hat{\mu}_i^{(t)}$: The value of $\hat{\mu}_i^{(t)}$ depends on how often we have pulled arm i so far and how the rewards turned out to be. If the first rewards were low, the value of $\hat{\mu}_i^{(t')}$ at the earlier time t' is low as well and arm i gets ignored.

Therefore, instead, we will consider the following way to determine all values of $\hat{\mu}_{i'}^{(t)}$. First, we draw T values for each arm i', which we denote by $X_{i',1},\ldots,X_{i',T}$. The meaning is that the j^{th} draw from arm i' has reward $X_{i',j}$. Note that fixing all these random outcomes, this also determines what the algorithm does and consequently also $\hat{\mu}_{i'}^{(t)}$.

Now, in order for there to be a t such that $|\hat{\mu}_i^{(t)} - \mu_i| \ge \sqrt{\frac{\ln T}{Q_i^{(t)}}}$, there has to be a k such that

 $\left|\frac{1}{k}\sum_{j=1}^{k}X_{i,j}-\mu_{i}\right|\geq\sqrt{\frac{\ln T}{k}}$. On these random variables $X_{i,1},\ldots,X_{i,k}$, we can apply Hoeffding's inequality and get

$$\mathbf{Pr}\left[\left|\frac{1}{k}\sum_{j=1}^{k}X_{i,j}-\mu_{i}\right| \geq \sqrt{\frac{\ln T}{k}}\right] \leq 2\exp\left(-2k\frac{\ln T}{k}\right) = \frac{2}{T^{2}}.$$

The event that there is a k for which $\left|\frac{1}{k}\sum_{j=1}^k X_{i,j} - \mu_i\right| \ge \sqrt{\frac{\ln T}{k}}$ is again a union of events for which we can apply the union bound. Therefore

$$\mathbf{Pr}\left[\exists k: \left|\frac{1}{k}\sum_{j=1}^{k}X_{i,j}-\mu_i\right| \geq \sqrt{\frac{\ln T}{k}}\right] \leq \sum_{k=1}^{T}\mathbf{Pr}\left[\left|\frac{1}{k}\sum_{j=1}^{k}X_{i,j}-\mu_i\right| \geq \sqrt{\frac{\ln T}{k}}\right] \leq T\frac{2}{T^2} = \frac{2}{T}.$$

By plugging in the definition of $\mathrm{Index}_i^{(t)}$, we immediately get that only with small probability an index $\mathrm{Index}_i^{(t)}$ falls below μ_i or is much higher than this.

Corollary 18.7. For all i, we have

$$\mathbf{Pr}\left[\exists t : \mathrm{Index}_i^{(t)} \leq \mu_i\right] \leq \frac{2}{T} \qquad and \qquad \mathbf{Pr}\left[\exists t : \mathrm{Index}_i^{(t)} \geq \mu_i + 2\sqrt{\frac{\ln T}{Q_i^{(t)}}}\right] \leq \frac{2}{T} .$$

This corollary is the key insight to complete our proof of Lemma 18.5.

Proof of Lemma 18.5. Note that for $Q_i > s_i$, there has to be some t_0 for which $Q_i^{(t_0)} = s_i$ and i is selected again. The algorithm selects i again because $\operatorname{Index}_i^{(t_0)}$ is the highest index. So in particular $\operatorname{Index}_i^{(t_0)} \geq \operatorname{Index}_{i^*}^{(t_0)}$.

Let us now apply Corollary 18.7 to i and i^* . We get that

$$\mathbf{Pr}\left[\exists t: \mathrm{Index}_{i^*}^{(t)} \leq \mu_{i^*}\right] \leq \frac{2}{T} \quad \text{and} \quad \mathbf{Pr}\left[\exists t: \mathrm{Index}_i^{(t)} \geq \mu_i + 2\sqrt{\frac{\ln T}{Q_i^{(t)}}}\right] \leq \frac{2}{T} .$$

By the union bound with probability at most $\frac{4}{T}$ one of the two events happens. If neither happens, then in particular at time t_0

Index_{i*}^(t₀) >
$$\mu_{i*}$$
 and Index_i^(t₀) < $\mu_{i} + 2\sqrt{\frac{\ln T}{s_{i}}} = \mu_{i} + \Delta_{i} = \mu_{i*}$.

This is a contradiction to $\operatorname{Index}_{i}^{(t_0)} \geq \operatorname{Index}_{i^*}^{(t_0)}$. This shows that $\operatorname{\mathbf{Pr}}\left[Q_i > s_i\right] \leq \frac{4}{T}$.

Reference

Peter Auer, Nicolò Cesa-Bianchi, Paul Fischer: Finite-time Analysis of the Multiarmed Bandit Problem. Mach. Learn. 47(2-3): 235-256 (2002)