Bandits 2

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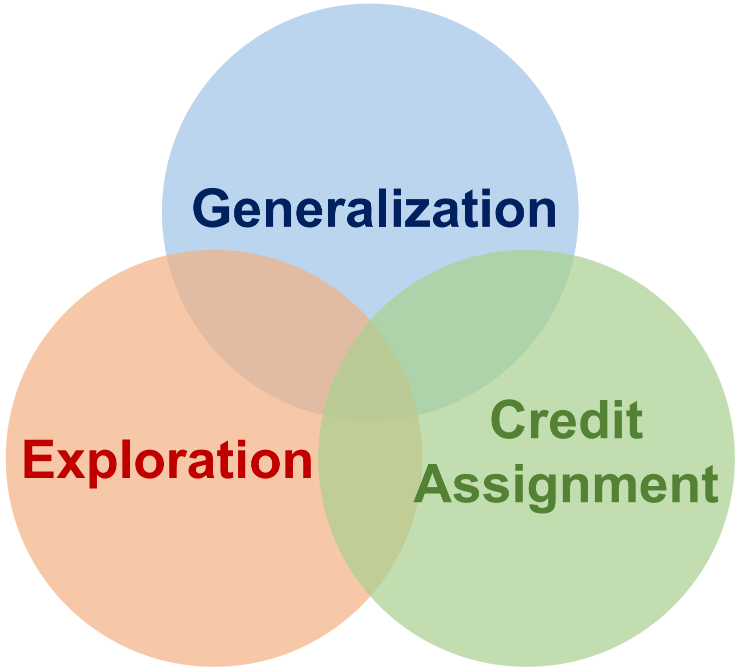
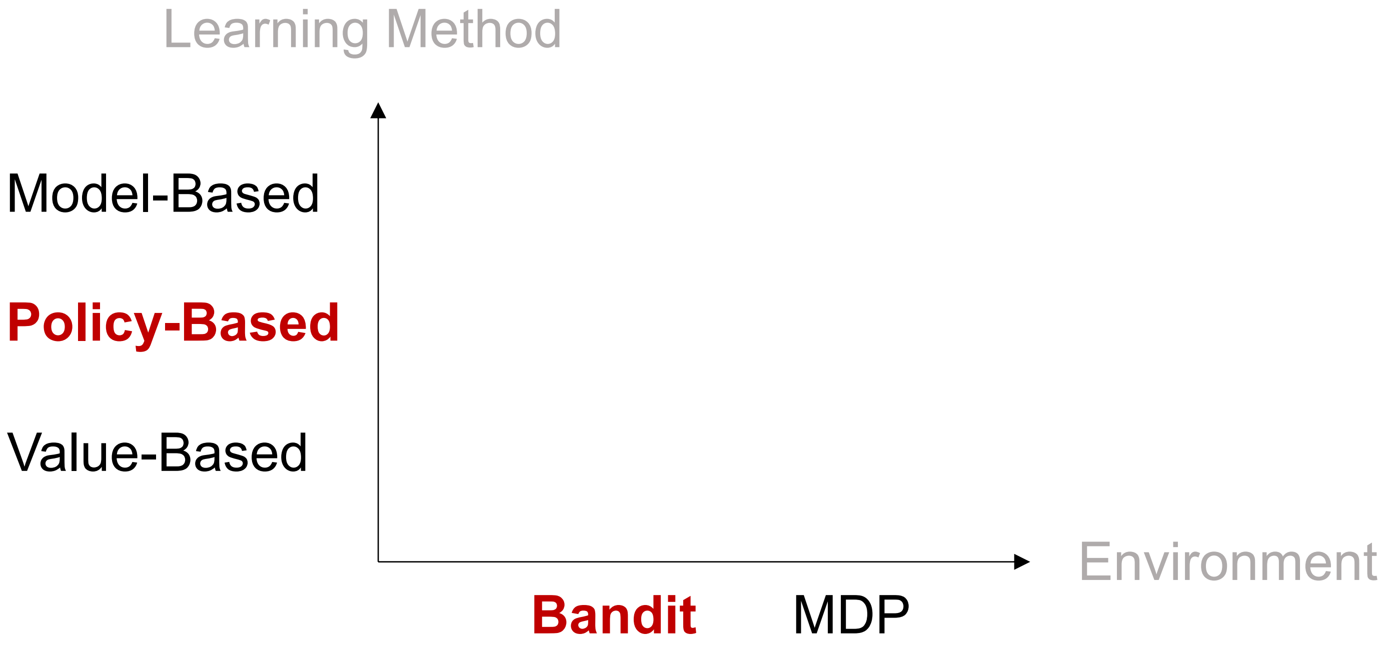
Roadmap


Generalization
Exploration
Credit
Assignment

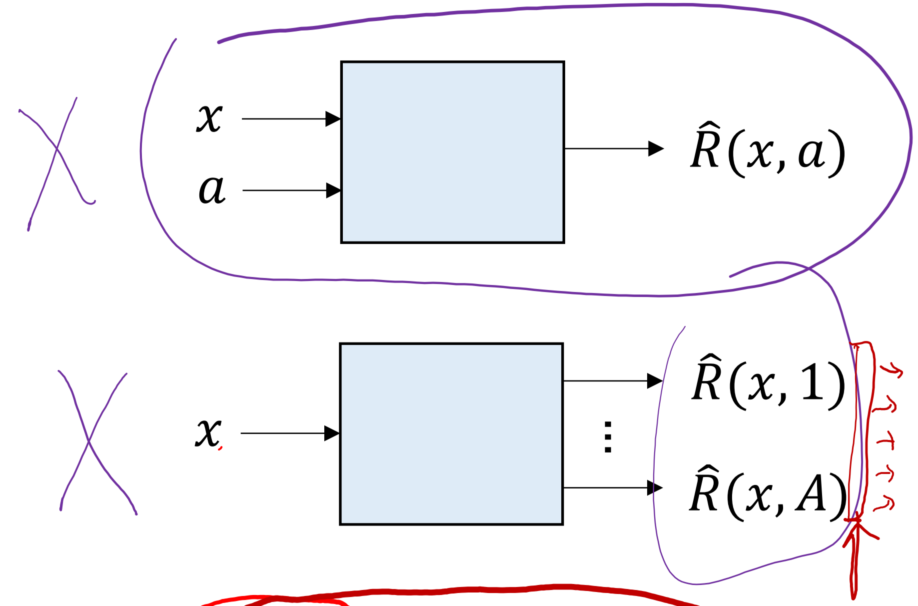

Learning Method
Model-Based
Policy-Based
Value-Based
Environment
Bandit
MDP

Policy-Based Bandits

- Key challenges: **Exploration** and **Generalization (if there are contexts)**
- Algorithms we will discuss:
  - KL-regularized policy updates (PPO)
  - Policy gradient (REINFORCE)

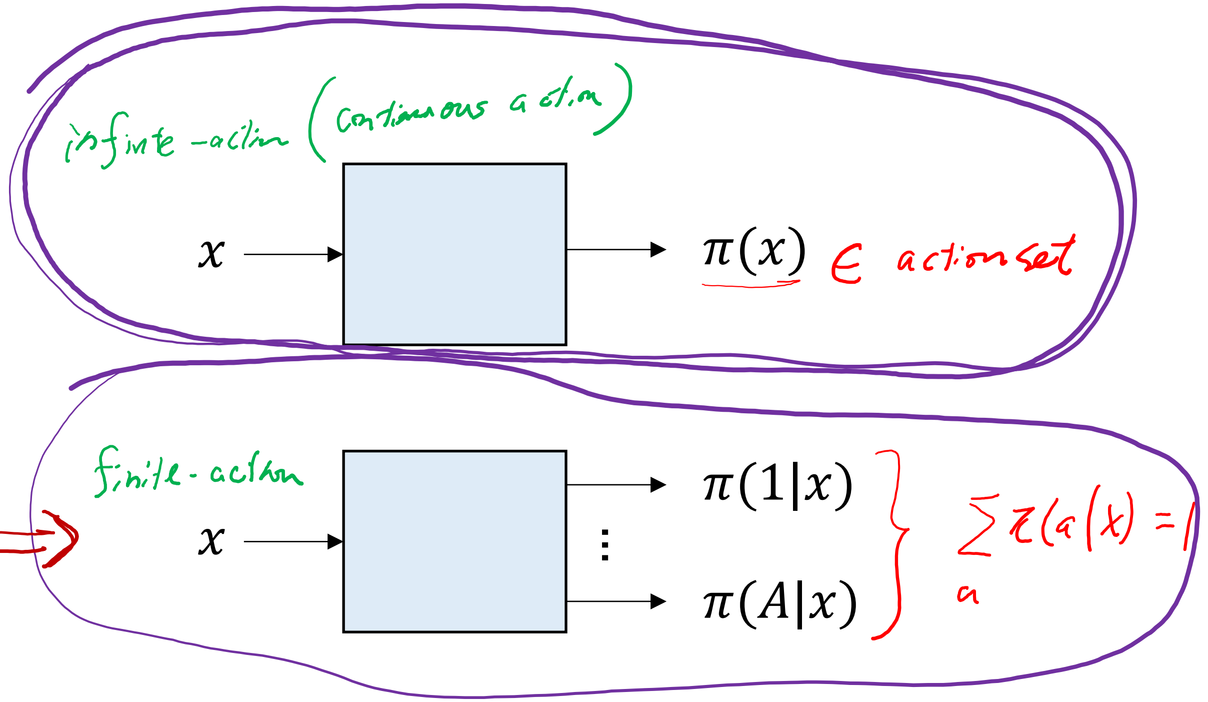
Policy-Based Bandits

x: context, a: action



$\pi(a|x) \propto \exp\left(\lambda \hat{R}(x,a)\right)$

softmax



Value-based approach

Policy-based approach

Policy-Based Bandits

Why policy-based bandit algorithms?

- Actually, in finite-action contextual bandit problems, value- and policy-based approaches are almost equivalent.
- But we have to use policy-based approaches to handle **continuous action space.**
- They are also different in MDPs. (later in the course)

The Full-Information MAB

Given: set of actions $\mathcal{A} = \{1, \dots, A\}$

For time $t = 1, 2, \dots, T$:

The learner chooses an action a_t

Environment reveals the reward $r_t(a) = R(a) + w_t(a)$ **of all actions**

Policy-based algorithm: Maintain a distribution $\pi_t(a)$ and update it with feedback

Sample $a_t \sim \pi_t$

How should we update from π_t to π_{t+1} using $r_t(1), \dots, r_t(A)$?

$\bar{r}_t \sim r_t$

$\pi_{t+1} \leftarrow \pi_t + \bar{r}_t$

$\pi_{t+1}(a) = \pi_t(a) + \bar{r}_t(a)$

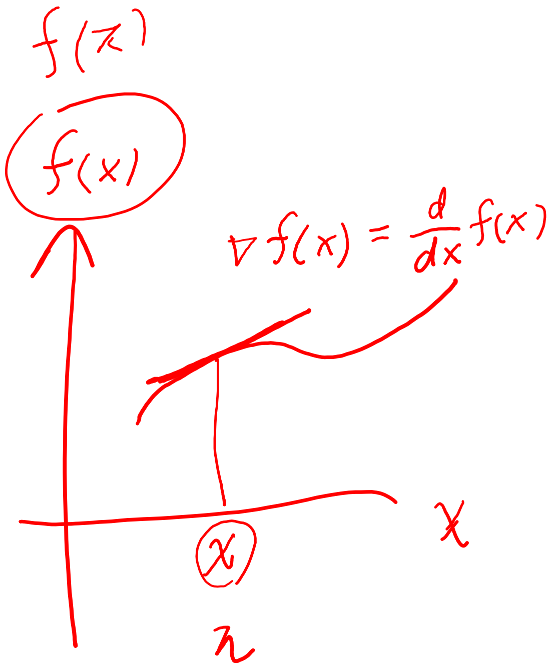
Algorithm for the Full-Information MAB

$$f(\pi) = \sum_{a=1}^{A} \pi(a)R(a)$$

← We want to find a π that **maximizes** this value

But we don't know $R(a)$

But we get noisy samples of $R(a)$, i.e., $r_t(a)$



Gradient Ascent

$\pi \in R^A$

$\langle \pi, R \rangle$

$$f(\pi) = \sum_{a=1}^{A} \pi(a) R(a) \quad \Rightarrow \quad \nabla_\pi f(\pi) = R$$

Gradient Ascent

learning rate

For $t = 1, 2 \ldots$

$$\pi_{t+1} \leftarrow \pi_t + \eta R$$

$$\pi_{t+1} \leftarrow \Pi(\pi_{t+1})$$

Stochastic Gradient Ascent

For $t = 1, 2 \ldots$

$$\pi_{t+1} \leftarrow \pi_t + \eta r_t$$

$$\pi_{t+1} \leftarrow \Pi(\pi_{t+1})$$

$\mathbb{E}[r_t] = R$

Exponential Weight Update

For $t = 1, 2 \ldots$

$$\pi_{t+1}(a) \propto \pi_t(a)\, e^{\eta r_t(a)}$$

or $$\pi_{t+1}(a) = \frac{\pi_t(a)\, e^{\eta r_t(a)}}{\sum_{b \in \mathcal{A}} \pi_t(b)\, e^{\eta r_t(b)}}$$

Better for bandit problems (because we never get $\pi_t(a) = 0$)

Exponential Weight Update = KL-Regularized Policy Updates

distance(π, π_t)

$$\pi_{t+1}(a) = \frac{\pi_t(a)\, e^{\eta r_t(a)}}{\sum_{b\in\mathcal{A}} \pi_t(b)\, e^{\eta r_t(b)}} \iff \pi_{t+1} = \operatorname*{argmax}_{\pi\in\Delta(\mathcal{A})} \left\{ \underbrace{\langle \pi - \pi_t, r_t\rangle - \frac{1}{\eta}\mathrm{KL}(\pi, \pi_t)}_{g(\pi)} \right\}$$

$$\underbrace{\langle \pi, r_t\rangle - \langle \pi_t, r_t\rangle}$$

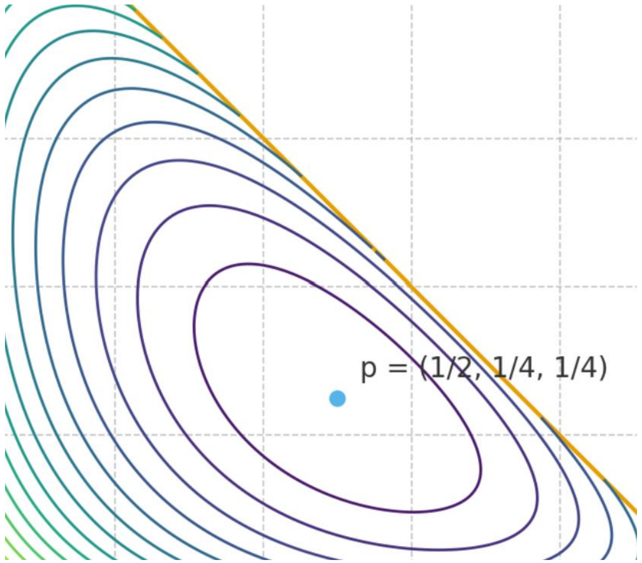
KL Divergence – A Distance Measure for Distributions

$$\boxed{\mathrm{KL}(\pi, \pi') = \sum_a \pi(a) \log \frac{\pi(a)}{\pi'(a)}}$$

$\mathrm{KL}(\pi, \pi') \geq 0$

$\mathrm{KL}(\pi, \pi') = 0$ if and only if $\pi = \pi'$

$\mathrm{KL}(\pi, \pi') \neq \mathrm{KL}(\pi', \pi)$

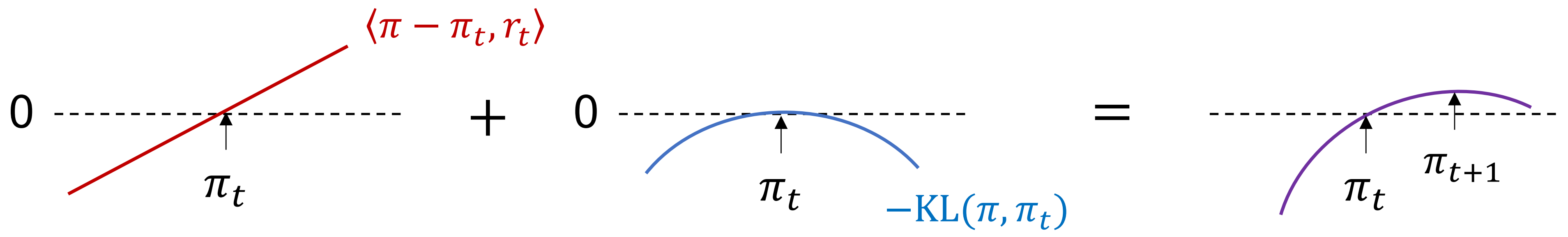


$KL\left(\pi, (1/2, 1/4, 1/4)\right)$

Regularized Policy Updates

$$\pi_{t+1} = \operatorname*{argmax}_{\pi \in \Delta(\mathcal{A})} \left\{ \langle \pi - \pi_t, r_t \rangle - \frac{1}{\eta} \mathrm{KL}(\pi, \pi_t) \right\}$$

$$= \operatorname*{argmax}_{\pi \in \Delta(\mathcal{A})} \left\{ \underbrace{\sum_a \big(\pi(a) - \pi_t(a)\big) r_t(a)}_{\text{The Improvement of } \pi \text{ over } \pi_t \text{ on } r_t} - \frac{1}{\eta} \mathrm{KL}(\pi, \pi_t) \right\}$$



Multi-Armed Bandits

Multi-Armed Bandits

Given: set of arms $\mathcal{A} = \{1, \dots, A\}$

For time $t = 1, 2, \dots, T$:

Learner chooses an arm $a_t \in \mathcal{A}$

Learner observes $r_t(a_t) = R(a_t) + w_t(a_t)$

Recall: Exponential Weight Updates

$$\pi_{t+1} = \operatorname*{argmax}_{\pi \in \Delta(\mathcal{A})} \left\{ \langle \pi - \pi_t, r_t \rangle - \frac{1}{\eta} \mathrm{KL}(\pi, \pi_t) \right\} \iff \pi_{t+1}(a) = \frac{\pi_t(a)\, e^{\eta r_t(a)}}{\sum_{b \in \mathcal{A}} \pi_t(b)\, e^{\eta r_t(b)}}$$

Exponential Weight Updates for Bandits?

$$\pi_{t+1} = \underset{\pi \in \Delta(\mathcal{A})}{\operatorname{argmax}} \left\{ \langle \pi - \pi_t, r_t \rangle - \frac{1}{\eta} \mathrm{KL}(\pi, \pi_t) \right\} \iff \pi_{t+1}(a) = \frac{\pi_t(a)\, e^{\eta r_t(a)}}{\sum_{b \in \mathcal{A}} \pi_t(b)\, e^{\eta r_t(b)}}$$

No longer observable

Only update the arm that we choose?

Exponential Weight Updates for Bandits?

$$\pi_{t+1} = \underset{\pi \in \Delta(\mathcal{A})}{\operatorname{argmax}} \left\{ \langle \pi - \pi_t, \hat{r}_t \rangle - \frac{1}{\eta} \mathrm{KL}(\pi, \pi_t) \right\} \quad \Longleftrightarrow \quad \pi_{t+1}(a) = \frac{\pi_t(a)\, e^{\eta \hat{r}_t(a)}}{\sum_{b \in \mathcal{A}} \pi_t(b)\, e^{\eta \hat{r}_t(b)}}$$

- $\hat{r}_t(a)$ is an **"estimator"** for $r_t(a)$
- But we can only observe the reward of one arm
- And let's set the restriction that we can only construct $\hat{r}_t$ from $r_t(a_t)$

What's the problem of setting $\hat{r}_t = (0, 0, \ldots, r_t(a_t), \ldots, 0)$?

Unbiased Reward / Gradient Estimator

Weight a sample by **the inverse of the probability we observe it**

$$\hat{r}_t(a) = \frac{r_t(a)}{\pi_t(a)} \mathbb{I}\{a_t = a\} = \begin{cases} \dfrac{r_t(a)}{\pi_t(a)} & \text{if } a_t = a \\ 0 & \text{otherwise} \end{cases}$$

$$\begin{aligned} \mathbb{E}[\hat{r}_t(a)] &= \Pr\{a_t = a\} \frac{r_t(a)}{\pi_t(a)} + \Pr\{a_t \neq a\} 0 \\ &= \pi_t(a) \frac{r_t(a)}{\pi_t(a)} \\ &= r_t(a) \end{aligned}$$

Importance Weighting

Directly Applying Exponential Weights

$\pi_1(a) = 1/A$ for all a

For $t = 1,2,\ldots,T$:

Sample $a_t \sim \pi_t$, and observe $r_t(a_t)$

Define for all a:

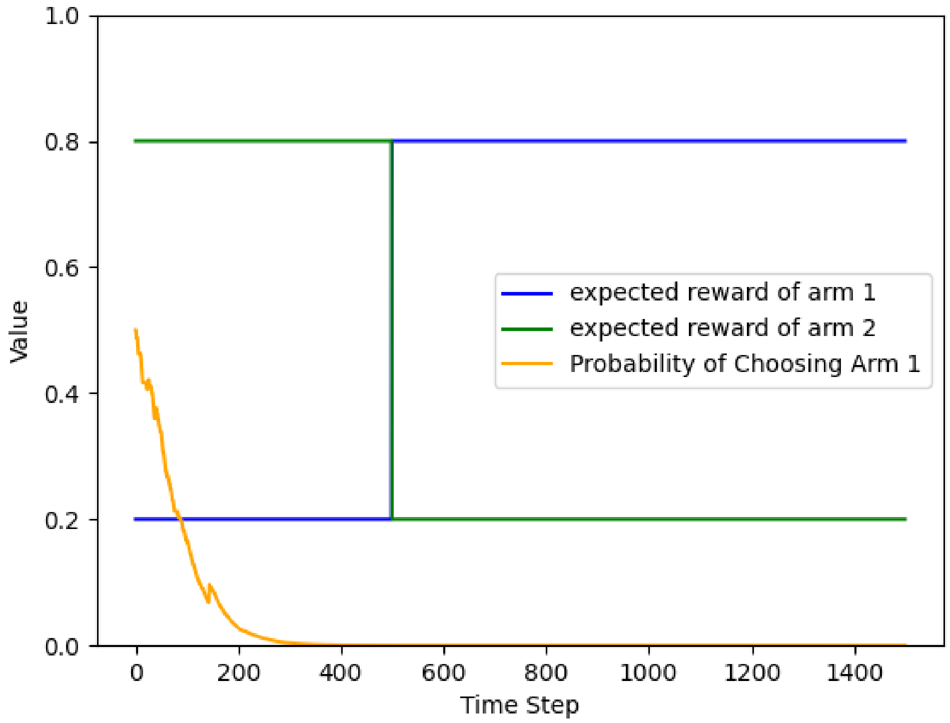
$$\hat{r}_t(a) = \frac{r_t(a)}{\pi_t(a)} \mathbb{I}\{a_t = a\}$$

Update policy:

$$\pi_{t+1}(a) = \frac{\pi_t(a)\exp(\eta \hat{r}_t(a))}{\sum_{a' \in \mathcal{A}} \pi_t(a')\exp(\eta \hat{r}_t(a'))}$$

Simple Experiment

- $A = 2,\ T = 1500,\ \eta = 1/\sqrt{T}$
- For $t \leq 500,\ r_t = [\text{Bernoulli}(0.2), \text{Bernoulli}(0.8)]$
- For $500 < t \leq 1500,\ r_t = [\text{Bernoulli}(0.8), \text{Bernoulli}(0.2)]$
- code



Solution 1: Adding Extra Exploration

- **Idea:** use at least η probability to choose each arm

- Instead of sampling a_t according to π_t, use

$$\pi'_t(a) = (1 - A\eta)\pi_t(a) + \eta$$

Then the unbiased reward estimator becomes

$$\hat{r}_t(a) = \frac{r_t(a)}{\pi'_t(a)} \mathbb{I}\{a_t = a\} = \frac{r_t(a)}{(1 - A\eta)\pi_t(a) + \eta} \mathbb{I}\{a_t = a\}$$

Applying Solution 1

$\pi_1(a) = 1/A$ for all a

For $t = 1,2,\ldots,T$:

Sample a_t from $\pi'_t = (1 - A\eta)\pi_t + A\eta\ \mathrm{uniform}(\mathcal{A})$, and observe $r_t(a_t)$

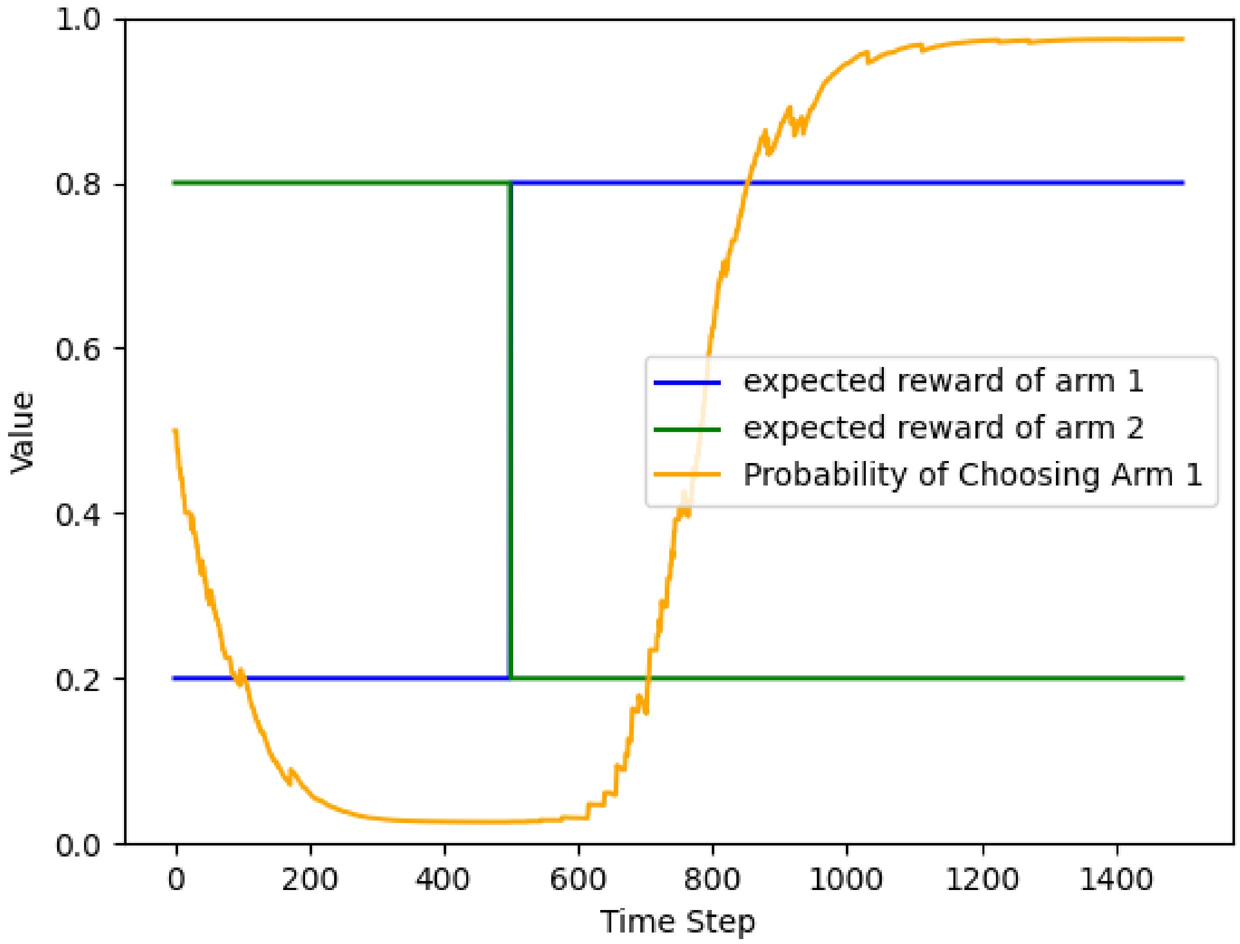
Define for all a:

$$\hat{r}_t(a) = \frac{r_t(a)}{\pi'_t(a)} \mathbb{I}\{a_t = a\}$$

Update policy:

$$\pi_{t+1}(a) = \frac{\pi_t(a)\exp(\eta \hat{r}_t(a))}{\sum_{a' \in \mathcal{A}} \pi_t(a')\exp(\eta \hat{r}_t(a'))}$$

Solution 1: Adding Extra Exploration



Solution 2: Reward Estimator with a Baseline

- The condition only requires $\eta \hat{r}_t(a) \le 1$. The reward estimator is allowed to be **very negative**!

  The fact that mirror ascent **cannot handle** very positive unbiased reward estimator but **can handle** a negative one is somewhat technical in the proof.

- Still sample a_t from π_t, but construct the reward estimator as

$$\hat{r}_t(a) = \frac{r_t(a) - 1}{\pi_t(a)} \mathbb{I}\{a_t = a\} + 1$$

- Why this resolves the issue?

Applying Solution 2

$\pi_1(a) = 1/A$ for all a

For $t = 1,2,\ldots,T$:

Sample a_t from π_t, and observe $r_t(a_t)$

Define for all a:

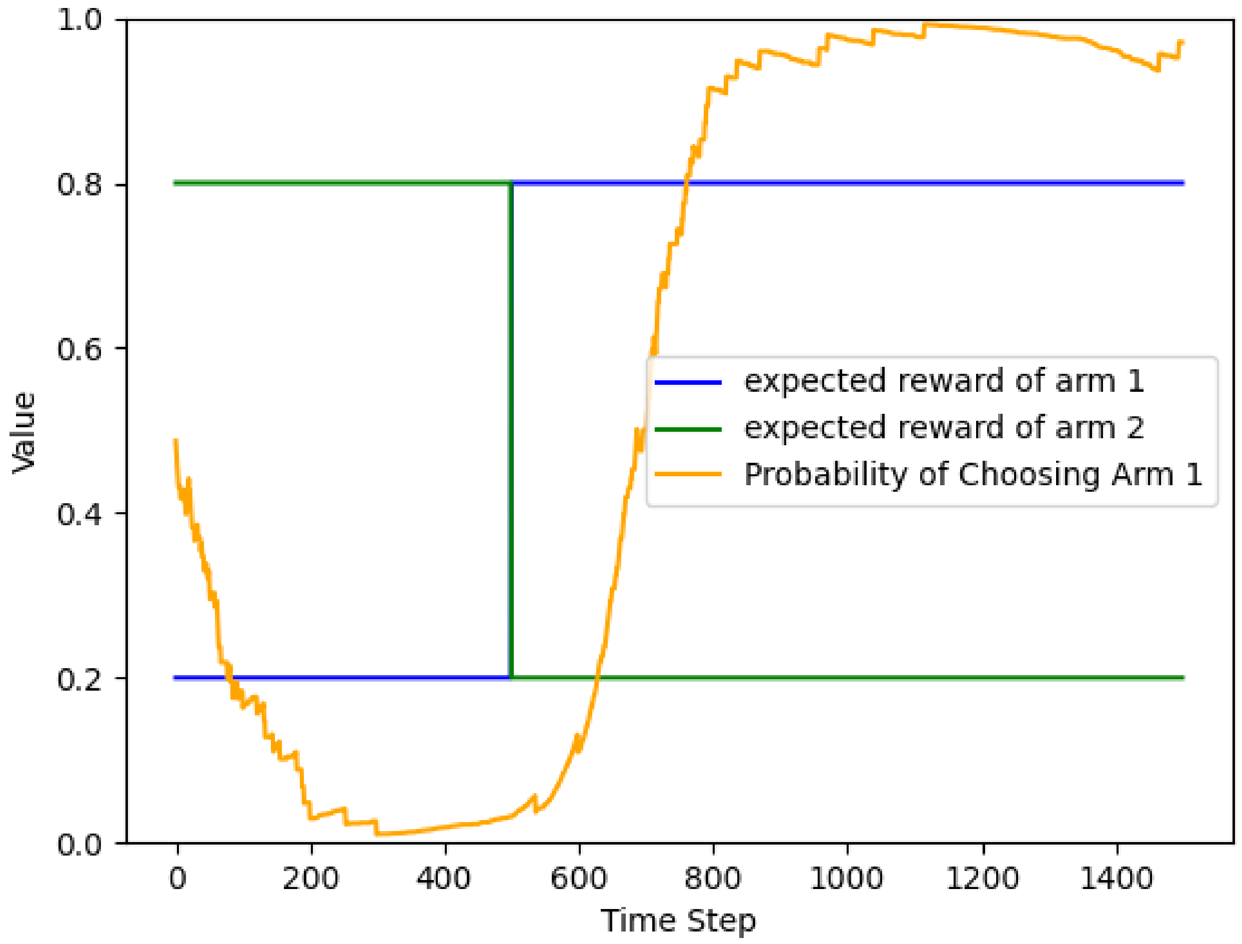
baseline

$$\hat{r}_t(a) = \frac{r_t(a) - 1}{\pi_t(a)} \mathbb{I}\{a_t = a\} + 1 \quad \text{or equivalently} \quad \hat{r}_t(a) = \frac{r_t(a) - 1}{\pi_t(a)} \mathbb{I}\{a_t = a\}$$

Update policy:

$$\pi_{t+1}(a) = \frac{\pi_t(a)\exp(\eta \hat{r}_t(a))}{\sum_{a' \in \mathcal{A}} \pi_t(a')\exp(\eta \hat{r}_t(a'))}$$

Solution 2: Reward Estimator with a Baseline



This is the EXP3 Algorithm

“**Exp**onential weight algorithm for **Exp**loration and **Exp**loitation”

- Exponential weights + either of the two solutions

The Role of Baseline

$$\hat{r}_t(a) = \frac{r_t(a) - b_t}{\pi_t(a)} \mathbb{I}\{a_t = a\}$$

$$\pi_{t+1}(a) = \frac{\pi_t(a)\exp(\eta \hat{r}_t(a))}{\sum_{a' \in \mathcal{A}} \pi_t(a')\exp(\eta \hat{r}_t(a'))} \quad \text{or} \quad \pi_{t+1} = \operatorname*{argmax}_{\pi \in \Delta(\mathcal{A})} \left\{ \langle \pi, \hat{r}_t \rangle - \frac{1}{\eta} \mathrm{KL}(\pi, \pi_t) \right\}$$

Larger b_t: More exploratory (tends to decrease the probability of the action just chosen)

– needed to detect changes in the environment.

We usually set b_t to be close to the recent performance level of the learner itself

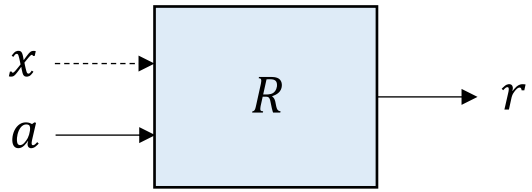
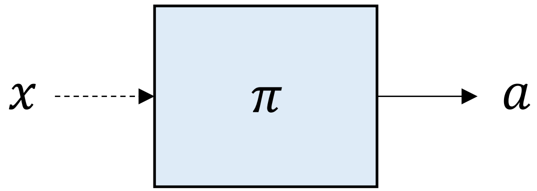
- When finding an action better than the learner itself, increase its probability
- Otherwise, decrease its probability

Summary

- Exponential weight update elements:
    - Incremental update (2 equivalent forms)
    - Importance weighting because we only observe the reward of the action we choose (otherwise the reward is **biased**)
    - **Baseline or extra uniform exploration** to encourage exploration

Review: Exploration Strategies for Bandits

x: context, a: action, r: reward

		MAB	CB
Value-based	 (context, action) to reward	Mean estimation + EG, BE Uncertainty as bonus	Regression + EG, BE
Policy-based	 context to action distribution	KL-regularized update with reward estimators (EXP3) + baseline, uniform exploration	**Next**

Contextual Bandits

Contextual Bandits

For time $t = 1, 2, \dots, T$:

Environment generates a context $x_t \in \mathcal{X}$

Learner chooses an action $a_t \in \mathcal{A}$

Learner observes $r_t(x_t, a_t)$

KL-Regularized Policy Updates

$$\pi_{t+1} = \underset{\pi \in \Delta(\mathcal{A})}{\operatorname{argmax}} \left\{ \sum_a \pi(a)\hat{r}_t(a) - \frac{1}{\eta} \sum_a \pi(a) \log \frac{\pi(a)}{\pi_t(a)} \right\}$$

$$\hat{r}_t(a) = \frac{r_t(a) - b_t}{\pi_t(a)} \, \mathbb{I}\{a_t = a\}$$

In practice, set b_t as a **running average** of $r_t(a_t)$ to track the learner's own performance.

The larger b_t is, the more exploration.

$$\theta_{t+1} = \underset{\theta}{\operatorname{argmax}} \left\{ \sum_a \pi_\theta(a|x_t) \, \hat{r}_t(x_t, a) - \frac{1}{\eta} \sum_a \pi_\theta(a|x_t) \log \frac{\pi_\theta(a|x_t)}{\pi_{\theta_t}(a|x_t)} \right\}$$

$$\hat{r}_t(x_t, a) = \frac{r_t(x_t, a) - b_t(x_t)}{\pi_{\theta_t}(a|x_t)} \, \mathbb{I}\{a_t = a\}$$

KL-Regularized Policy Updates

For $t = 1, 2, \dots, T$:

Receive context x_t

Take action $a_t \sim \pi_{\theta_t}(\cdot|x_t)$ and receive reward $r_t(x_t, a_t)$

Create reward estimator $\hat{r}_t(x_t, a) = \frac{r_t(x_t,a) - b_t(x_t)}{\pi_{\theta_t}(a|x_t)} \mathbb{I}\{a_t = a\}$

Update

$$\theta_{t+1} = \underset{\theta}{\operatorname{argmax}} \left\{ \sum_a \pi_\theta(a|x_t)\, \hat{r}_t(x_t, a) - \frac{1}{\eta} \sum_a \pi_\theta(a|x_t) \log \frac{\pi_\theta(a|x_t)}{\pi_{\theta_t}(a|x_t)} \right\}$$

KL-Regularized Policy Updates with Batches (PPO for CB)

For $t = 1, 2, \ldots, T$:

For $i = 1, \ldots, N$:

Receive context x_i

Take action $a_i \sim \pi_{\theta_t}(\cdot|x_i)$ and receive reward $r_i(x_i, a_i)$

Create reward estimator $\hat{r}_i(x_i, a) = \frac{r_i(x_i,a) - b_t(x_i)}{\pi_{\theta_t}(a|x_i)} \mathbb{I}\{a_i = a\}$

For $j = 1, \ldots, M$:

Solve argmax

For minibatch $\mathcal{B} \subset \{1, 2, \ldots, N\}$ of size B:

$$\theta \leftarrow \theta + \nabla_\theta \frac{1}{B} \sum_{i \in \mathcal{B}} \left(\sum_a \pi_\theta(a|x_i)\, \hat{r}_i(x_i, a) - \frac{1}{\eta} \sum_a \pi_\theta(a|x_i) \log \frac{\pi_\theta(a|x_i)}{\pi_{\theta_t}(a|x_i)} \right)$$

$$= \theta + \nabla_\theta \frac{1}{B} \sum_{i \in \mathcal{B}} \left(\frac{\pi_\theta(a_i|x_i)}{\pi_{\theta_t}(a_i|x_i)} \left(r_i(x_i, a_i) - b_t(x_i)\right) - \frac{1}{\eta} \sum_a \pi_\theta(a|x_i) \log \frac{\pi_\theta(a|x_i)}{\pi_{\theta_t}(a|x_i)} \right)$$

$\theta_{t+1} \leftarrow \theta$

KL-Regularized Policy Updates with Batches (PPO for CB)

$$\theta \leftarrow \theta + \nabla_\theta \frac{1}{B} \sum_{i \in \mathcal{B}} \left(\frac{\pi_\theta(a_i|x_i)}{\pi_{\theta_t}(a_i|x_i)} (r_i(x_i, a_i) - b_t(x_i)) - \frac{1}{\eta} \underbrace{\sum_a \pi_\theta(a|x_i) \log \frac{\pi_\theta(a|x_i)}{\pi_{\theta_t}(a|x_i)}}_{\mathrm{KL}\left(\pi_\theta(\cdot\,|x_i),\, \pi_{\theta_t}(\cdot\,|x_i)\right)} \right)$$

Estimating KL by Samples

http://joschu.net/blog/kl-approx.html

Sample $a_i \sim \pi_{\theta_t}(\cdot\,|x_i)$ and define $kl_i(\theta_t, \theta) = \boxed{\frac{\pi_\theta(a_i|x_i)}{\pi_{\theta_t}(a_i|x_i)} - 1 - \log \frac{\pi_\theta(a_i|x_i)}{\pi_{\theta_t}(a_i|x_i)}}$

Just need one sample of a_i

Then $\mathbb{E}_{a_i}[kl_i(\theta_t, \theta)] = \mathrm{KL}\left(\pi_{\theta_t}(\cdot\,|x_i), \pi_\theta(\cdot\,|x_i)\right)$

PPO with KL Estimator

$$kl_i(\theta_t, \theta) = \frac{\pi_\theta(a_i|x_i)}{\pi_{\theta_t}(a_i|x_i)} - 1 - \log \frac{\pi_\theta(a_i|x_i)}{\pi_{\theta_t}(a_i|x_i)}$$

For $t = 1, 2, \dots, T$:

For $i = 1, \dots, N$:

Receive context x_i

Take action $a_i \sim \pi_{\theta_t}(\cdot|x_i)$ and receive reward $r_i(x_i, a_i)$

Create reward estimator $\hat{r}_i(x_i, a) = \frac{r_i(x_i,a) - b_t(x_i)}{\pi_{\theta_t}(a|x_i)} \mathbb{I}\{a_i = a\}$

For $j = 1, \dots, M$:

For minibatch $\mathcal{B} \subset \{1, 2, \dots, N\}$ of size B:

$$\theta \leftarrow \theta + \nabla_\theta \frac{1}{B} \sum_{i \in \mathcal{B}} \left(\frac{\pi_\theta(a_i|x_i)}{\pi_{\theta_t}(a_i|x_i)} (r_i(x_i, a_i) - b_t(x_i)) - \frac{1}{\eta} kl_i(\theta_t, \theta) \right)$$

$\theta_{t+1} \leftarrow \theta$

Summary: PPO (Proximal Policy Optimization)

- PPO-CB is an extension of EXP3 to contextual bandits. The central idea is KL-regularized policy updates
- PPO is a strong algorithm for RL in MDPs