Multi-Armed Bandits: Exploration versus Exploitation

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Exploration versus Exploitation

- Many situations in business (& life!) present dilemma on choices
- **Exploitation:** Pick choices that *seem* best based on past outcomes
- **Exploration:** Pick choices not yet tried out (or not tried enough)
- Exploitation has notions of "being greedy" and being "short-sighted"
- Too much Exploitation $\Rightarrow$ Regret of missing unexplored "gems"
- Exploration has notions of "gaining info" and being "long-sighted"
- Too much Exploration $\Rightarrow$ Regret of wasting time on "duds"
- How to balance Exploration and Exploitation so we combine *information-gains* and *greedy-gains* in the most optimal manner
- Can we set up this problem in a mathematically disciplined manner?

Examples

- Restaurant Selection
  - **Exploitation:** Go to your favorite restaurant
  - **Exploration:** Try a new restaurant
- Online Banner Advertisement
  - **Exploitation:** Show the most successful advertisement
  - **Exploration:** Show a new advertisement
- Oil Drilling
  - **Exploitation:** Drill at the best known location
  - **Exploration:** Drill at a new location
- Learning to play a game
  - **Exploitation:** Play the move you believe is best
  - **Exploration:** Play an experimental move

The Multi-Armed Bandit (MAB) Problem

- Multi-Armed Bandit is spoof name for "Many Single-Armed Bandits"
- A Multi-Armed bandit problem is a 2-tuple $(\mathcal{A}, \mathcal{R})$
- $\mathcal{A}$ is a known set of m actions (known as "arms")
- $\mathcal{R}^a(r) = \mathbb{P}[r|a]$ is an **unknown** probability distribution over rewards
- At each step t, the AI agent (algorithm) selects an action $a_t \in \mathcal{A}$
- Then the environment generates a reward $r_t \sim \mathcal{R}^{a_t}$
- The AI agent's goal is to maximize the **Cumulative Reward**:

$$\sum_{t=1}^{T} r_t$$

- Can we design a strategy that does well (in Expectation) for any T?
- Note that any selection strategy risks wasting time on "duds" while exploring and also risks missing untapped "gems" while exploiting

Is the MAB problem a Markov Decision Process (MDP)?

- Note that the environment doesn't have a notion of *State*
- Upon pulling an arm, the arm just samples from its distribution
- However, the agent might maintain a statistic of history as it's *State*
- To enable the agent to make the arm-selection (action) decision
- The action is then a (*Policy*) function of the agent's *State*
- So, agent's arm-selection strategy is basically this *Policy*
- Note that many MAB algorithms don't take this formal MDP view
- Instead, they rely on heuristic methods that don't aim to *optimize*
- They simply strive for "good" Cumulative Rewards (in Expectation)
- Note that even in a simple heuristic algorithm, a_t is a random variable simply because it is a function of past (random) rewards

Regret

- The *Action Value* $Q(a)$ is the (unknown) mean reward of action a

$$Q(a) = \mathbb{E}[r|a]$$

- The *Optimal Value* V^* is defined as:

$$V^* = Q(a^*) = \max_{a \in \mathcal{A}} Q(s)$$

- The *Regret* l_t is the opportunity loss on a single step t

$$l_t = \mathbb{E}[V^* - Q(a_t)]$$

- The *Total Regret* L_T is the total opportunity loss

$$L_T = \sum_{t=1}^{T} \mathbb{E}[V^* - Q(a_t)]$$

- Maximizing *Cumulative Reward* is same as Minimizing *Total Regret*

Counting Regret

- Let $N_t(a)$ be the (random) number of selections of a across t steps
- Define *Count*$_t$ of a (for given action-selection strategy) as $\mathbb{E}[N_t(a)]$
- Define *Gap* Δ_a of a as the value difference between a and optimal a^*

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

- Total Regret is sum-product (over actions) of *Gaps* and *Counts*$_T$

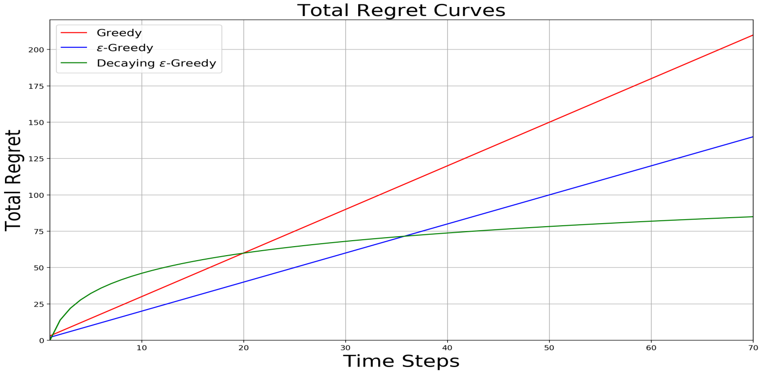
$$L_T = \sum_{t=1}^{T} \mathbb{E}[V^* - Q(a_t)]$$

$$= \sum_{a \in \mathcal{A}} \mathbb{E}[N_T(a)](V^* - Q(a))$$

$$= \sum_{a \in \mathcal{A}} \mathbb{E}[N_T(a)]\Delta_a$$

- A good algorithm ensures small *Counts* for large *Gaps*
- Little problem though: *We don't know the Gaps*!

Linear or Sublinear Total Regret



- If an algorithm *never* explores, it will have linear total regret
- If an algorithm *forever* explores, it will have linear total regret
- Is it possible to achieve sublinear total regret?

Greedy Algorithm

- We consider algorithms that estimate $\hat{Q}_t(a) \approx Q(a)$
- Estimate the value of each action by rewards-averaging

$$\hat{Q}_t(a) = \frac{1}{N_t(a)} \sum_{s=1}^{t} r_s \cdot \mathbb{1}_{a_s = a}$$

- The *Greedy* algorithm selects the action with highest estimated value

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

- Greedy algorithm can lock onto a suboptimal action forever
- Hence, Greedy algorithm has linear total regret

ϵ-Greedy Algorithm

- The ϵ-Greedy algorithm continues to explore forever
- At each time-step t:
  - With probability $1 - \epsilon$, select $a_t = \arg\max_{a \in \mathcal{A}} \hat{Q}_t(a)$
  - With probability ϵ, select a random action (uniformly) in $\mathcal{A}$
- Constant ϵ ensures a minimum regret proportional to mean gap

$$l_t \geq \frac{\epsilon}{|\mathcal{A}|} \sum_{a \in \mathcal{A}} \Delta_a$$

- Hence, ϵ-Greedy algorithm has linear total regret

Optimistic Initialization

- Simple and practical idea: Initialize $\hat{Q}_0(a)$ to a high value for all $a \in \mathcal{A}$
- Update action value by incremental-averaging
- Starting with $N_0(a) \geq 0$ for all $a \in \mathcal{A}$,

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

$$\hat{Q}_t(a) = \hat{Q}_{t-1}(a) \text{ for all } a \neq a_t$$

- Encourages systematic exploration early on
- One can also start with a high value for $N_0(a)$
- But can still lock onto suboptimal action
- Hence, Greedy + optimistic initialization has linear total regret
- ϵ-Greedy + optimistic initialization also has linear total regret

Decaying ϵ_t-Greedy Algorithm

- Pick a decay schedule for $\epsilon_1, \epsilon_2, \ldots$
- Consider the following schedule

$$c > 0$$

$$d = \min_{a|\Delta_a > 0} \Delta_a$$

$$\epsilon_t = \min(1, \frac{c|\mathcal{A}|}{d^2 t}\}$$

- Decaying ϵ_t-Greedy algorithm has *logarithmic* total regret
- Unfortunately, above schedule requires advance knowledge of gaps
- Practically, implementing *some* decay schedule helps considerably
- Educational Code for decaying ϵ-greedy with optimistic initialization

Lower Bound

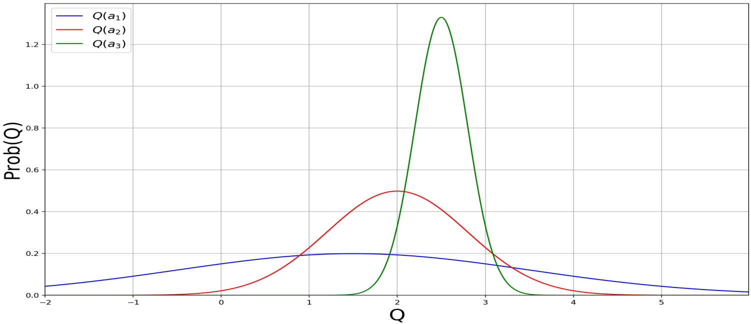
- Goal: Find an algorithm with sublinear total regret for any multi-armed bandit (without any prior knowledge of $\mathcal{R}$)
- The performance of any algorithm is determined by the similarity between the optimal arm and other arms
- Hard problems have similar-looking arms with different means
- Formally described by KL-Divergence $KL(\mathcal{R}^a || \mathcal{R}^{a^*})$ and gaps Δ_a

Theorem (Lai and Robbins)

Asymptotic Total Regret is at least logarithmic in number of steps

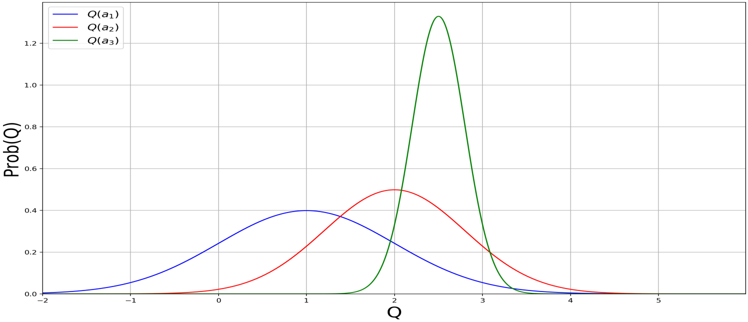
$$\lim_{T \to \infty} L_T \geq \log T \sum_{a|\Delta_a > 0} \frac{1}{\Delta_a} \geq \log T \sum_{a|\Delta_a > 0} \frac{\Delta_a}{KL(\mathcal{R}^a || \mathcal{R}^{a^*})}$$

Optimism in the Face of Uncertainty



- Which action should we pick?
- The more uncertain we are about an action-value, the more important it is to explore that action
- It could turn out to be the best action

Optimism in the Face of Uncertainty (continued)



- After picking *blue* action, we are less uncertain about the value
- And more likely to pick another action
- Until we home in on the best action

Upper Confidence Bounds

- Estimate an upper confidence $\hat{U}_t(a)$ for each action value
- Such that $Q(a) \leq \hat{Q}_t(a) + \hat{U}_t(a)$ with high probability
- This depends on the number of times $N_t(a)$ that a has been selected
  - Small $N_t(a) \Rightarrow$ Large $\hat{U}_t(a)$ (estimated value is uncertain)
  - Large $N_t(a) \Rightarrow$ Small $\hat{U}_t(a)$ (estimated value is accurate)
- Select action maximizing Upper Confidence Bound (UCB)

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

Hoeffding's Inequality

Theorem (Hoeffding's Inequality)

Let $X_1, \ldots, X_t$ be i.i.d. random variables in $[0, 1]$, and let

$$\bar{X}_t = \frac{1}{t} \sum_{s=1}^{t} X_s$$

be the sample mean. Then,

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

- Apply Hoeffding's Inequality to rewards of $[0, 1]$-support bandits
- Conditioned on selecting action a

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

Calculating Upper Confidence Bounds

- Pick a small probability p that $Q(a)$ exceeds UCB $\{\hat{Q}_t(a) + \hat{U}_t(a)\}$
- Now solve for $\hat{U}_t(a)$

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

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

- Reduce p as we observe more rewards, eg: $p = t^{-\alpha}$ (for fixed $\alpha > 0$)
- This ensures we select optimal action as $t \to \infty$

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

UCB1

Yields UCB1 algorithm for arbitrary-distribution arms bounded in $[0, 1]$

$$a_t = \underset{a \in \mathcal{A}}{\arg\max}\{\hat{Q}_t(a) + \sqrt{\frac{\alpha \log t}{2N_t(a)}}\}$$

Theorem

The UCB1 Algorithm achieves logarithmic total regret

$$L_T \leq \sum_{a | \Delta_a > 0} \frac{4\alpha \cdot \log T}{\Delta_a} + \frac{2\alpha \cdot \Delta_a}{\alpha - 1}$$

Educational Code for UCB1 algorithm

Bayesian Bandits

- So far we have made no assumptions about the rewards distribution $\mathcal{R}$ (except bounds on rewards)
- *Bayesian Bandits* exploit prior knowledge of rewards distribution $\mathbb{P}[\mathcal{R}]$
- They compute posterior distribution of rewards $\mathbb{P}[\mathcal{R}|h_t]$ where $h_t = a_1, r_1, \ldots, a_{t-1}, r_{t-1}$ is the history
- Use posterior to guide exploration
  - Upper Confidence Bounds (Bayesian UCB)
  - Probability Matching (Thompson sampling)
- Better performance if prior knowledge of $\mathcal{R}$ is accurate

Bayesian UCB Example: Independent Gaussians

- Assume reward distribution is Gaussian, $\mathcal{R}^a(r) = \mathcal{N}(r; \mu_a, \sigma_a^2)$
- Compute Gaussian posterior over μ_a, σ_a^2 (Bayes update details here)

$$\mathbb{P}[\mu_a, \sigma_a^2 | h_t] \propto \mathbb{P}[\mu_a, \sigma_a^2] \cdot \prod_{t | a_t = a} \mathcal{N}(r_t; \mu_a, \sigma_a^2)$$

- Pick action that maximizes Expectation of c std-devs above mean

$$a_t = \arg\max_{a \in \mathcal{A}} \mathbb{E}[\mu_a + \frac{c\sigma_a}{\sqrt{N_t(a)}}]$$

Probability Matching

- *Probability Matching* selects action a according to probability that a is the optimal action

$$\pi(a_t|h_t) = \mathbb{P}_{\mathcal{D}_t \sim \mathbb{P}[\mathcal{R}|h_t]}[\mathbb{E}_{\mathcal{D}_t}[r|a_t] > \mathbb{E}_{\mathcal{D}_t}[r|a], \forall a \neq a_t]$$

- Probability matching is optimistic in the face of uncertainty
- Because uncertain actions have higher probability of being max
- Can be difficult to compute analytically from posterior

Thompson Sampling

- *Thompson Sampling* implements probability matching

$$\pi(a_t|h_t) = \mathbb{P}_{\mathcal{D}_t \sim \mathbb{P}[\mathcal{R}|h_t]}[\mathbb{E}_{\mathcal{D}_t}[r|a_t] > \mathbb{E}_{\mathcal{D}_t}[r|a], \forall a \neq a_t]$$

$$= \mathbb{E}_{\mathcal{D}_t \sim \mathbb{P}[\mathcal{R}|h_t]}[\mathbb{1}_{a_t = \arg\max_{a \in \mathcal{A}} \mathbb{E}_{\mathcal{D}_t}[r|a]}]$$

- Use Bayes law to compute posterior distribution $\mathbb{P}[\mathcal{R}|h_t]$
- *Sample* a reward distribution $\mathcal{D}_t$ from posterior $\mathbb{P}[\mathcal{R}|h_t]$
- Estimate Action-Value function with sample $\mathcal{D}_t$ as $\hat{Q}_t(a) = \mathbb{E}_{\mathcal{D}_t}[r|a]$
- Select action maximizing value of sample

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

- Thompson Sampling achieves Lai-Robbins lower bound!
- Educational Code for Thompson Sampling for Gaussian Distributions
- Educational Code for Thompson Sampling for Bernoulli Distributions

Gradient Bandit Algorithms

- Gradient Bandit Algorithms are based on Stochastic Gradient Ascent
- We optimize *Score* parameters s_a for $a \in \mathcal{A} = \{a_1, \ldots, a_m\}$
- Objective function to be maximized is the Expected Reward

$$J(s_{a_1}, \ldots, s_{a_m}) = \sum_{a \in \mathcal{A}} \pi(a) \cdot \mathbb{E}[r|a]$$

- $\pi(\cdot)$ is probabilities of taking actions (based on a stochastic policy)
- The stochastic policy governing $\pi(\cdot)$ is a function of the *Scores*:

$$\pi(a) = \frac{e^{s_a}}{\sum_{b \in \mathcal{A}} e^{s_b}}$$

- *Scores* represent the relative value of actions based on seen rewards
- Note: π has a Boltzmann distribution (Softmax-function of *Scores*)
- We move the *Score* parameters s_a (hence, action probabilities $\pi(a)$) such that we ascend along the direction of gradient of objective $J(\cdot)$

Gradient of Expected Reward

- To construct Gradient of $J(\cdot)$, we calculate $\frac{\partial J}{\partial s_a}$ for all $a \in \mathcal{A}$

$$\frac{\partial J}{\partial s_a} = \frac{\partial}{\partial s_a}(\sum_{a' \in \mathcal{A}} \pi(a') \cdot \mathbb{E}[r|a']) = \sum_{a' \in \mathcal{A}} \mathbb{E}[r|a'] \cdot \frac{\partial \pi(a')}{\partial s_a}$$

$$= \sum_{a' \in \mathcal{A}} \pi(a') \cdot \mathbb{E}[r|a'] \cdot \frac{\partial \log \pi(a')}{\partial s_a} = \mathbb{E}_{a' \sim \pi, r \sim \mathcal{R}^{a'}}[r \cdot \frac{\partial \log \pi(a')}{\partial s_a}]$$

- We know from standard softmax-function calculus that:

$$\frac{\partial \log \pi(a')}{\partial s_a} = \frac{\partial}{\partial s_a}(\log \frac{e^{s_{a'}}}{\sum_{b \in \mathcal{A}} e^{s_b}}) = \mathbb{1}_{a=a'} - \pi(a)$$

- Therefore $\frac{\partial J}{\partial s_a}$ can we re-written as:

$$= \mathbb{E}_{a' \sim \pi, r \sim \mathcal{R}^{a'}}[r \cdot (\mathbb{1}_{a=a'} - \pi(a))]$$

- At each step t, we approximate the gradient with (a_t, r_t) sample as:

$$r_t \cdot (\mathbb{1}_{a=a_t} - \pi_t(a)) \text{ for all } a \in \mathcal{A}$$

Score updates with Stochastic Gradient Ascent

- $\pi_t(a)$ is the probability of a at step t derived from score $s_t(a)$ at step t
- Reduce variance of estimate with baseline B that's independent of a:

$$(r_t - B) \cdot (\mathbb{1}_{a=a_t} - \pi_t(a)) \text{ for all } a \in \mathcal{A}$$

- This doesn't introduce bias in the estimate of gradient of $J(\cdot)$ because

$$\mathbb{E}_{a' \sim \pi}[B \cdot (\mathbb{1}_{a=a'} - \pi(a))] = \mathbb{E}_{a' \sim \pi}[B \cdot \frac{\partial \log \pi(a')}{\partial s_a}]$$

$$= B \cdot \sum_{a' \in \mathcal{A}} \pi(a') \cdot \frac{\partial \log \pi(a')}{\partial s_a} = B \cdot \sum_{a' \in \mathcal{A}} \frac{\partial \pi(a')}{\partial s_a} = B \cdot \frac{\partial}{\partial s_a} (\sum_{a' \in \mathcal{A}} \pi(a')) = 0$$

- We can use $B = \bar{r}_t = \frac{1}{t} \sum_{s=1}^{t} r_s =$ average rewards until step t
- So, the update to scores $s_t(a)$ for all $a \in \mathcal{A}$ is:

$$s_{t+1}(a) = s_t(a) + \alpha \cdot (r_t - \bar{r}_t) \cdot (\mathbb{1}_{a=a_t} - \pi_t(a))$$

- Educational Code for this Gradient Bandit Algorithm

Value of Information

- Exploration is useful because it gains information
- Can we quantify the value of information?
  - How much would a decision-maker be willing to pay to have that information, prior to making a decision?
  - Long-term reward after getting information minus immediate reward
- Information gain is higher in uncertain situations
- Therefore it makes sense to explore uncertain situations more
- If we know value of information, we can trade-off exploration and exploitation *optimally*

Information State Space

- We have viewed bandits as *one-step* decision-making problems
- Can also view as *sequential* decision-making problems
- At each step there is an *information state* $\tilde{s}$
  - $\tilde{s}$ is a statistic of the history, i.e., $\tilde{s}_t = f(h_t)$
  - summarizing all information accumulated so far
- Each action a causes a transition to a new information state $\tilde{s}'$ (by adding information), with probability $\tilde{\mathcal{P}}^a_{\tilde{s},\tilde{s}'}$
- This defines an MDP $\tilde{M}$ in information state space

$$\tilde{M} = (\tilde{\mathcal{S}}, \mathcal{A}, \tilde{\mathcal{P}}, \mathcal{R}, \gamma)$$

Example: Bernoulli Bandits

- Consider a Bernoulli Bandit, such that $\mathcal{R}^a = \mathcal{B}(\mu_a)$
- For arm a, reward=1 with probability μ_a (=0 with probability $1 - \mu_a$)
- Assume we have m arms $a_1, a_2, \ldots, a_m$
- The information state is $\tilde{s} = (\alpha_{a_1}, \beta_{a_1}, \alpha_{a_2}, \beta_{a_2} \ldots, \alpha_{a_m}, \beta_{a_m})$
- α_a records the pulls of arms a for which reward was 1
- β_a records the pulls of arm a for which reward was 0
- In the long-run, $\frac{\alpha_a}{\alpha_a+\beta_a} \rightarrow \mu_a$

Solving Information State Space Bandits

- We now have an infinite MDP over information states
- This MDP can be solved by Reinforcement Learning
- Model-free Reinforcement learning, eg: Q-Learning (Duff, 1994)
- Or Bayesian Model-based Reinforcement Learning
  - eg: Gittins indices (Gittins, 1979)
  - This approach is known as Bayes-adaptive RL
  - Finds Bayes-optimal exploration/exploitation trade-off with respect of prior distribution

Bayes-Adaptive Bernoulli Bandits

- Start with $Beta(\alpha_a, \beta_a)$ prior over reward function $\mathcal{R}^a$
- Each time a is selected, update posterior for $\mathcal{R}^a$ as:
  - $Beta(\alpha_a + 1, \beta_a)$ if $r = 1$
  - $Beta(\alpha_a, \beta_a + 1)$ if $r = 0$
- This defines transition function $\tilde{\mathcal{P}}$ for the Bayes-adaptive MDP
- (α_a, β_a) in information state provides reward model $Beta(\alpha_a, \beta_a)$
- Each state transition corresponds to a Bayesian model update

Gittins Indices for Bernoulli Bandits

- Bayes-adaptive MDP can be solved by Dynamic Programming
- The solution is known as the Gittins Index
- Exact solution to Bayes-adaptive MDP is typically intractable
- Guez et al. 2020 applied Simulation-based search
  - Forward search in information state space
  - Using simulations from current information state

Summary of approaches to Bandit Algorithms

- Naive Exploration (eg: ϵ-Greedy)
- Optimistic Initialization
- Optimism in the face of uncertainty (eg: UCB, Bayesian UCB)
- Probability Matching (eg: Thompson Sampling)
- Gradient Bandit Algorithms
- Information State Space MDP, incorporating value of information

Contextual Bandits

- A Contextual Bandit is a 3-tuple $(\mathcal{A}, \mathcal{S}, \mathcal{R})$
- $\mathcal{A}$ is a known set of m actions ("arms")
- $\mathcal{S} = \mathbb{P}[s]$ is an **unknown** distribution over states ("contexts")
- $\mathcal{R}_s^a(r) = \mathbb{P}[r|s, a]$ is an **unknown** probability distribution over rewards
- At each step t, the following sequence of events occur:
    - The environment generates a states $s_t \sim \mathcal{S}$
    - Then the AI Agent (algorithm) selects an actions $a_t \in \mathcal{A}$
    - Then the environment generates a reward $r_t \in \mathcal{R}_{s_t}^{a_t}$
- The AI agent's goal is to maximize the Cumulative Reward:

$$\sum_{t=1}^{T} r_t$$

- Extend Bandit Algorithms to Action-Value $Q(s, a)$ (instead of $Q(a)$)