Econ 2148, fall 2019 Multi-armed bandits

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Agenda

- ► Thus far: "Supervised machine learning" data are given. Next: "Active learning" – experimentation.
- Setup: The multi-armed bandit problem.
 Adaptive experiment with exploration / exploitation trade-off.
- Two popular approximate algorithms:
 - 1. Thompson sampling
 - 2. Upper Confidence Bound algorithm
- Characterizing regret.
- Characterizing an exact solution: Gittins Index.
- Extension to settings with covariates (contextual bandits).

Takeaways for this part of class

- ▶ When experimental units arrive over time, and we can adapt our treatment choices, we can learn optimal treatment quickly.
- Treatment choice: Trade-off between
 - 1. choosing good treatments now (exploitation),
 - 2. and learning for future treatment choices (exploration).
- Optimal solutions are hard, but good heuristics are available.
- We will derive a bound on the regret of one heuristic.
 - Bounding the number of times a sub-optimal treatment is chosen,
 - using large deviations bounds (cf. testing!).
- We will also derive a characterization of the optimal solution in the infinite-horizon case. This relies on a separate index for each arm.

Setup

- ▶ Treatments $D_t \in 1, ..., k$
- Experimental units come in sequentially over time. One unit per time period t = 1, 2, ...
- ▶ Potential outcomes: i.i.d. over time, $Y_t = Y_t^{D_t}$,

$$Y_t^d \sim F^d$$
 $E[Y_t^d] = \theta^d$

Treatment assignment can depend on past treatments and outcomes,

$$D_{t+1} = d_t(D_1, \ldots, D_t, Y_1, \ldots, Y_t).$$

Setup continued

Optimal treatment:

$$d^* = \operatorname*{argmax}_d \theta^d \qquad \qquad \theta^* = \operatorname*{max}_d \theta^d = \theta^{d^*}$$

Expected regret for treatment d:

$$\Delta^d = E\left[Y^{d^*} - Y^d\right] = \theta^{d^*} - \theta^d.$$

Finite horizon objective: Average outcome,

$$U_T = \frac{1}{T} \sum_{1 \le t \le T} Y_t.$$

Infinite horizon objective: Discounted average outcome,

$$U_{\infty} = \sum_{t>1} \beta^t Y_t$$

The multi-armed bandit

Expectations of objectives

Expected finite horizon objective:

$$E[U_T] = E\left[\frac{1}{T}\sum_{1 \leq t \leq T} \theta^{D_t}\right]$$

Expected infinite horizon objective:

$$E[U_{\infty}] = E\left[\sum_{t\geq 1} eta^t heta^{D_t}
ight]$$

Expected finite horizon regret:

Compare to always assigning optimal treatment d^* .

$$R_T = E\left[\frac{1}{T}\sum_{1 \le t \le T} \left(Y_t^{d^*} - Y_t\right)\right] = E\left[\frac{1}{T}\sum_{1 \le t \le T} \Delta^{D_t}\right]$$

Practice problem

- Show that these equalities hold.
- Interpret these objectives.
- Relate them to our decision theory terminology.

Two popular algorithms

Upper Confidence Bound (UCB) algorithm

Define

$$egin{aligned} ar{Y}_t^d &= rac{1}{T_t^d} \sum_{1 \leq s \leq t} \mathbf{1}(D_s = d) \cdot Y_s, \ T_t^d &= \sum_{1 \leq s \leq t} \mathbf{1}(D_s = d) \ B_t^d &= B(T_t^d). \end{aligned}$$

- \triangleright $B(\cdot)$ is a decreasing function, giving the width of the "confidence interval." We will specify this function later.
- At time t+1, choose

$$D_{t+1} = \underset{d}{\operatorname{argmax}} \ \bar{Y}_t^d + B_t^d.$$

"Optimism in the face of uncertainty."

Two popular algorithms

Thompson sampling

- Start with a Bayesian prior for θ .
- Assign each treatment with probability equal to the posterior probability that it is optimal.
- Put differently, obtain one draw $\hat{\theta}_{t+1}$ from the posterior given $(D_1, \dots, D_t, Y_1, \dots, Y_t)$, and choose

$$D_{t+1} = \underset{d}{\operatorname{argmax}} \ \hat{\theta}_{t+1}^{d}.$$

Easily extendable to more complicated dynamic decision problems, complicated priors, etc.!

Two popular algorithms

Thompson sampling - the binomial case

- ▶ Assume that $Y \in \{0,1\}$, $Y_t^d \sim Ber(\theta^d)$.
- Start with a uniform prior for θ on $[0,1]^k$.
- ▶ Then the posterior for θ^d at time t+1 is a *Beta* distribution with parameters

$$\alpha_t^d = 1 + T_t^d \cdot \bar{Y}_t^d,$$

$$\beta_t^d = 1 + T_t^d \cdot (1 - \bar{Y}_t^d).$$

Thus

$$D_t = \underset{d}{\operatorname{argmax}} \hat{\theta}_t.$$

where

$$\hat{ heta}_t^{d} \sim \textit{Beta}(lpha_t^{d}, eta_t^{d})$$

is a random draw from the posterior.

Regret bounds

- Back to the general case.
- Recall expected finite horizon regret,

$$R_T = E\left[\frac{1}{T}\sum_{1 \leq t \leq T} \left(Y_t^{d^*} - Y_t\right)\right] = E\left[\frac{1}{T}\sum_{1 \leq t \leq T} \Delta^{D_t}\right].$$

Thus,

$$T \cdot R_T = \sum_d E[T_T^d] \cdot \Delta^d.$$

- ▶ Good algorithms will have $E[T_T^d]$ small when $\Delta^d > 0$.
- ▶ We will next derive upper bounds on $E[T_T^d]$ for the UCB algorithm.
- ▶ We will then state that for large *T* similar upper bounds hold for Thompson sampling.
- There is also a lower bound on regret across all possible algorithms which is the same, up to a constant.

Probability theory preliminary

Large deviations

Suppose that

$$E[\exp(\lambda \cdot (Y - E[Y]))] \le \exp(\psi(\lambda)).$$

Let $\bar{Y}_T = \frac{1}{T} \sum_{1 \le t \le T} Y_t$ for i.i.d. Y_t . Then, by Markov's inequality and independence across t,

$$P(\bar{Y}_T - E[Y] > \varepsilon) \le \frac{E[\exp(\lambda \cdot (\bar{Y}_T - E[Y]))]}{\exp(\lambda \cdot \varepsilon)}$$

$$= \frac{\prod_{1 \le t \le T} E[\exp((\lambda/T) \cdot (Y_t - E[Y]))]}{\exp(\lambda \cdot \varepsilon)}$$

$$\le \exp(T\psi(\lambda/T) - \lambda \cdot \varepsilon).$$

Large deviations continued

ightharpoonup Define the Legendre-transformation of ψ as

$$\psi^*(\varepsilon) = \sup_{\lambda \geq 0} \left[\lambda \cdot \varepsilon - \psi(\lambda)\right].$$

ightharpoonup Taking the inf over λ in the previous slide implies

$$P(\bar{Y}_T - E[Y] > \varepsilon) \le \exp(-T \cdot \psi^*(\varepsilon)).$$

- For distributions bounded by [0,1]: $\psi(\lambda) = \lambda^2/8$ and $\psi^*(\varepsilon) = 2\varepsilon^2$.
- For normal distributions: $\psi(\lambda) = \lambda^2 \sigma^2/2$ and $\psi^*(\varepsilon) = \varepsilon^2/(2\sigma^2)$.

Applied to the Bandit setting

Suppose that for all d

$$E[\exp(\lambda \cdot (Y^d - \theta^d))] \le \exp(\psi(\lambda))$$

$$E[\exp(-\lambda \cdot (Y^d - \theta^d))] \le \exp(\psi(\lambda)).$$

Recall / define

$$ar{Y}_t^d = rac{1}{T_t^d} \sum_{1 \leq s \leq t} \mathbf{1}(D_s = d) \cdot Y_s, \qquad \qquad B_t^d = (\psi^*)^{-1} \left(rac{lpha \log(t)}{T_t^d}
ight).$$

Then we get

$$P(\bar{Y}_t^d - \theta^d > B_t^d) \le \exp(-T_t^d \cdot \psi^*(B_t^d))$$

$$= \exp(-\alpha \log(t)) = t^{-\alpha}$$

$$P(\bar{Y}_t^d - \theta^d < -B_t^d) \le t^{-\alpha}.$$

Why this choice of $B(\cdot)$?

- ightharpoonup A smaller $B(\cdot)$ is better for exploitation.
- ▶ A larger $B(\cdot)$ is better for exploration.
- Special cases:
 - Distributions bounded by [0,1]:

$$B_t^d = \sqrt{rac{lpha \log(t)}{2T_t^d}}.$$

Normal distributions:

$$B_t^d = \sqrt{2\sigma^2 rac{lpha \log(t)}{T_t^d}}.$$

The $\alpha \log(t)$ term ensures that coverage goes to 1, but slow enough to not waste too much in terms of exploitation.

When d is chosen by the UCB algorithm

> By definition of UCB, at least one of these three events has to hold when d is chosen at time t+1:

$$\bar{Y}_t^{d^*} + B_t^{d^*} \le \theta^* \tag{1}$$

$$\bar{Y}_t^d - B_t^d > \theta^d \tag{2}$$

$$2B_t^d > \Delta^d. \tag{3}$$

1 and 2 have low probability. By previous slide,

$$P\left(\bar{Y}_t^{d^*} + B_t^{d^*} \leq \theta^*\right) \leq t^{-\alpha}, \qquad P\left(\bar{Y}_t^d - B_t^d > \theta^d\right) \leq t^{-\alpha}.$$

 \triangleright 3 only happens when T_t^d is small. By definition of B_t^d , 3 happens iff

$$T_t^d < rac{lpha \log(t)}{\psi^*(\Delta^d/2)}.$$

Regret bounds

Practice problem

Show that at least one of the statements 1, 2, or 3 has to be true whenever $D_{t+1} = d$, for the UCB algorithm.

Bounding $E[T_t^d]$

Let

$$ilde{T}_T^d = \left \lfloor rac{lpha \log(T)}{\psi^*(\Delta^d/2)}
ight
floor.$$

- Forcing the algorithm to pick d the first \tilde{T}_T^d periods can only increase T_T^d .
- We can collect our results to get

$$\begin{split} E[T_T^d] &= \sum_{1 \leq t \leq T} \mathbf{1}(D_t = d) \leq \tilde{T}_T^d + \sum_{\tilde{T}_T^d < t \leq T} E[\mathbf{1}(D_t = d)] \\ &\leq \tilde{T}_T^d + \sum_{\tilde{T}_T^d < t \leq T} E[\mathbf{1}((1) \text{ or } (2) \text{ is true at } t)] \\ &\leq \tilde{T}_T^d + \sum_{\tilde{T}_T^d < t \leq T} E[\mathbf{1}((1) \text{is true at } t)] + E[\mathbf{1}((2) \text{ is true at } t)] \\ &\leq \tilde{T}_T^d + \sum_{\tilde{T}_T^d < t \leq T} 2t^{-\alpha + 1} \leq \tilde{T}_T^d + \frac{\alpha}{\alpha - 2}. \end{split}$$

Upper bound on expected regret for UCB

We thus get:

$$E[T_T^d] \le rac{lpha \log(T)}{\psi^*(\Delta^d/2)} + rac{lpha}{lpha - 2},
onumber \ R_T \le rac{1}{T} \sum_d \left(rac{lpha \log(T)}{\psi^*(\Delta^d/2)} + rac{lpha}{lpha - 2}
ight) \cdot \Delta^d.$$

- Expected regret (difference to optimal policy) goes to 0 at a rate of $O(\log(T)/T)$ pretty fast!
- While the cost of "getting treatment wrong" is Δ^d , the difficulty of figuring out the right treatment is of order $1/\psi^*(\Delta^d/2)$. Typically, this is of order $(1/\Delta^d)^2$.

Related bounds - rate optimality

Lower bound: Consider the Bandit problem with binary outcomes and any algorithm such that $E[T_t^d] = o(t^a)$ for all a > 0. Then

$$\liminf_{t\to\infty} \frac{\tau}{\log(\tau)} \bar{R}_{\tau} \geq \sum_{d} \frac{\Delta^{d}}{kl(\theta^{d}, \theta^{*})},$$

where
$$kl(p,q) = p \cdot \log(p/q) + (1-p) \cdot \log((1-p)/(1-q))$$
.

▶ **Upper bound for Thompson sampling**: In the binary outcome setting, Thompson sampling achieves this bound, i.e.,

$$\liminf_{t\to\infty} \frac{\tau}{\log(\tau)} \bar{R}_T = \sum_{d} \frac{\Delta^d}{kl(\theta^d, \theta^*)}.$$

Gittins index

Setup

- Consider now the discounted infinite-horizon objective, $E[U_{\infty}] = E\left[\sum_{t\geq 1} \beta^t \theta^{D_t}\right]$, averaged over independent (!) priors across the components of θ .
- We will characterize the optimal strategy for maximizing this objective.
- ▶ To do so consider the following, simpler decision problem:
 - You can only assign treatment d.
 - You have to pay a charge of γ^d each period in order to continue playing.
 - You may stop at any time, then the game ends.
- Define γ_t^d as the charge which would make you indifferent between playing or not, given the period t posterior.

Gittins index

Formal definition

- ▶ Denote by π_t the posterior in period t, by $\tau(\cdot)$ an arbitrary stopping rule.
- Define

$$\begin{split} \gamma_t^d &= \sup \left\{ \gamma : \sup_{\tau(\cdot)} E_{\pi_t} \left[\sum_{1 \leq s \leq \tau} \beta^s \left(\theta^d - \gamma \right) \right] \geq 0 \right\} \\ &= \sup_{\tau(\cdot)} \frac{E_{\pi_t} \left[\sum_{1 \leq s \leq \tau} \beta^s \theta^d \right]}{E_{\pi_t} \left[\sum_{1 \leq s \leq \tau} \beta^s \right]} \end{split}$$

 Gittins and Jones (1974) prove: The optimal policy in the bandit problem always chooses

$$D_t = \underset{d}{\operatorname{argmax}} \ \gamma_t^d.$$

Heuristic proof (sketch)

- Imagine a per-period charge for each treatment is set initially equal to γ_1^d .
 - Start playing the arm with the highest charge, continue until it is optimal to stop.
 - At that point, the charge is reduced to γ_t^d .
 - Repeat.
- This is the optimal policy, since:
 - 1. It maximizes the amount of charges paid.
 - 2. Total expected benefits are equal to total expected charges.
 - There is no other policy that would achieve expected benefits bigger than expected charges.

Contextual bandits

- A more general bandit problem:
 - \triangleright For each unit (period), we observe covariates X_t .
 - ightharpoonup Treatment may condition on X_t .
 - ightharpoonup Outcomes are drawn from a distribution $F^{x,d}$, with mean $\theta^{x,d}$.
- In this setting Gittins' theorem fails when the prior distribution of $\theta^{x,d}$ is not independent across x or across d.
- But Thompson sampling is easily generalized. For instance to a hierarchical Bayes model:

$$egin{aligned} egin{aligned} egin{aligned} Y^d | X = x, heta, lpha, eta &\sim extit{Ber}(heta^{x,d}) \ heta^{x,d} | lpha, eta &\sim extit{Beta}(lpha^d, eta^d) \ &(lpha^d, eta^d) \sim \pi. \end{aligned}$$

This model updates the prior for $\theta^{x,d}$ not only based on observations with D = d, X = x, but also based on observations with D = d but different values for X.

References

- ▶ Bubeck, S. and Cesa-Bianchi, N. (2012). Regret Analysis of Stochastic and Nonstochastic Multi-armed Bandit Problems. Foundations and Trends® in Machine Learning, 5(1):1–122.
- Russo, D. J., Roy, B. V., Kazerouni, A., Osband, I., and Wen, Z. (2018). A Tutorial on Thompson Sampling. Foundations and Trends® in Machine Learning, 11(1):1–96.
- Weber, R. et al. (1992). On the Gittins index for multiarmed bandits. The Annals of Applied Probability, 2(4):1024–1033.