CMPT 419/983: Theoretical Foundations of Reinforcement Learning

Lecture 1

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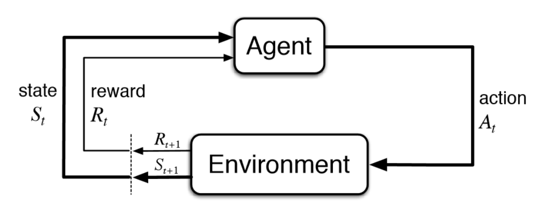
Introduction

- Supervised machine learning involves learning from a fixed, static dataset.
- Once a dataset is collected, supervised learning does not typically reason about how the data was acquired nor does it involve further interactions with the world.
- Applications in computational advertising, robotics, clinical trials involve collecting data in an online fashion, and reasoning about the decisions used to gather it.
- **Sequential decision-making** under uncertainty focuses on problems that involve interacting with the world, collecting data and reasoning about it, all with incomplete information about the world.

Introduction



- A typical problem in sequential decision-making involves an *agent* (e.g: marketer, robot, investor) sequentially interacting with the *environment* (e.g: online advertising platform, Mars terrain, stock market).
- An interaction involves the agent choosing an *action* and receiving feedback.
- For example, the feedback can be in the form of a *reward*) designed to measure the agent's performance in achieving its goal.
- One possible objective: Find a sequence of actions (referred to as a *policy*) that maximizes the *cumulative reward* across the sequence of interactions.

Motivating Applications

- Games. E.g: Go and Atari by DeepMind.
- Conversational agents. Eg: ChatGPT by OpenAI.
- Chip design by Google AI
- Cooling the interior of large commercial buildings by DeepMind
- Recommendation system by Microsoft
- Healthcare and Clinical Trials by Durand et al.
- Autonomous Navigation of Stratospheric Balloons by Google AI.
- For more applications, refer to Glen Berseth's and Csaba Szepesvari's lists.

This Course

Motivation

- Typical algorithms used in practice are often (a) brittle (their performance is sensitive to hyper-parameters) (b) inefficient (require a large number of interactions to learn to make good decisions) and (c) do not have theoretical guarantees on their performance and can fail on simple problems.
- Numerous fundamental theoretical questions remain unanswered and there is a large discrepancy between the theory and practice.

Objective:

- Understand the foundational concepts in bandits and reinforcement learning (RL) from a theoretical perspective.
- Use this knowledge to inform the design of theoretically-principled, statistically and computationally efficient algorithms.

Course Logistics

Topics:

- **Bandits**: Multi-armed/Contextual Bandit framework, Algorithms for regret minimization
- **Markov Decision Processes**: Structural properties, (Approximate) Value/Policy Iteration, Linear Programming, Temporal Difference Learning, Policy Gradients
- **Online & Batch RL**: Q Learning, LSVI-UCB, Learning with access to a simulator

What we won't cover: Continuous state-action spaces, Constrained MDPs, Multi-objective RL

- **Instructor**: Sharan Vaswani. [`sharan_vaswani@sfu.ca`]
- **Teaching Assistant**: Michael Lu. [`michael_lu_3@sfu.ca`]
- **Course Webpage**: `https://vaswanis.github.io/419_983-F23.html`
- **Piazza**: `https://piazza.com/sfu.ca/fall2023/cmpt419983/home`
- **Prerequisites**: Probability, Linear Algebra, Calculus, Undergraduate Machine Learning

Course Logistics – Grading

Assignments $[4 \times 12\% = 48\%]$

- Assignments to be submitted online (via Coursys), typed up in Latex with accompanying code submitted as a zip file.
- Each assignment will be due in 3 weeks (at 11.59 pm PST).

Final Project [50%]

- Aim is to give you a taste of research in RL Theory.
- Projects to be done in groups of 3-4. Will maintain a list of possible topics. Can choose from the list or propose your own topic. (more details will be on Piazza)
- Project Proposal [10%] – Discussion (before 20 October) + Report (due 20 October)
- Project Milestone [5%] – Update (before 20 November)
- Project Presentation [10%] – (*tentatively* 1, 4 December)
- Project Report [25%] (15 December)

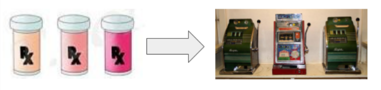
Participation [2%] In class (during lectures, project presentations), on Piazza

Stochastic Multi-armed Bandits

Motivating Application: Clinical Trials

- Do not have complete information about the effectiveness or side-effects of the drugs.
- **Aim**: Maximize the number of patients healed.

- Each drug choice is mapped to an *arm* and the drug's effectiveness is mapped to the arm's *mean reward*.
- Administering a drug is an *action* that is equivalent to *pulling* the corresponding arm.
- Each time an arm is pulled, we get a *noisy* reward that models a patients reaction to the drug.
- The trial goes on for T *rounds*.



  - Other motivating applications: Recommendation systems, computational advertising.

Problem Formulation

Input: K arms (possible actions) and their corresponding unknown reward distributions $\{\nu_a\}_{i=1}^{K}$. Define $\mu_a := \mathbb{E}_{r\sim\nu_a}[r]$ as the expected reward obtained by choosing action a.

Algorithm Generic Bandit Framework (K arms, T rounds)

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for $t = 1 \to T$ **do**
- **SELECT**: Use a bandit algorithm to decide which arm(s) to pull.
- **OBSERVE**: Pull the selected arm $a_t \in [K]$ and observe reward $R_t \sim \nu_{a_t}$.
- **UPDATE**: Update the estimated reward for arm a_t.

end for

Bandit Feedback: Can only observe the noisy reward R_t from the pulled arm a_t.

Objective: Maximize $\mathbb{E}[\sum_{t=1}^{T} R_t]$ where the expectation is over both the randomness of the algorithm (if any) and the distribution of rewards.

Bandit problems are a special case of RL problems, and capture a lot of the intricacy.

Problem Formulation

- Define $a^* := \arg\max_{a \in [K]} \mu_a$ as the *best or optimal arm* in hindsight, and $\mu_* := \max_a \mu_a$.
- Maximizing cumulative rewards $\implies$ Select a^* as much as possible $\implies$ Minimize the *cumulative regret*.
- **Cumulative Regret**: $\text{Regret}(T) := \sum_{t=1}^{T} [\mu^* - \mathbb{E}[R_t]] = T\mu^* - \sum_{t=1}^{T} \mathbb{E}[R_t]$.
- Since the optimal arm is unknown, the algorithm needs to *explore* to narrow down on the best arm. If we can identify the best arm, the algorithm should *exploit* and always choose it.
- Need to find a *policy* that trades off exploration and exploitation to minimize $\text{Regret}(T)$.
- Ideally, want $\text{Regret}(T) = o(T)$ i.e. the regret grows sub-linearly with T, meaning that $\lim_{T \to \infty} \frac{\text{Regret}(T)}{T} = 0$.

Regret Decomposition

Claim: If $\Delta_a := \mu^* - \mu_a$ and $N_a(T)$ is the number of times arm a was chosen *until* round T, then,

$$\text{Regret}(T) = \sum_{a=1}^{K} \Delta_a \, \mathbb{E}[N_a(T)] \, .$$

Proof:

$$\text{Regret}(T) = \mu^* T - \sum_{t=1}^{T} \mathbb{E}[R_t] = \mu^* T - \sum_{t=1}^{T} \mathbb{E}[\mu_{a_t}] = \sum_{t=1}^{T} \mathbb{E}\left[\mu^* - \mu_{a_t}\right]$$

(Taking the expectation w.r.t to the reward distribution)

$$= \sum_{a=1}^{K} [\mu^* - \mu_a] \, \mathbb{E}\left[\sum_{t=1}^{T} \mathcal{I}\left\{a_t = a\right\}\right] = \sum_{a=1}^{K} [\mu^* - \mu_a] \, \mathbb{E}[N_a(T)]$$

$$\implies \text{Regret}(T) = \sum_{a=1}^{K} \Delta_a \, \mathbb{E}[N_a(T)] \, .$$

- Hence, to minimize the regret, an algorithm should (i) not pull arms with $\Delta_a > 0$ too often (**exploit**) which requires (ii) estimating the values of Δ_a to sufficient accuracy (**explore**).

Naive Strategy

Algorithm Naive Strategy

for $t = 1 \to K$ **do**
  Select arm $a_t = t$ and observe reward R_t
end for
Calculate empirical mean reward for arm $a \in [K]$ as $\hat{\mu}_a(K) := \frac{\sum_{t=1}^{K} R_t \, \mathcal{I}\{a_t = a\}}{N_a(K)}$
for $t = K + 1 \to T$ **do**
  Pull arm $\hat{a} := \arg\max_{a \in [K]} \hat{\mu}_a(K)$ *(choose lower-indexed arm if there is a tie)*.
end for

Q: Will this naive strategy result in sublinear regret?

Explore-Then-Commit (ETC)

Algorithm Explore-Then-Commit

Input: $m \in \left\{1, \ldots, \lfloor \frac{T}{K} \rfloor\right\}$.
for $t = 1 \to m\,K$ **do**
  Select arm $a_t = t \bmod K + 1$ and observe reward R_t **(Explore)**
end for
Calculate empirical mean reward for arm $a \in [K]$ as $\hat{\mu}_a(mK) := \frac{\sum_{t=1}^{mK} R_t\, \mathcal{I}\{a_t = a\}}{N_a(mK)}$
for $t = mK + 1 \to T$ **do**
  Pull arm $\hat{a} := \arg\max_{a \in [K]} \hat{\mu}_a(mK)$ **(Commit)**
end for

Q: Will ETC result in sublinear regret?

Yes! under suitable distributional assumptions on the rewards.

In particular, if $r \sim \nu_a$, we will assume that $r - \mu_a$ are sub-Gaussian random variables, then we will prove that ETC results in sub-liner regret. For this, we need to first recap some concentration (tail) inequalities from undergraduate probability.

Digression – Concentration inequalities

Concentration inequalities bound the probability that the r.v. takes a value much different from its mean.

Example: Consider a r.v. X that can take on only non-negative values and $\mathbb{E}[X] = 99.99$. Show that $\Pr[X \geq 300] \leq \frac{1}{3}$.

$$\begin{aligned} \textit{Proof}: \mathbb{E}[X] &= \sum_{x \in \text{Range}(X)} x \Pr[X = x] = \sum_{x | x \geq 300} x \Pr[X = x] + \sum_{x | 0 \leq x < 300} x \Pr[X = x] \\ &\geq \sum_{x | x \geq 300} (300) \Pr[X = x] + \sum_{x | 0 \leq x < 300} x \Pr[X = x] \\ &= (300) \Pr[X \geq 300] + \sum_{x | 0 \leq x < 300} x \Pr[X = x] \end{aligned}$$

If $\Pr[X \geq 300] > \frac{1}{3}$, then, $\mathbb{E}[X] > (300)\,\frac{1}{3} + \sum_{x | 0 \leq x < 300} x \Pr[X = x] > 100$ (since the second term is always non-negative). Hence, if $\Pr[X \geq 300] > \frac{1}{3}$, $\mathbb{E}[X] > 100$ which is a contradiction since $\mathbb{E}[X] = 99.99$.

Digression – Markov's Theorem

Markov's theorem formalizes the intuition on the previous slide, and can be stated as follows.

Markov's Theorem: If X is a non-negative random variable, then for all $x > 0$,

$$\Pr[X \geq x] \leq \frac{\mathbb{E}[X]}{x}.$$

Proof: Define $\mathcal{I}\{X \geq x\}$ to be the indicator r.v. for the event $[X \geq x]$. Then for all values of X, $x\mathcal{I}\{X \geq x\} \leq X$.

$$\mathbb{E}[x\mathcal{I}\{X \geq x\}] \leq \mathbb{E}[X] \implies x\,\mathbb{E}[\mathcal{I}\{X \geq x\}] \leq \mathbb{E}[X] \implies x\Pr[X \geq x] \leq \mathbb{E}[X]$$

$$\implies \Pr[X \geq x] \leq \frac{\mathbb{E}[X]}{x}. \quad \square$$

Since the above theorem holds for all $x > 0$, we can set $x = c\mathbb{E}[X]$ for $c \geq 1$. In this case, $\Pr[X \geq c\mathbb{E}[X]] \leq \frac{1}{c}$. Hence, the probability that X is "far" from the mean in terms of the multiplicative factor c is upper-bounded by $\frac{1}{c}$.

Digression – Sub-Gaussian random variables

If a centered r.v. X (meaning that $\mathbb{E}[X] = 0$) is σ sub-Gaussian, then for all $\lambda \in \mathbb{R}$,

$$\mathbb{E}\left[\exp(\lambda X)\right] \leq \exp\left(\frac{\lambda^2 \sigma^2}{2}\right) .$$

Example 1: If $X \sim N(0, 1)$, then its moment generating function $\mathbb{E}\left[\exp(\lambda X)\right] = \exp\left(\frac{\lambda^2 \sigma^2}{2}\right)$, meaning that Gaussian r.v. are sub-Gaussian.

Example 2: If $X \in [a, b]$ and $\mathbb{E}[X] = 0$, then X is $(b - a)$ sub-Gaussian.

Properties: If X is centered and σ sub-Gaussian, then,

(a) $\mathbb{E}[X] = 0$, $\mathrm{Var}[X] \leq \sigma^2$
(b) For a constant $c \in \mathbb{R}$, cX is $|c|\,\sigma$ sub-Gaussian.
(c) If $\{X_i\}_{i=1}^n$ are independent and σ_i sub-Gaussian respectively, then, $\sum_{i=1}^n X_i$ is $\sqrt{\sum_{i=1}^n \sigma_i^2}$ sub-Gaussian.

Need to prove some of these properties in Assignment 1!

Digression – Concentration inequalities for sub-Gaussian r.v's

Claim: If X is σ sub-Gaussian, then for any $\epsilon \geq 0$, $\Pr[X \geq \epsilon] \leq \exp\left(-\frac{\epsilon^2}{2\sigma^2}\right)$.

Proof: For some constant $c > 0$ to be tuned later,

$$\begin{aligned}
\Pr[X \geq \epsilon] &= \Pr[cX \geq c\epsilon] = \Pr[\exp(c\,X) \geq \exp(c\,\epsilon)] \\
&\leq \mathbb{E}[\exp(c\,X)]\,\exp(-c\,\epsilon) && \text{(Markov's inequality)} \\
&\leq \exp\left(\frac{c^2\sigma^2}{2} - c\,\epsilon\right) && \text{(Def. of sub-Gaussian r.v's)} \\
&= \exp\left(-\frac{\epsilon^2}{2\sigma^2}\right) \quad \square && \text{(Setting } c = \epsilon/\sigma^2\text{)}
\end{aligned}$$

Similarly, $\Pr[X \leq -\epsilon] \leq \exp\left(-\frac{\epsilon^2}{2\sigma^2}\right)$. By the union bound, $\Pr[|X| \geq \epsilon] \leq 2\,\exp\left(-\frac{\epsilon^2}{2\sigma^2}\right)$.

Setting $\delta = 2\,\exp\left(-\frac{\epsilon^2}{2\sigma^2}\right) \implies \epsilon = \sqrt{2\sigma^2\,\log(2/\delta)}$. Hence, w.p. $1-\delta$, X will take on values in the range $\left[-\sqrt{2\sigma^2\,\log(2/\delta)}, +\sqrt{2\sigma^2\,\log(2/\delta)}\right]$.

Claim: Consider n i.i.d r.v's X_i such that $\mathbb{E}[X_i] = \mu$. If $X_i - \mu$ are σ sub-Gaussian and $\hat{\mu} := \frac{1}{n}\sum_{i=1}^{n} X_i$ is the empirical mean, then, $\Pr[|\hat{\mu} - \mu| \geq \epsilon] \leq \exp\left(-\frac{n\epsilon^2}{2\sigma^2}\right)$.

Proof: Using property (c) of σ sub-Gaussian r.v's, $\sum_{i=1}^{n}[X_i - \mu]$ is $\sqrt{n\sigma^2}$ sub-Gaussian.
Using property (b) of σ sub-Gaussian r.v's, $\frac{\sum_{i=1}^{n}[X_i - \mu]}{n}$ is $\frac{\sigma}{\sqrt{n}}$ sub-Gaussian.
$\implies \hat{\mu} - \mu$ is $\frac{\sigma}{\sqrt{n}}$ sub-Gaussian. Using the concentration result from the previous slide,
$\Pr[|\hat{\mu} - \mu| \geq \epsilon] \leq \exp\left(-\frac{n\epsilon^2}{2\sigma^2}\right)$. $\square$

Hence, as we collect more data, the empirical mean concentrates around the true mean at an exponential rate.

Back to Explore-Then-Commit (ETC)

Algorithm Explore-Then-Commit

Input: $m \in \left\{1, \dots, \lfloor \frac{T}{K} \rfloor \right\}$.
for $t = 1 \to m\,K$ **do**
  Select arm $a_t = (t \bmod K) + 1$ and observe reward R_t **(Explore)**
end for
Calculate empirical mean reward for arm $a \in [K]$ as $\hat{\mu}_a(mK) := \frac{\sum_{t=1}^{mK} R_t \, \mathcal{I}\{a_t = a\}}{N_a(mK)}$
for $t = mK + 1 \to T$ **do**
  Pull arm $\hat{a} := \arg\max_{a \in [K]} \hat{\mu}_a(mK)$ **(Commit)**
end for

Distributional Assumption: The *noise* $\eta_t := R_t - \mu_{a_t}$ is 1 sub-Gaussian. $\implies$ after pulling each arm m times in the **exploration** phase, for all $a \in [K]$, $|\hat{\mu}_a - \mu_a|$ is $\frac{\sigma}{\sqrt{m}}$ sub-Gaussian and hence, $\Pr[|\hat{\mu}_a - \mu_a| \geq \epsilon] \leq 2 \exp\left(-\frac{m\epsilon^2}{2\sigma^2}\right)$.

Intuitively, the **exploration** phase estimates the gap Δ_a for each arm upto a certain error. After this initial estimation, the algorithm **commits** to the *best empirical arm*.

Explore-Then-Commit – Regret Analysis

Claim: For any $m \in \{1, \ldots, \lfloor T/K \rfloor\}$,

$$\text{Regret}(\text{ETC}, T) \leq m \sum_{a=1}^{K} \Delta_a + (T - m\,K) \sum_{a=1}^{K} \Delta_a \exp\left(-\frac{m\,\Delta_a^2}{4}\right)$$

Proof: Without loss of generality, assume that arm 1 is the best arm. Using the regret decomposition, we know that $\text{Regret}(\text{ETC}, T) = \sum_a \Delta_a \, \mathbb{E}[N_a(T)]$. For each arm $a \in [K]$, $\mathbb{E}[N_a(T)] = m + (T - m\,K)\ \Pr[\text{algorithm commits to arm } a]$.

$$\Pr[\text{algorithm commits to arm } a] = \Pr[\hat{\mu}_a > \max_{j \neq a} \hat{\mu}_j] \leq \Pr[\hat{\mu}_a > \hat{\mu}_1]$$

(Since $\{\hat{\mu}_a > \max_{j \neq a} \hat{\mu}_j\}$ is a subset of $\{\hat{\mu}_a > \hat{\mu}_1\}$)

$$= \Pr[\hat{\mu}_a - \mu_a > \hat{\mu}_1 - \mu_1 + [\mu_1 - \mu_a]] = \Pr[\underbrace{[\hat{\mu}_a - \mu_a]}_{X_a} - \underbrace{[\hat{\mu}_1 - \mu_1]}_{X_1} \geq \Delta_a]$$

$$= \Pr[X_a - X_1 \geq \Delta_a]$$

Explore-Then-Commit – Regret Analysis

Recall that $\text{Regret}(\text{ETC}, T) = \sum_a \Delta_a \left[m + (T - m\,K) \Pr[\text{algorithm commits to arm } a]\right]$ and $\Pr[\text{algorithm commits to arm } a] \leq \Pr[X_a - X_1 \geq \Delta_a]$ where $X_a = \hat{\mu}_a - \mu_a$. Because of our assumption, both X_a and X_1 are $\frac{1}{\sqrt{m}}$ sub-Gaussian. Using property (c) of sub-Gaussian r.v's, $X_a - X_1$ is $\frac{\sqrt{2}}{\sqrt{m}}$ sub-Gaussian. Using the concentration result for sub-Gaussian r.v's,

$$\Pr[X_a - X_1 \geq \Delta_a] \leq \exp\left(-\frac{m\,\Delta_a^2}{4}\right)$$

Putting everything together,

$$\text{Regret}(\text{ETC}, T) \leq \sum_a \Delta_a \left[m + (T - m\,K)\exp\left(-\frac{m\,\Delta_a^2}{4}\right)\right]$$

$$\implies \text{Regret}(\text{ETC}, T) \leq m \sum_{a=1}^{K} \Delta_a + (T - m\,K) \sum_{a=1}^{K} \Delta_a \exp\left(-\frac{m\,\Delta_a^2}{4}\right) \quad \square$$

Explore-Then-Commit – Regret Analysis

Recall that $\text{Regret}(\text{ETC}, T) \leq m \sum_{a=1}^{K} \Delta_a + (T - m\,K) \sum_{a=1}^{K} \Delta_a \exp\left(-\frac{m\,\Delta_a^2}{4}\right)$.

In order to gain some intuition about how to set m, consider $K = 2$ with $\Delta := \mu_1 - \mu_2$.

$$\text{Regret}(\text{ETC}, T) \leq m\Delta + (T - 2m)\Delta \exp\left(-\frac{m\,\Delta^2}{4}\right) < m\Delta + T\Delta \exp\left(-\frac{m\,\Delta^2}{4}\right)$$

Optimizing the RHS w.r.t m, we get $m = \frac{4}{\Delta^2} \log\left(\frac{\Delta^2 T}{4}\right)$. Since m is an integer ≥ 1, we should set $m = \max\left\{1, \lceil \frac{4}{\Delta^2} \log\left(\frac{\Delta^2 T}{4}\right) \rceil\right\}$. Plugging this value back,

$$\implies \text{Regret}(\text{ETC}, T) \leq \Delta + \frac{4}{\Delta}\left[1 + \log_{+}\left(\frac{\Delta^2 T}{4}\right)\right] \qquad (\log_{+}(x) := \max\{0, \log(x)\})$$

Hence, ETC with $m = O(1/\Delta^2)$ achieves $O\left(\frac{\log(T)}{\Delta}\right)$ *instance or gap-dependent* regret.

Q: What is the problem with this bound?

Explore-Then-Commit – Regret Analysis

To overcome the previous problem, one can bound the *worst-case problem-independent regret*.

Claim: For $\Delta \leq 1$, ETC results in an $O(1+\sqrt{T})$ worst-case bound on the regret.

Proof: In the worst-case, we pull the sub-optimal arm in every round. Hence, the regret for any algorithm is upper-bounded by $T\Delta$. Putting this together with the bound on the previous slide,

$$\text{Regret}(\text{ETC}, T) \leq \min\left\{T\Delta, \Delta + \frac{4}{\Delta}\left[1 + \log_+\left(\frac{\Delta^2 T}{4}\right)\right]\right\}$$

If $\Delta < \frac{1}{\sqrt{T}}$, $\text{Regret}(\text{ETC}, T) \leq \sqrt{T}$. On the other hand, if $\Delta \geq \frac{1}{\sqrt{T}}$,

$$\text{Regret}(\text{ETC}, T) \leq \Delta + 4\sqrt{T} + \left[\frac{4}{\Delta}\log_+\left(\frac{\Delta^2 T}{4}\right)\right] = \Delta + 4\sqrt{T} + 4\max_{z>0}\frac{\log_+(Tz^2/4)}{z}$$

$$\text{Regret}(\text{ETC}, T) \leq \Delta + 4\sqrt{T} + \frac{4\sqrt{T}}{e} \leq 1 + \sqrt{T}\left(4 + \frac{4}{e}\right) \qquad \text{(Since } \Delta \leq 1\text{)}$$

- In general, for K arms, it can be shown that ETC results in $O(\sqrt{KT})$ worst-case regret.

Explore-Then-Commit – Regret Analysis

We have seen that ETC with $m = O(1/\Delta^2)$ achieves an $O(\Delta + \sqrt{T})$ regret for any instance.

Q: What is the problem with the ETC algorithm?

Claim: For $\Delta \leq 1$, there exists $C > 0$ s.t. ETC with $m = T^{2/3}$ results in $(1 + C)\, T^{2/3}$ regret.

Proof: Need to prove this in Assignment 1!

Hint: Starting from the expression, $\text{Regret}(\text{ETC}, T) \leq m\Delta + T\Delta \exp\left(-\frac{m\Delta^2}{4}\right)$, upper-bound the second term independent of Δ and then choose m.

ϵ-greedy Algorithm

Algorithm ϵ-greedy

Input: $\{\epsilon_t\}_{t=1}^{T}$
for $t = 1 \to K$ **do**
  Select arm $a_t = t$ and observe R_t
end for
Calculate empirical mean reward for arm $a \in [K]$ as $\hat{\mu}_a(K) := \frac{\sum_{t=1}^{K} R_t \, \mathcal{I}\{a_t = a\}}{N_a(K)}$
for $t = K + 1 \to T$ **do**
  Select arm $\begin{cases} a_t = \arg\max_{a \in [K]} \hat{\mu}_a(t-1) \; w.p \; 1 - \epsilon_t \\ a_t \sim \mathcal{U}\{1, 2, \ldots, K\} \; w.p \; \epsilon_t \end{cases}$
  Observe reward R_t and update for $a \in [K]$:
$$N_a(t) = N_a(t-1) + \mathcal{I}\{a_t = a\} \quad ; \quad \hat{\mu}_a(t) = \frac{N_a(t-1)\,\hat{\mu}_a(t-1) + R_t \, \mathcal{I}\{a_t = a\}}{N_a(t)}$$
end for

- ϵ-greedy with a fixed $\epsilon_t = \epsilon$ can result in linear regret.
- For $K = 2$, ϵ-greedy with $\epsilon_t = O\left(\frac{1}{\Delta^2 T}\right)$ incurs $O\left(\frac{\log(T)}{\Delta^2}\right)$ regret.

Upper Confidence Bound (UCB) Algorithm

- Based on the principle of *optimism in the face of uncertainty*.

Algorithm Upper Confidence Bound

1: **Input**: δ
2: For each arm $a \in [K]$, initialize $U_a(0, \delta) := \infty$.
3: **for** $t = 1 \to T$ **do**
4: Select arm $a_t = \arg\max_{a \in [K]} U_a(t-1, \delta)$ *(Choose the lower-indexed arm in case of a tie)*
5: Observe reward R_t and update for $a \in [K]$:

$$N_a(t) = N_a(t-1) + \mathcal{I}\{a_t = a\} \quad ; \quad \hat{\mu}_a(t) = \frac{N_a(t-1)\,\hat{\mu}_a(t-1) + R_t\,\mathcal{I}\{a_t = a\}}{N_a(t)}$$

$$U_a(t, \delta) = \hat{\mu}_a(t) + \sqrt{\frac{2\log(1/\delta)}{N_a(t)}}$$

6: **end for**

- Intuitively, UCB pulls a "promising" arm (with higher empirical mean $\hat{\mu}_a$) or one that has not been explored enough (with lower $N_a(t)$).

UCB – Regret Analysis

Claim: UCB with $\delta = \frac{1}{T^2}$ achieves the following problem-dependent bound on the regret,

$$\text{Regret}(\text{UCB}, T) \leq 2\sum_{a=1}^{K} \Delta_a + \sum_{a \in [K] \mid \Delta_a > 0} \frac{16 \log(T)}{\Delta_a}$$

Proof: Without loss of generality, assume that arm 1 is the best arm. Using the regret decomposition, we know that $\text{Regret}(\text{UCB}, T) = \sum_a \Delta_a \mathbb{E}[N_a(T)]$. Define a threshold τ_a and $\hat{\mu}_{a,\tau_a}$ as the mean for arm a after pulling it for the first τ_a times. Define a "good" event G_a for each $a \neq 1$.

$$G_a = \left\{\mu_1 < \min_{t \in [T]} U_1(t, \delta)\right\} \cap \left\{\hat{\mu}_{a,\tau_a} + \sqrt{\frac{2\log(1/\delta)}{\tau_a}} < \mu_1\right\}$$

Consider two cases when bounding $\mathbb{E}[N_a(T)]$. Using the law of total expectation,

$$\begin{aligned}
\mathbb{E}[N_a(T)] &= \mathbb{E}[N_a(T) | G_a] \Pr[G_a] + \mathbb{E}[N_a(T) | G_a^c] \Pr[G_a^c] \\
&\leq \underbrace{\mathbb{E}[N_a(T) | G_a]}_{\text{Term (i)}} + T \underbrace{\Pr[G_a^c]}_{\text{Term (ii)}} \qquad (N_a(T) \leq T \text{ for all } a,\ \Pr[G_a] \leq 1)
\end{aligned}$$

UCB – Regret Analysis

Recall that $G_a = \{\mu_1 < \min_{t\in[T]} U_1(t,\delta)\} \cap \left\{\hat{\mu}_{a,\tau_a} + \sqrt{\frac{2\log(1/\delta)}{\tau_a}} < \mu_1\right\}$. We will show (by contradiction) that Term (i) $= \mathbb{E}[N_a(T)|G_a] \le \tau_a$.

Suppose $\mathbb{E}[N_a(T)|G_a] > \tau_a$, then there is a round t s.t. $N_a(t-1) = \tau_a$, $a_t = a$. Since $a_t = \arg\max_a U_a(t-1,\delta)$, it follows that $U_a(t-1,\delta) > U_1(t-1,\delta)$. However, we know that,

$$U_a(t-1,\delta) = \hat{\mu}_a(t-1) + \sqrt{\frac{2\log(1/\delta)}{N_a(t-1)}} = \hat{\mu}_a(t-1) + \sqrt{\frac{2\log(1/\delta)}{\tau_a}}$$

(By assumption, $N_a(t-1) = \tau_a$)

$$= \hat{\mu}_{a,\tau_a} + \sqrt{\frac{2\log(1/\delta)}{\tau_a}} \qquad \text{(Since arm } a \text{ has been pulled } \tau_a \text{ times)}$$

$$\le \mu_1 < U_1(t-1,\delta)\,, \qquad \text{(Since we are conditioning on } G_a\text{)}$$

which is a contradiction. Hence, $\mathbb{E}[N_a(T)|G_a] \le \tau_a$.

UCB – Regret Analysis

$$\text{Bounding Term (ii)} = \Pr[G_a^c] \le \Pr\left[\mu_1 \ge \min_{t\in[T]} U_1(t,\delta)\right] + \Pr\left[\hat{\mu}_{a,\tau_a} + \sqrt{\frac{2\log(1/\delta)}{\tau_a}} \ge \mu_1\right].$$

$$\begin{aligned}
\left\{\mu_1 \ge \min_{t\in[T]} U_1(t,\delta)\right\} &= \left\{\mu_1 \ge \min_{t\in[T]}\left\{\hat{\mu}_1(t) + \sqrt{\frac{2\log(1/\delta)}{N_1(t)}}\right\}\right\} \\
&= \left\{\mu_1 \ge \min_{s\in[T]}\left\{\hat{\mu}_{1,s} + \sqrt{\frac{2\log(1/\delta)}{s}}\right\}\right\} \\
&= \bigcup_{s=1}^{T}\left\{\mu_1 \ge \hat{\mu}_{1,s} + \sqrt{\frac{2\log(1/\delta)}{s}}\right\} \\
\implies \Pr\left[\mu_1 \ge \min_{t\in[T]} U_1(t,\delta)\right] &\le \sum_{s=1}^{T} \Pr\left[\mu_1 \ge \hat{\mu}_{1,s} + \sqrt{\frac{2\log(1/\delta)}{s}}\right] \qquad \text{(Union Bound)} \\
&\le \sum_{s=1}^{T} \delta = \delta T \qquad \text{(Using concentration for sub-Gaussian r.v's)}
\end{aligned}$$

UCB – Regret Analysis

Recall that Term (ii) $= \Pr[G_a^c] \le \delta T + \Pr\left[\hat{\mu}_{a,\tau_a} + \sqrt{\frac{2\log(1/\delta)}{\tau_a}} \ge \mu_1\right]$. Assume that τ_a is chosen such that $\Delta_a - \frac{2\log(1/\delta)}{\tau_a} \ge \frac{\Delta_a}{2}$.

$$\Pr\left[\hat{\mu}_{a,\tau_a} + \sqrt{\frac{2\log(1/\delta)}{\tau_a}} \ge \mu_1\right] = \Pr\left[\hat{\mu}_{a,\tau_a} - \mu_a + \sqrt{\frac{2\log(1/\delta)}{\tau_a}} \ge \Delta_a\right] \quad \le \Pr\left[\hat{\mu}_{a,\tau_a} - \mu_a \ge \frac{\Delta_a}{2}\right]$$

$$\le \exp\left(-\frac{\tau_a \Delta_a^2}{8}\right)$$

(Using concentration for sub-Gaussian r.v's)

Putting everything together,

$$\implies \Pr[G_a^c] \le \delta T + \exp\left(-\frac{\tau_a \Delta_a^2}{8}\right)$$

$$\implies \mathbb{E}[N_a(T)] \le \tau_a + T\left[\delta T + \exp\left(-\frac{\tau_a \Delta_a^2}{8}\right)\right]$$

UCB – Regret Analysis

Recall that $\mathbb{E}[N_a(T)] \le \tau_a + T\left[\delta T + \exp\left(-\frac{\tau_a \Delta_a^2}{8}\right)\right]$.

$$\begin{aligned}
\mathbb{E}[N_a(T)] &\le \frac{8\log(1/\delta)}{\Delta_a^2} + T\,[\delta T + \delta] && \left(\text{Setting } \tau_a = \tfrac{8\log(1/\delta)}{\Delta_a^2}\right)\\
&\le \frac{8\log(1/\delta)}{\Delta_a^2} + 2\delta T^2 \\
&= \frac{16\log(T)}{\Delta_a^2} + 2 && \left(\text{Setting } \delta = 1/T^2\right)
\end{aligned}$$

$$\implies \text{Regret}(\text{UCB}, T) = \sum_a \Delta_a\,\mathbb{E}[N_a(T)] = 2\sum_{a=1}^{K}\Delta_a + \sum_{a=2}^{K}\frac{16\log(T)}{\Delta_a} \quad \square$$

UCB – Regret Analysis

Claim: For $\Delta \leq 1$, UCB with $\delta = \frac{1}{T^2}$ achieves the following worst-case regret,

$$\text{Regret}(\text{UCB}, T) \leq 2K + 8\sqrt{K\ T\ \log(T)}$$

Proof: Define $C > 0$ to be a constant to be tuned later. From the regret decomposition result,

$$\begin{aligned}
\text{Regret}(\text{UCB}, T) &= \sum_{a=1}^{K} \Delta_a \, \mathbb{E}[N_a(T)] = \sum_{a \mid \Delta_a < C} \Delta_a \, \mathbb{E}[N_a(T)] + \sum_{a \mid \Delta_a \geq C} \Delta_a \, \mathbb{E}[N_a(T)] \\
&\leq CT + \sum_{a \mid \Delta_a \geq C} \Delta_a \, \mathbb{E}[N_a(T)] && \left(\text{Since } \textstyle\sum_{a=1}^{K} N_a(T) = T\right) \\
&\leq CT + \sum_{a \mid \Delta_a \geq C} \left[\frac{16 \log(T)}{\Delta_a} + 2\Delta_a\right] && \text{(From the previous slide)} \\
&\leq CT + \left[\frac{16K\ \log(T)}{C} + \sum_{a \mid \Delta_a \geq C} 2\Delta_a\right] && \left(\text{Setting } C = \sqrt{\tfrac{16K\ \log(T)}{T}}\right)
\end{aligned}$$

$$\implies \text{Regret}(\text{UCB}, T) \leq 8\sqrt{K\ T\ \log(T)} + 2K\Delta_a \leq 2K + 8\sqrt{K\ T\ \log(T)}$$

UCB vs ETC

- Similar to best-tuned ETC, UCB results in an $\tilde{O}(\sqrt{KT})$ problem-independent regret.
- Unlike best-tuned ETC, UCB does not need to know the gaps Δ to set algorithm parameters, but does require knowledge of the horizon T.

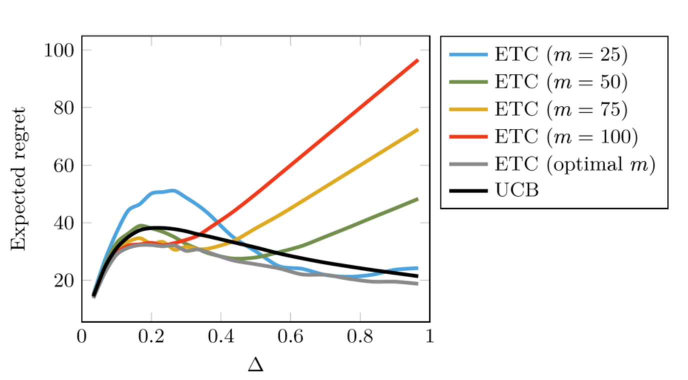

Figure 1: For $K = 2$, $T = 1000$, Gaussian rewards, comparing UCB and ETC(m) as a function of the gap Δ.

Improvements to UCB

- **Problem**: UCB requires knowledge of T and hence, the number of rounds needs to be fixed.
- *Sol*: Define UCB as $\hat{\mu}_a(t) + \sqrt{\frac{2\,\log(f(t))}{N_a(t)}}$ where $f(t) := 1 + t\log^2(t)$. No dependence on T, but results in the same $O(\sqrt{KT\log(T)})$ worst-case regret. (see [LS20, Chapter 8])
- **Lower-Bound**: For a fixed T and for every bandit algorithm, there exists a stochastic bandit problem with rewards in $[0, 1]$ such that $\text{Regret}(T) = \Omega(\sqrt{KT})$. (see [LS20, Chapter 15]).
- **Problem**: UCB is sub-optimal by a $\sqrt{\log(T)}$ factor compared to the lower-bound. Is it possible to develop an algorithm that does not incur this log factor?
- *Sol*: [Lat18, MG17] propose modifications of UCB that achieve $O(\sqrt{KT})$ regret.

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