CS292F StatRL Lecture 8 Exploration in Bandits

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Recap: Lecture 7

- Multi-Armed Bandits
  - Problem setup
  - Regret definition
- No regret learning algorithms
  - Exploration first
  - Eps-greedy
  - Upper Confidence Bound

Recap: Regret bounds

- Exploration first / eps-greedy

$$\tilde{O}(T^{2/3}k^{1/3})$$

- UCB

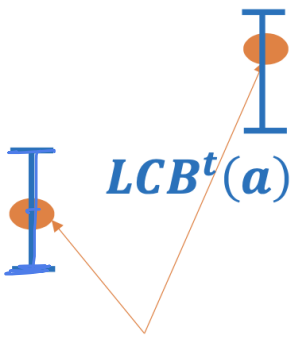
$$\tilde{O}(\sqrt{Tk})$$

$$\tilde{O}\left(\sum_{a \neq a^*} \frac{1}{\Delta_a}\right) \log T$$

Recap: UCB algorithm for MAB

$$UCB^t(a) = \tilde{\mu}^t(a) + \sqrt{\frac{\log(2kT/\delta)}{2n^t(a)}}$$

$$LCB^t(a) = \tilde{\mu}^t(a) - \sqrt{\frac{\log(2kT/\delta)}{2n^t(a)}}$$



Actual reward means

By Hoeffding and union bound, with probability $\geq 1-\delta$, it holds $\forall a \in [k], t \in [T]$:

$$\boldsymbol{\mu(a) \in [LCB^t(a), UCB^t(a)]}$$

Claim : In the event that all confidence intervals confidence intervals hold, the regret is at most $\sum_t (UCB^t(a^t) - LCB^t(a^t)) + \delta \cdot T$

Proof: $Reg^t = \mu(a^\star) - \mu(a^t)$

$\leq UCB^t(a^\star) - LCB^t(a^t)$

$\leq UCB^t(a^t) - LCB^t(a^t)$

$2 \cdot \epsilon$

Recap: UCB algorithm for MAB

Gap-independent analysis:

$$\sum_{t=0}^{T-1} \mu^\star - \mu_{A_t} \le 4\sqrt{\ln(TK/\delta)} \sum_{t=0}^{T-1} \sqrt{\frac{1}{N^t(A_t)}}$$

$$= 4\sqrt{\ln(TK/\delta)} \sum_a \sum_{i=1}^{N^T(a)} \frac{1}{\sqrt{i}} \le 8\sqrt{\ln(TK/\delta)} \sum_a \sqrt{N^T(a)} \le 8\sqrt{\ln(TK/\delta)} \sqrt{K \sum_a N^T(a)}$$

$$\le 8\sqrt{\ln(TK/\delta)}\sqrt{KT}.$$

Gap-dependent analysis:

$$N^T(a) \le \frac{4\ln(TK/\delta)}{\Delta_a^2}.$$

whenever

$\bar{Q}(a) \le \mu(a^*)$

then a will not be chosen ever again

$\mu(a^*) - \bar{Q}(a) \le \Delta_a$

Recap: Linear bandits: problem setup

("Dani et al., 2008")

- Action space is a compact set

decision $x_t \in D \subset R^d$.

- Reward is linear + i.i.d. noise.

$\mathbb{E}[r_t | x_t = x] = \mu^\star \cdot x \in [-1, 1]$, $\eta_t = r_t - \mu^\star \cdot x_t$

($\mu^\star$: unknown vector)

- Agent chooses a sequence of actions

$$x_1, \ldots, x_T$$

- The regret is defined similarly

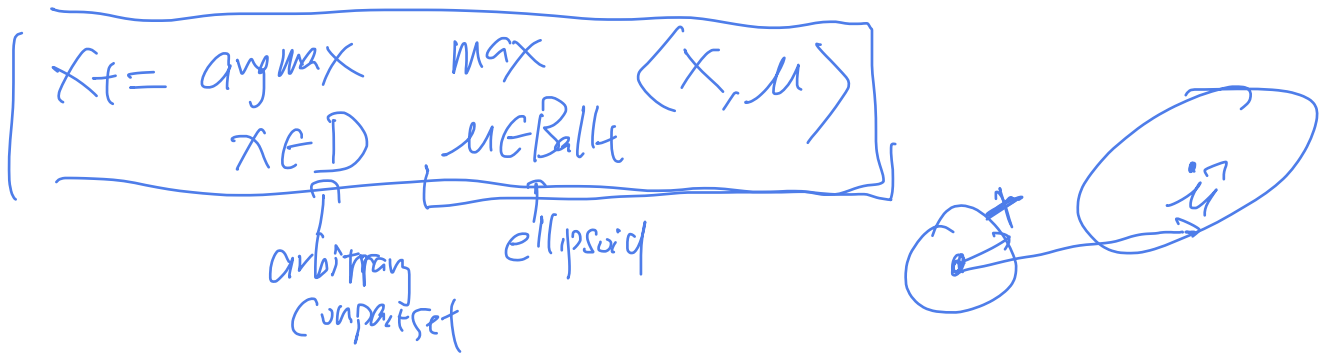
$$\mathrm{Reg}_T = T \cdot \langle \mu^*, x^* \rangle - \sum_{t=1}^{T} \langle \mu^*, x_t \rangle$$

$\mathbb{E}[\mathrm{Reg}_T]$: over randomness of the agent.

$$x^\star \in \mathrm{argmax}_{x \in D}\, \mu^\star \cdot x$$

Recap: The LinUCB algorithm: Optimism in the Face of Uncertainty.

- Consider the ridge regression at each time t.
- Construct high probability confidence set of the parameter vector
- Choose actions that maximize the UCB.



This lecture

- The regret analysis of LinUCB
- Exploration in Tabular RL
  - Problem setup

Regret bound of LinUCB

Sublinear regret: $R_T \leq O^\star(d\sqrt{T})$
poly dependence on d , no dependence on the cardinality $|D|$.

η_t is independent $\mathcal{Q}$ G^2-subgaussian

Theorem 5.3 (AJKS)

Suppose: bounded noise $|\eta_t| \leq \sigma$, that $\|\mu^\star\| \leq W$, and that $\|x\| \leq B$ for all $x \in D$. Set $\lambda = \sigma^2/W^2$ and

$$\beta_t := \sigma^2\left(2 + 4d\log\left(1 + \frac{TB^2W^2}{d}\right) + 8\log(4/\delta)\right).$$

With probability greater than $1-\delta$, that for all $t \geq 0$,

$$R_T \leq c\sigma\sqrt{T}\left(d\log\left(1 + \frac{TB^2W^2}{d\sigma^2}\right) + \log(4/\delta)\right) \asymp O(\sqrt{T})$$

where c is an absolute constant.

(Dani, Hayes & Kakde, 2009)

(From this slide onwards mostly taken from Sham Kakade)

Two components of the regret analysis

- Uniform (over all t) confidence bound

Proposition 5.5 (AJKS)

(Confidence) Let $\delta > 0$. We have that

$$\Pr(\forall t,\ \mu^\star \in \text{BALL}_t) \geq 1 - \delta.$$

- Sum of Squares Regret bound

Proposition 5.6 (AJKS)

(Sum of Squares Regret Bound) Define:

$$\text{regret}_t = \mu^\star \cdot x^* - \mu^\star \cdot x_t$$

Suppose $\|x\| \leq B$ for $x \in D$. Suppose β_t is increasing and larger than 1. Suppose $\mu^\star \in \text{BALL}_t$ for all t, then

$$\sum_{t=0}^{T-1} \text{regret}_t^2 \leq 4\beta_T d \log\left(1 + \frac{TB^2}{d\lambda}\right)$$

Proof of the main regret bound

- By Cauchy-Schwarz

$$\sum_{t=0}^{T-1} \text{regret}_t \leq \sqrt{T \sum_{t=0}^{T-1} \text{regret}_t^2} \leq \sqrt{4 T \beta_T d \log\left(1 + \frac{TB^2}{d\lambda}\right)}.$$

$\sum_{t=1}^{T-1} 1 \cdot \text{regret}_t \leq \sqrt{\sum 1^2 \sum \text{regret}_t^2}$

substitute $\beta_t = G^2\left[2 + d\log\left(1 + \frac{TB^2}{d\lambda}\right) + 8\log\left(\frac{4}{\delta}\right)\right]$

Plan of the proof

1. First prove the Proposition that bounds the sum of square regret
   - By bounding instantaneous regret
   - And then bounding the sum of squares with "Information Gain"

2. Prove the uniform confidence bound
   - Basically show that the choice of β_t "works".

"Width" of Confidence Ball

Lemma 5.7 (AJKS)

Let $x \in D$. If $\mu \in \text{BALL}_t$ and $x \in D$. Then

$$|(\mu - \widehat{\mu}_t)^\top x| \le \sqrt{\beta_t x^\top \Sigma_t^{-1} x}$$

Proof: By Cauchy-Schwarz, we have:

$$|(\mu - \widehat{\mu}_t)^\top x| = |(\mu - \widehat{\mu}_t)^\top \Sigma_t^{1/2} \Sigma_t^{-1/2} x| = |(\Sigma_t^{1/2}(\mu - \widehat{\mu}_t))^\top \Sigma_t^{-1/2} x|$$

$$\le \|\Sigma_t^{1/2}(\mu - \widehat{\mu}_t)\| \|\Sigma_t^{-1/2} x\| = \|\Sigma_t^{1/2}(\mu - \widehat{\mu}_t)\| \sqrt{x^\top \Sigma_t^{-1} x} \le \sqrt{\beta_t x^\top \Sigma_t^{-1} x}$$

where the last inequality holds since $\mu \in \text{BALL}_t$. ■

Instantaneous Regret is bounded by the width of the ellipsoid.

Define

$$w_t := \sqrt{x_t^\top \Sigma_t^{-1} x_t}$$

which is the "normalized width" at time t in the direction of our decision.

Lemma 5.8 (AJKS)

Fix $t \le T$. If $\mu^\star \in \text{BALL}_t$, then

$$\text{regret}_t \le 2 \min\left(\sqrt{\beta_t} w_t, 1\right) \le 2\sqrt{\beta_T} \min\left(w_t, 1\right)$$

Proof: Let $\widetilde{\mu} \in \text{BALL}_t$ denote the vector which minimizes the dot product $\widetilde{\mu}^\top x_t$. By choice of x_t, we have

$$\widetilde{\mu}^\top x_t = \max_{\mu \in \text{BALL}_t} \max_{x \in D} \mu^\top x \ge (\mu^\star)^\top x^*,$$

where the inequality used the hypothesis $\mu^\star \in \text{BALL}_t$. Hence,

$$\begin{aligned} \text{regret}_t &= (\mu^\star)^\top x^* - (\mu^\star)^\top x_t \le (\widetilde{\mu} - \mu^\star)^\top x_t \\ &= (\widetilde{\mu} - \widehat{\mu}_t)^\top x_t + (\widehat{\mu}_t - \mu^\star)^\top x_t \le 2\sqrt{\beta_t} w_t \end{aligned}$$

"Geometric potential" argument: Converting summation to product

Lemma 5.9 (AJKS)

We have:

$$\det \Sigma_T = \det \Sigma_0 \prod_{t=0}^{T-1} (1 + w_t^2).$$

Proof: By the definition of Σ_{t+1}, we have

$$\begin{aligned}\det \Sigma_{t+1} &= \det(\Sigma_t + x_t x_t^\top) = \det(\Sigma_t^{1/2}(I + \Sigma_t^{-1/2} x_t x_t^\top \Sigma_t^{-1/2})\Sigma_t^{1/2}) \\ &= \det(\Sigma_t) \det(I + \Sigma_t^{-1/2} x_t (\Sigma_t^{-1/2} x_t)^\top) = \det(\Sigma_t) \det(I + v_t v_t^\top),\end{aligned}$$

where $v_t := \Sigma_t^{-1/2} x_t$. Now observe that $v_t^\top v_t = w_t^2$ and ... ■

Taking logarithm (get information gain), then bounding it with data-independent terms.

Lemma

For any sequence $x_0, \dots x_{T-1}$ such that, for $t < T$, $\|x_t\|_2 \le B$, we have:

$$\log\left(\det \Sigma_{T-1} / \det \Sigma_0\right) = \log\det\left(I + \frac{1}{\lambda}\sum_{t=0}^{T-1} x_t x_t^\top\right) \le d\log\left(1 + \frac{TB^2}{d\lambda}\right).$$

Proof: Denote the eigenvalues of $\sum_{t=0}^{T-1} x_t x_t^\top$ as $\sigma_1, \dots \sigma_d$, and note:

$$\sum_{i=1}^{d} \sigma_i = \mathrm{Trace}\left(\sum_{t=0}^{T-1} x_t x_t^\top\right) = \sum_{t=0}^{T-1} \|x_t\|^2 \le TB^2.$$

Using the AM-GM inequality,

$$\log\det\left(I + \frac{1}{\lambda}\sum_{t=0}^{T-1} x_t x_t^\top\right) = \log\left(\prod_{i=1}^{d}(1 + \sigma_i/\lambda)\right)$$

$$= d\log\left(\prod_{i=1}^{d}\left(1 + \sigma_i/\lambda\right)\right)^{1/d} \le d\log\left(\frac{1}{d}\sum_{i=1}^{d}(1 + \sigma_i/\lambda)\right) \le d\log\left(1 + \frac{TB^2}{d\lambda}\right)$$

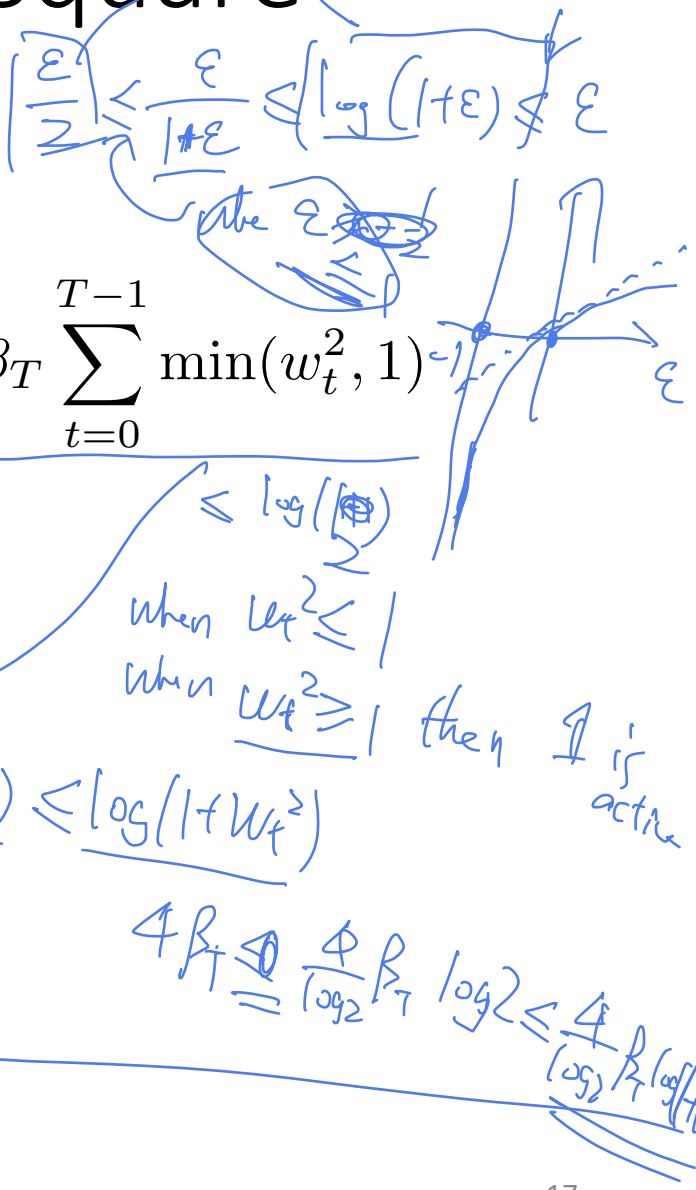
Bounding the Sum of Square Instantaneous Regret

$$\sum_{t=0}^{T-1} \text{regret}_t^2 \leq \sum_{t=0}^{T-1} 4\beta_t \min(w_t^2, 1) \leq 4\beta_T \sum_{t=0}^{T-1} \min(w_t^2, 1)$$

$$\leq \max\left\{8, \frac{4}{\log 2}\right\} \beta_T \sum_{t=1}^{T-1} \log(1 + w_t^2)$$

$$= C\beta_T \log\left(\det \Sigma_T / \det \Sigma_0\right)$$

$$\leq C\beta_T d \log\left(1 + \frac{T\beta^2}{d\lambda}\right).$$



Plan of the proof

1. First prove the Proposition that bounds the sum of square regret
   - By bounding instantaneous regret
   - And then bounding the sum of squares with "Information Gain"

2. Prove the uniform confidence bound
   - Basically show that the choice of β_t "works".

We need to prove that the true parameter is in the version space w.h.p.

- Recall the version space is:

Proof: Since $r_\tau = x_\tau \cdot \mu^\star + \eta_\tau$, we have:

$$\widehat{\mu}_t - \mu^\star = \Sigma_t^{-1} \sum_{\tau=0}^{t-1} r_\tau x_\tau - \mu^\star = \Sigma_t^{-1} \sum_{\tau=0}^{t-1} x_\tau (x_\tau \cdot \mu^\star + \eta_\tau) - \mu^\star$$

$$= \Sigma_t^{-1} \left(\sum_{\tau=0}^{t-1} x_\tau (x_\tau)^\top \right) \mu^\star - \mu^\star + \Sigma_t^{-1} \sum_{\tau=0}^{t-1} \eta_\tau x_\tau$$

$$= \lambda \Sigma_t^{-1} \mu^\star + \Sigma_t^{-1} \sum_{\tau=0}^{t-1} \eta_\tau x_\tau$$

By the triangle inequality,

$$\sqrt{(\widehat{\mu}_t - \mu^\star)^\top \Sigma_t (\widehat{\mu}_t - \mu^\star)} \le \left\| \lambda \Sigma_t^{-1/2} \mu^\star \right\| + \left\| \Sigma_t^{-1/2} \sum_{\tau=0}^{t-1} \eta_\tau x_\tau \right\|$$

$$\le \sqrt{\lambda} \|\mu^\star\| + ??.$$

How can we bound "??" To be continued... ■

Self-normalized Martingale concentration bound.

Lemma (Self-Normalized Bound for Vector-Valued Martingales)

(Abassi et. al '11) Suppose $\{\varepsilon_i\}_{i=1}^{\infty}$ *are mean zero random variables (can be generalized to martingales), and* ε_i *is bounded by* σ*. Let* $\{X_i\}_{i=1}^{\infty}$ *be a stochastic process. Define* $\Sigma_t = \Sigma_0 + \sum_{i=1}^{t} X_i X_i^\top$*. With probability at least* $1-\delta$*, we have for all* $t \geq 1$*:*

$$\left\| \sum_{i=1}^{t} X_i \varepsilon_i \right\|^2_{\Sigma_t^{-1}} \leq \sigma^2 \log\left(\frac{\det(\Sigma_t)\det(\Sigma_0)^{-1}}{\delta^2} \right).$$

Continue the proof by applying concentration, and the bound for information-gain

$$\sqrt{(\widehat{\mu}_t - \mu^\star)^\top \Sigma_t (\widehat{\mu}_t - \mu^\star)} = \|(\Sigma_t)^{1/2}(\widehat{\mu}_t - \mu^\star)\|$$

$$\leq \left\|\lambda \Sigma_t^{-1/2} \mu^\star\right\| + \left\|\Sigma_t^{-1/2} \sum_{\tau=0}^{t-1} \eta_\tau x_\tau\right\|$$

$$\leq \sqrt{\lambda}\|\mu^\star\| + \sqrt{2\sigma^2 \log\left(\det(\Sigma_t)\det(\Sigma^0)^{-1}/\delta_t\right)}.$$

$$\delta_t = (3/\pi^2)/t^2$$

$$1 - \Pr(\forall t,\, \mu^\star \in \textsc{Ball}_t) = \Pr(\exists t,\, \mu^\star \notin \textsc{Ball}_t) \leq \sum_{t=1}^{\infty} \Pr(\mu^\star \notin \textsc{Ball}_t) < \sum_{t=1}^{\infty} (1/t^2)(3/\pi^2) = 1/2.$$

Final remarks on Linear Bandits

- The regret of LinUCB is optimal up to $\tilde{O}(d\sqrt{T})$
- Strong assumption on realizability.
  - Agnostic linear bandits?
- Contextual version: a finite list of available actions are given at each t.

Exploration in Reinforcement Learning

- Why is it challenging?
  - The reward depends on both s, a
  - Unlike the generative model setting, we cannot just choose any s to explore.
  - The data needs to be actively collected

- We will study
  - Tabular MDP
  - Linear MDPs
  - Both in the finite horizon episodic setting.

Recap: Finite horizon MDPs

- Parameterization / Setup

$$M = (\mathcal{S}, \mathcal{A}, \{P\}_h, \{r\}_h, H, \mu)$$

- Additional notations
  - Q functions
  - V functions
  - Policies

Problem setup: online learning of Finite horizon MDPs

- Agent decides on a policy
- Collect a trajectory
- Agent updates the policy.
- Regret definition

Recap: The need for strategic exploration

UCB-VI: model-based learning by optimistic value Iterations

- Construct estimates of the transition kernels
- Design exploration bonuses
  - Idea: based on the uncertainty in the transition kernel estimates
- Update the policy by optimistic value iteration

How do we estimate the model parameters (P and r)?

- Simple plug-in estimator

- What happens if we observe no state-action pairs?

What does value iteration does in finite horizion?

$$\widehat{V}_H^k(s) = 0, \forall s,$$

$$\widehat{Q}_h^k(s,a) = \min\left\{r_h(s,a) + b_h^k(s,a) + \widehat{P}_h^k(\cdot|s,a)\cdot \widehat{V}_{h+1}^k,\ H\right\},$$

$$\widehat{V}_h^k(s) = \max_a \widehat{Q}_h^k(s,a), \pi_h^k(s) = \mathrm{argmax}_a\, \widehat{Q}_h^k(s,a), \forall h, s, a.$$

- Remark:
  - It converges in H steps
  - It produces a non-stationary policy indexed by h

How do we design exploration bonuses?

$$b_h^k(s,a) = H\sqrt{\frac{L}{N_h^k(s,a)}} \quad \text{where} \quad L := \ln(SAHK/\delta)$$

- Intuitively, this encourages exploring new state-action pairs.
- Idea: propagate errors from the estimated transitions over to the rewards.

The regret of UCB-VI

- Theorem (AJKS Thm 6.1):

$$Regret := \mathbb{E}\left[\sum_{k=0}^{K-1}\left(V^{\star} - V^{\pi^k}\right)\right] \leq 2H^2 S\sqrt{AK \cdot \ln(SAH^2K^2)} = \widetilde{O}\left(H^2 S\sqrt{AK}\right)$$

- This is not optimal in H, S, but a simple analysis to start.
- We will talk about the proof next Monday.