Multi-Arm Bandits - II

Easwar Subramanian

TCS Innovation Labs, Hyderabad

Email : easwar.subramanian@tcs.com / cs5500.2020@iith.ac.in

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Overview

1. Introduction to Bandit Problem
2. Naive Approaches
3. Optimism in the Face of Uncertainty
4. Thompson Sampling

Introduction to Bandit Problem

Multi Arm Bandit

- **Learning Problem :** Which arm is the best ?
- **Decision Problem :** Which arm to pull next ?

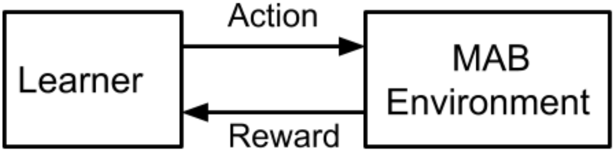
Bandit Problems – Motivations

- Managing exploration-exploitation trade-off
- Baby reinforcement learning
- Lots of appliations in online learning

Applications

- Music Recommeder System
- Clinical trials
- Dynamic Pricing
- Ad Placement
- A/B Testing
- Network Routing
- Game Tree Search

Multi Arm Bandit : Setting



- There are K arms to pull and there are N rounds
- The agent can pull any of the K arms in each round $t \in \{0, 1, \cdots, N\}$
- On pulling arm a, the agent gets a random reward r_a sampled from a distribution (independent of previous choices and rewards)
- Goal is to find an algorithm that maximizes the sum of rewards obtained by pulling arm (in expectation)

Multi Arm Bandit : Formulation

- A multi-arm bandit is defined as a tuple $< \mathcal{A}, \mathcal{R} >$
- $< \mathcal{A} >$ is the set of arms available
- $\mathcal{R}^a(r) = \mathbb{P}(r|a)$ is the unknown of distribution of rewards of arm a
- At each step t the agent selects an action $a_t \in \mathcal{A}$ and gets a reward $r_t \sim \mathcal{R}^{a_t}$
- The goal is to maximise cumulative reward $\sum_{t=1}^{N} r_t$

Regret Minimization

- The goal is to maximize cumulative reward $\sum_{t=1}^{t} r_t$
- Define the action value function $Q(a)$ to be the mean reward for action a i.e. $Q(a) = \mathbb{E}(r|a)$
- The optimal value V^* is
$$V^* = Q(a^*) = \max_{a \in \mathcal{A}} Q(a)$$
- The regret is the lost opportunity at one step
$$l_t = \mathbb{E}[V^* - r_t] = V^* - \mathbb{E}[r_t]$$
- Total regret is the total opportunity loss
$$L_N = \mathbb{E}\left[\sum_{t=1}^{N} (V^* - r_t)\right] = NV^* - \mathbb{E}\left[\sum_{t=1}^{N} r_t\right]$$
- Maximize cumulative reward $\equiv$ Minimize total regret

Regret Minimization : Alternative Formulation

- Let the **count** $N_t(a)$ be the number of times arm a is pulled upto time t $(N_t(a) \equiv \sum_{\tau=1}^{t} \mathbb{1}_{A_\tau = a})$
- Let Δ_a be the **gap** between optimal reward (from optimal action a^*) and reward of arm a

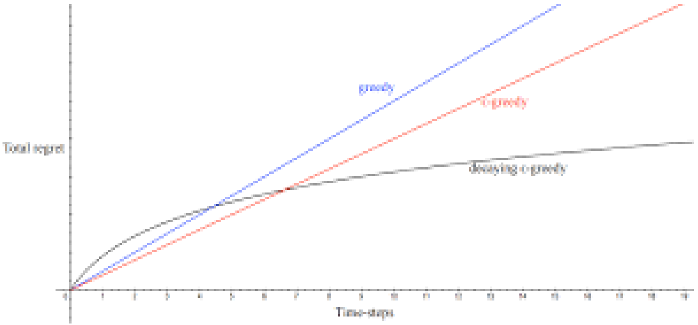
$$\Delta_a = V^* - Q(a)$$

- Regret is a function of gaps and counts given as

$$\begin{aligned} L_N &= \mathbb{E}\left[\sum_{t=1}^{N} (V^* - r_t)\right] = \mathbb{E}\left[\sum_{t=1}^{N} \Delta_{A_t}\right] \\ &= \mathbb{E}\left[\sum_{t=1}^{N} \sum_{a \in \mathcal{A}} \mathbb{1}_{A_t = a}\, \Delta_a\right] = \sum_{a \in \mathcal{A}} \Delta_a \, \mathbb{E}\left(N_n(a)\right) \end{aligned}$$

- A good algorithm ensures small counts for large gaps

Linear or Sub-Linear Regret



- Algorithms that explore forever have total linear regret
- Algorithms that never explore have total linear regret
- **Question** : Is it possible for develop algorithms have sub-linear regret ?

On Estimating Mean Rewards

- We consider algorithms that estimate $\hat{Q}_\tau(a) \approx Q(a)$
- The sample estimate $\hat{Q}(a)$ is estimated via Monte-Carlo simulations

$$\hat{Q}_t(a) = \frac{1}{N_t(a)} \sum_{\tau=1}^{N} r_t \mathbb{1}(A_t = a)$$

Naive Approaches

Greedy Algorithm

- At any time t, a greedy algorithm selects the action with highest $\hat{Q}_t(a)$, i.e.

$$a_t^* = \arg\max_{a \in \mathcal{A}} \hat{Q}_t(a)$$

- Greedy algorithm can lock into a sub-optimal arm forever
- $\implies$ Greedy has linear total regret

Explore Then Commit

Algorithm Explore then Commit

```
Let $K$ be the number of arms; $N$ be the total rounds; Initialize $M$
for $m = 1, 2, \cdots M$ do
    for $a = 1, 2, \cdots, K$ do
        Pull arm $a$; Observe reward $r_a$; Compute mean reward $\hat{Q}(a)$ for arm $a$;
    end for
end for
for $i = MK + 1, \cdots, N$ do
    Pull the arm with the best mean reward [i.e. $a^* = \arg\max_a \hat{Q}(a)$]
end for
```

Question : Which parts of the algorithm explores and which part exploits ?

Explore Then Commit

Algorithm Explore then Commit

```
Let K be the number of arms; N be the total rounds; Initialize M
Exploration Phase
for m = 1, 2, ··· M  do
    for a = 1, 2, ··· , K do
        Pull arm a; Observe reward r_a; Compute mean reward Q̂(a) for arm a;
    end for
end for
Exploitation Phase
for t = MK + 1, ··· , N do
    Pull the arm with the best mean reward [i.e. a* = arg max_a Q̂(a)]
end for
```

Question : Why do we expect this algorithm to work ?

Law of Large Numbers

- Suppose $X_1, X_2, \cdots$ are independent samples of a random variable X having mean μ
- Denote empirical mean of m samples by $\hat{\mu}_m$ defined as

$$\hat{\mu}_m = \frac{1}{m}\sum_{i=1}^{m} X_i$$

- Weak law of large numbers states that $\hat{\mu}_m \to \mu$ in probability as $m \to \infty$
- Strong law of large numbers states that $\hat{\mu}_m \to \mu$ almost surely as $m \to \infty$

Explore and Commit : Analysis

- At round m, upon pulling arm a, the agent gets a random reward $r^a_m \sim \mathcal{R}^a$
- After M rounds, we have $\hat{Q}(a)$ as the empirical mean reward for pulling arm a

$$\hat{Q}(a) = \frac{1}{m}\sum_{i=1}^{m} r^a_m$$

$$\hat{Q}(a) \rightarrow Q(a)$$

as the number of rounds gets large

Question : Is there a shortcoming to ETC ?

ETC does not use the experience generated after the initial explore phase

Greedy Approach

Algorithm Greedy Algorithm

Let K be the number of arms; N be the total rounds; Initialize M
for $m = 1, 2, \cdots M$ **do**
  for $a = 1, 2, \cdots, K$ **do**
    Pull arm a; Observe reward r_a; Compute mean reward $\hat{Q}(a)$ for arm a;
  end for
end for
for $t = MK + 1, \cdots, N$ **do**
  Pull the arm with the **current** best mean reward [i.e. $a^* = \arg\max_a \hat{Q}(a)$]
  Update the mean observed rewards with the latest observation
end for

Question : Will this work well ? Can we improve exploration ?

The greedy algorithm is unlikely to explore during the exploitation phase

The ϵ - Greedy Approach

Algorithm ϵ - Greedy Algorithm

```
Let K be the number of arms; N be the total rounds; Initialize M and choose ε ∈ (0,1) small
for m = 1, 2, ··· M  do
    for a = 1, 2, ··· , K do
        Pull arm k; Observe reward r_a; Compute mean reward Q̂(a) for arm a;
    end for
end for
for t = MK + 1, ··· , N do
    With probability 1 − ε, pull the arm with the current best mean reward [i.e. a* = argmax_a Q̂(a)], else play another arm uniformly at random
    Update the mean observed rewards with the latest observation
end for
```

Quesiton : Do you see possible drawback ?

The ϵ-greedy algorithm explores forever. Also, has total linear regret.

Optimistic Initialization

- **Idea** : Initialise $Q(a)$ for all actions to high value
- Update action value by incremental Monte-Carlo evaluation; Let $a \in \mathcal{A}$ be the arm pulled at round t, Then,

$$\hat{Q}_t(a) = \hat{Q}_{t-1}(a) + \frac{1}{N_t(a)}\left(r_t - \hat{Q}_{t-1}\right)$$

  where $r_t \sim \mathcal{R}^a$ is the reward obtained at round t
- Encourages systematic exploration early on
- Locking onto sub-optimal arm is a possibility
- Greedy + optimistic initialization has linear total regret
- ϵ - Greedy + optimistic initialization has linear total regret

The ϵ - Greedy with Decay Approach

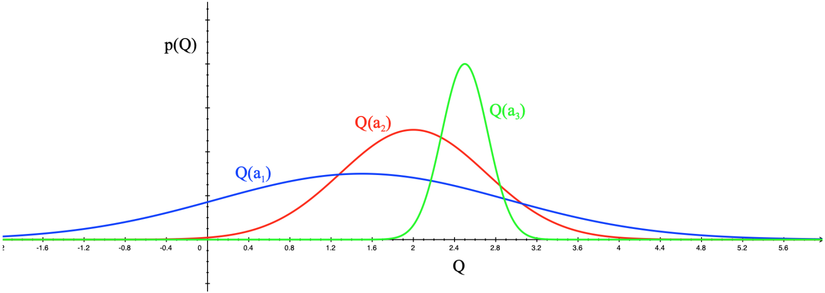
Algorithm ϵ - Greedy with Decay Algorithm

Let K be the number of arms; N be the total rounds; Initialize M and choose $\epsilon \in (0,1)$ small and choose a small decay rate $r \in (0,1)$
for $m = 1, 2, \cdots M$ **do**
    for $a = 1, 2, \cdots, K$ **do**
        Pull arm a; Observe reward r_a; Compute mean reward $\hat{Q}(a)$ for arm a;
    end for
end for
for $t = MK + 1, \cdots, N$ **do**
    With probability $1 - \epsilon$, pull the arm with the **current** best mean reward [i.e. $a^* = \arg\max_a \hat{Q}(a)$], else play another arm uniformly at random
    Update the mean observed rewards with the latest observation
    Reduce ϵ by fraction r
end for

Certain choices of decay schedule can achieve lograthmic asymptotic total regret

Optimism in the Face of Uncertainty

Optimism in the Face of Uncertainty



- Which arm (among the three) should we choose at next round ?
- **Optimism in the Face of Uncertainty** $\implies$ pick the arm that we are most uncertain about
- The more uncertain we are about the action-value of an arm, the more we should explore that action; as it could turn out to be the best action

Upper Confidence Bound

- Estimate an upper confidence $\hat{U}_t(a)$ for action a at time t such that

$$Q(a) \leq \hat{Q}_t(a) + \hat{U}_t(a)$$

- The upper confidence bound depends on the number of times an arm a has been pulled so far
  - ★ Small $N_t(a) \implies$ Large $\hat{U}_t(a)$
  - ★ Large $N_t(a) \implies$ Small $\hat{U}_t(a)$
- Select action a, at time t, that maximizes

$$a_t = \arg\max_a \left[\hat{Q}_{t-1}(a) + \hat{U}_{t-1}(a)\right]$$

- Hoeffding's inequality provides a way to arrive at the formulation for $\hat{U}_t(a)$

Hoeffding's Inequality

Theorem

Let $X_1, \ldots, X_t$ be i.i.d. (independent and identically distributed) random variables and they are all bounded by the interval $[0, 1]$. The sample mean is $\overline{X}_t = \frac{1}{t}\sum_{\tau=1}^{t} X_\tau$. Then for $u > 0$, we have,

$$\mathbb{P}[\mathbb{E}[X] > \overline{X}_t + u] \leq e^{-2tu^2}$$

- We will apply Hoeffding's inequality to the rewards of the bandit

$$\mathbb{P}[Q(a) > \hat{Q}_t(a) + \hat{U}_t(a)] \leq e^{-2N_t(a)\hat{U}_t(a)^2}$$

Calculating Upper Confidence Bound

- Pick a probability p that true value exceeds UCB
- Now solve for $\hat{U}_t(a)$ by setting

$$p = e^{-2N_t(a)\hat{U}_t(a)^2}$$

then,

$$\hat{U}_t(a) = \sqrt{\frac{-\log p}{2N_t(a)}}$$

- Reduce p as t^{-4} as we observe more rewards
- Ensures optimal action selection asymptotically (as $t \to \infty$)

$$\hat{U}_t(a) = \sqrt{\frac{2\log t}{N_t(a)}}$$

UCB1 Algorithm

Algorithm UCB1 Algorithm

Let K be the number of arms;
for $a = 1, 2, \cdots, K$ **do**
    Pull arm a; Observe reward r_a; Compute mean reward $\hat{Q}(a)$ for arm a;
end for
for $t = K+1, \cdots, N$ **do**
    Pull arm a such that

$$a_t = \arg\max_a \left[\underbrace{\hat{Q}_t(a)}_{\text{Exploitation}} + \underbrace{\sqrt{\frac{2 \log t}{N_t(a)}}}_{\text{Exploration}} \right]$$

    Update the mean observed rewards and UCB coefficient of the arm chosen
end for

Assumptions Matter

- So far we have made no assumptions about the reward distribution $\mathcal{R}$ (except bound on rewards)
- Neccessary to make assumptions; Strong assumptions, when made the right way, lead to better algorithms
- Examples :
  - ★ Bernoulli
  - ★ Gaussian with unknown mean and unit variance
  - ★ Many more ...

Bayesian Bandits

- So far we have made no assumptions about the reward distribution $\mathcal{R}$ (except bound on rewards)
- Bayesian bandits exploit prior knowledge of rewards, $p[\mathcal{R}]$
- They compute posterior distribution of rewards $p[\mathcal{R}|h_t]$ where $h_t = \{a_1, r_1, \cdots, a_{t-1}, r_{t-1}\}$
- Use posterior to guide exploration (Bayesian UCB, probability matching)
- Better performance if prior knowledge is accurate

Bayesian UCB

- Assume reward distribution is Gaussian
  - ★ Reward of every arm is given by $\mathcal{N}(\mu_a, \sigma_a)$
- Upon pulling arm a, observe reward r_a ; Compute posterior using Baye's law
- Pick arm a that maximizes standard deviation of $\hat{Q}_t(a)$

$$a_t = \arg\max_a \left[\underbrace{\mu_{t,a}}_{\text{Exploitation}} + \underbrace{\sqrt{\frac{c\sigma_{t,a}}{N_t(a)}}}_{\text{Exploration}} \right]$$

Thompson Sampling

Bernoulli Bandits

- Consider a Bernoulli bandit
  - ★ Each one of the K machines has a probability θ_k of providing a reward to the player

Let us consider a single Bernoulli bandit with probability θ of obtaining a reward

- Suppose R be the random variable that denotes the outcome of pulling the arm of a bandit
  - ★ $\mathbb{P}(R = 1) = \theta$ and $\mathbb{P}(R = 0) = 1 - \theta$
  - ★ The probability mass function can be written as

$$\mathbb{P}(R = r) = \theta^r (1 - \theta)^{1-r}$$

  - ★ The expected reward after one round is given by $\mathbb{E}(R) = \theta$

Frequentist vs Bayesian Approach

Let $R_1, R_2, \cdots, R_n$ be outcomes of n rounds of pulling the bandit arm

- **Frequentist approach :** Estimate the fixed but unknown parameter θ using the average of $R_1, \cdots, R_n$ for large n
- **Bayesian approach :** Treat θ as an uncertain parameter, and estimate its distribution from the data $D_n = \{R_1, \cdots, R_n\}$ by computing the posterior distribution using Baye's formula

$$\mathbb{P}(\theta|D_n) = \frac{\mathbb{P}(D_n|\theta) \cdot \eta(\theta)}{\mathbb{P}(D)}$$

where $\eta(\theta)$ is a suitable prior distribution on θ

A suitable prior distribution for a Bernoulli bandit is uniform prior

Choice of Initial Prior

- Suppose we take a uniform prior, then,

$$\mathbb{P}(\theta|D_n) = \underbrace{c\theta^{S_n}(1-\theta)^{n-S_n}}_{\text{Beta Distribution}}$$

  with $S_n = R_1 + R_2 + \cdots + R_n$

- The posterior $c\theta^{S_n}(1-\theta)^{n-S_n}$ is of the form that resembles Beta distribution with parameters α and γ given by

$$\beta_{\alpha,\gamma}(\theta) = \frac{\Gamma(\alpha+\gamma)}{\Gamma(\alpha)\Gamma(\gamma)}\theta^{\alpha-1} \cdot (1-\theta)^{\gamma-1}$$

- Note that $\beta_{1,1}$ is a uniform distribution
- Initialize the Beta parameters α and β such that prior is uniform
  - ★ $\alpha = 1$ and $\gamma = 1$; we expect the reward probability to be 50% (uniform prior)
  - ★ $\alpha = 9000$ and $\gamma = 1000$; we strongly believe that the reward probability is 90% (not a recommended choice for prior)

Posterior Updates of Beta Distribution

- Assuming uniform prior, after n rounds, we have, $\theta|D_n \sim \beta_{S_n+1, n-S_n+1}$
- Recursive posterior updates :
  - ★ If $\theta|D_n \sim \beta_{\alpha_n, \gamma_n}$ then $\theta|D_{n+1} \sim \beta_{\alpha_{n+1}, \gamma_{n+1}}$ with

$$\begin{aligned} \alpha_{n+1} &= \alpha_n + R_{n+1} \\ \gamma_{n+1} &= \gamma_n + (1 - R_{n+1}) \end{aligned}$$

Thompson Sampling : Algorithm

Algorithm Thompson Sampling Algorithm

1: Let K be the number of arms;
2: **for** $t = 1, \cdots, N$ **do**
3:     **for** $a = 1, 2, \cdots K$ **do**
4:         Sample θ_t^a from its posterior; $\theta_t^a \sim \beta_{\alpha_t^a, \gamma_t^a}$
5:     **end for**
6:     Play the arm $a^* = \arg\max_a \theta_t^a$ and observe the reward R_t
7:     Update the posterior of the chosen arm by updating the parameters of the corresponding Beta distribution

$$\begin{aligned} \alpha_{t+1}^{a^*} &= \alpha_t^{a^*} + R_t \\ \gamma_{t+1}^{a^*} &= \gamma_t^{a^*} + (1 - R_t) \end{aligned}$$

8: **end for**

Closing Remarks

- Information state space approach involves modelling the arm selection problem as an MDP with state comprising of history (h_t) of past decisions and rewards. Subsequently, use model free RL or Bayesian RL to solve the MDP
- There are other variants of bandit problems that include **Best arm identification**, **PAC** and **Contextual Bandits**
  - ★ PAC : find an arm within ϵ of the best arm with probability at least $1 - \delta$
- The exploration techniques mentioned here can easily be extended to full reinforcement learning setting