

- HW2 due 2/18
- PRA3 due 2/22
- Course project progress report I due 2/27
- Come to OH for course project discussion!

Artificial Intelligence Methods for Social Good Lecture 10 Basics of Multi-Armed Bandit

17-537 (9-unit) and 17-737 (12-unit) Instructor: Fei Fang <u>feifang@cmu.edu</u>



- Multi-Armed Bandit (MAB) Problems
- Bandit Data-Driven Optimization in Food Rescue
- Markov Decision Process
- Restless Multi-Armed Bandits

Learning Objectives

- Understand the concept of
 - Multi-Armed Bandit (MAB)
 - Zero-regret strategy
 - Upper Confidence Bound (UCB)
 - Probably approximately correct (PAC)
 - Markov Decision Process
 - Restless Multi-Armed Bandits

A Simple Sequential Decision Making Problem

- Multi-Armed Bandit (MAB)
 - K arms (slot machines)
 - Each arm k is associated with a reward distribution R_k (pdf $p_k(r)$), with expected reward μ_k

$$\mu_k = \mathbb{E}_{r \sim R_k}[r] = \int_r r p_k(r) dr$$



- Gambler does not know R_k , μ_k
- In each round $t \in \{1 \dots T\}$, gambler chooses one arm I_t , and observe a reward r_t drawn from the distribution R_{I_t}

Multi-Armed Bandit (MAB)

- A special case: Binary MAB
 - Reward is either 0 or 1
 - $\Pr(r = 1) = p_k$, $\Pr(r = 0) = 1 p_k$, $\mu_k = p_k$

	Arm I	Arm 2	Arm 3
μ_k	0.2	0.3	0.7

Multi-Armed Bandit (MAB)

• Let
$$\mu^* = \max_k \mu_k$$

- Define regret $\rho_T = T\mu^* \sum_{t=1}^T r_t$
- A typical task in MAB: find zero-regret strategy
 lim_{T→∞} p_{T/T} = 0

	Arm I	Arm 2	Arm 3
μ_k	0.2	0.3	0.7

If always choose arm 1, what is the expected regret?

 $\mathbb{E}[\rho_T] =$

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If always choose arm 1, what is the expected regret?

$$\mathbb{E}[\rho_T] = \mathbb{E}\left[T\mu^* - \sum_{t=1}^T \widehat{r_t}\right] = T\mathbb{E}[\mu^*] - \mathbb{E}\left[\sum_{t=1}^T \widehat{r_t}\right] = T*0.7 - T*0.3 = 0.4T$$

Poll I

$$\mu^* = \max_k \mu_k$$
$$\rho_T = T\mu^* - \sum_{t=1}^T \widehat{r_t}$$

- Consider a MAB with 3 arms and the expected reward for arm $k \in \{1..3\}$ is $\mu_k = k/3$. If we randomly choose an arm to pull in each round for T rounds, what would be the expected average regret $\mathbb{E}[\frac{\rho_T}{T}]$?
- A: I B: $\frac{1}{2}$ C: $\frac{1}{3}$ D: $\frac{2}{3}$
- E: None of the above
- F: I don't know

	Arm I	Arm 2	Arm 3
μ_k	I/3	2/3	I

Poll I

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$$\mu^* = \max_k \mu_k$$
$$\rho_T = T\mu^* - \sum_{t=1}^T \widehat{r_t}$$

• Consider a MAB with 3 arms and the expected reward for arm $k \in \{1..3\}$ is $\mu_k = k/3$. If we randomly choose an arm to pull in each round for T rounds, what would be the expected average regret $\mathbb{E}[\frac{\rho_T}{T}]$?

$$\mathbb{E}\left[\frac{\rho_T}{T}\right] = \mathbb{E}\left[\frac{T\mu^* - \sum_{t=1}^T \hat{r_t}}{T}\right] = \mathbb{E}[\mu^*] - \mathbb{E}\left[\frac{\sum_{t=1}^T \hat{r_t}}{T}\right] = 1 - \frac{\sum_k \mu_k}{n}$$
$$= 1 - \frac{n(n+1)}{2n^2} = 1 - \frac{n+1}{2n} = 1 - \frac{1}{2} - \frac{1}{2n} = \frac{1}{2} - \frac{1}{2n} = \frac{1}{2} - \frac{1}{6} = \frac{1}{3}$$

Discussion

- What problems you encounter in your daily life can be viewed / modeled as an MAB problem?
- In those problems, how do you choose the arm to pull in each time step?

Probably approximately correct (PAC) and MAB

- Probably approximately correct (PAC): with high probability, it is close to being correct $Pr(error \le \epsilon) \ge 1 \delta$
- ► PAC version of zero-regret strategy $\Pr(\lim_{T \to \infty} \frac{\rho}{T} \le \epsilon) \ge 1 - \delta$

- In binary MAB, reward is either 0 or 1
- Let N(k) be the number of times that k is chosen
- Let H(k) be the number of times that k is chosen and reward is 1
- Let $\widehat{\mu_k} = H(k)/N(k)$, average reward when k is chosen
- Given N(k), H(k), $\widehat{\mu_k}$, we can estimate the range of μ_k

$$\widehat{\mu_k} = H(k)/N(k)$$

According to Chernoff-Hoeffding Bound

$$\Pr(\widehat{\mu_k} \ge \mu_k + a) \le e^{-2a^2 N(k)}$$

$$\Pr(\widehat{\mu_k} \le \mu_k - a) \le e^{-2a^2 N(k)}$$

• So
$$\Pr(\widehat{\mu_k} - a \le \mu_k \le \widehat{\mu_k} + a) \ge 1 - 2e^{-2a^2N(k)}$$

What do we know from this?

If we set
$$a = \sqrt{\frac{2 \ln t}{N(k)}}$$
 and $\mu_{LB}^k = \widehat{\mu_k} - a$, $\mu_{UB}^k = \widehat{\mu_k} + a$
Then $\Pr(\mu_{LB}^k \le \mu_k \le \mu_{UB}^k) \ge 1 - 2t^{-4}$

- Chernoff-Hoeffding Bound: Let X_1, X_2, \ldots, X_n be independent random variables in the range [0, 1] with $\mathbb{E}[X_i] = \mu$. Then for a > 0 $\Pr(\frac{1}{n}\sum_{i}X_{i} \ge \mu + a) \le e^{-2a^{2}n}$ $\Pr(\frac{1}{n}\sum_{i=1}^{n}X_{i} \le \mu - a) \le e^{-2a^{2}n}$
- That is, with high probability, the observed average value of X_i is very close to the expected value of X_i

- UCBI Algorithm:
 - Always choose the arm with the highest upper confidence bound defined as $\mu_{UB}^k = \widehat{\mu_k} + \sqrt{\frac{2 \ln t}{N(k)}}$
 - Intuition: If μ_{UB}^k is large, either arm k is a good arm or N(k) is small (not enough data is gathered)
 - General principle: optimism in the face of uncertainty

UCBI Algorithm

Initialize $H(\cdot) = 0, N(\cdot) = 0, \mu_{UB} = 0, \hat{\mu} = 0$ For t = 1..TChoose arm $k_t = \operatorname{argmax}_k \mu_{UB}^k$ Get reward $r_t \sim Bernoulli(\mu_k)$ Update $H(k_t) \leftarrow H(k_t) + r_t$ Update $N(k_t) \leftarrow N(k_t) + 1$ Update $\hat{\mu}_{k_t} = \frac{H(k_t)}{N(k_t)}$ For k = 1..NUpdate $\mu_{UB}^k \leftarrow \hat{\mu}_k + \sqrt{\frac{2 \ln t}{N(k)}}$

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UCBI Algorithm

```
Initialize H(\cdot) = 0, N(\cdot) = 0, \mu_{UB} = 0, \hat{\mu} = 0

For t = 1..T

Choose arm k_t =

Get reward r_t \sim

Update H(k_t) \leftarrow H(k_t) + r_t

Update N(k_t) \leftarrow N(k_t) + 1

Update \hat{\mu}_{k_t} = \frac{H(k_t)}{N(k_t)}

For k = 1..N

Update \mu_{UB}^k \leftarrow
```

- (T/F) Follow UCBI algorithm. Assume that in round t, arm 1 has the highest upper confidence bound µ^k_{UB} among all arms
- If µ¹_{UB} − µ¹_{LB} ≤ ε, then the difference between the optimal expected reward among all arms and the average value of arm 1 is guaranteed to be no larger than ε with high probability, i.e.,

$$\Pr\left(\max_{k}\mu_{k}-\mu_{1}\leq\epsilon\right)\geq1-2t^{-4}?$$

Poll 2

• (T/F) If $\mu_{UB}^1 - \mu_{LB}^1 \le \epsilon$, then the difference between the optimal expected reward among all arms and the average value of arm I is guaranteed to be no larger than ϵ with high probability, i.e.,

$$\Pr\left(\max_{k}\mu_{k}-\mu_{1}\leq\epsilon\right)\geq1-2t^{-4}?$$

$$v_{1}-\tau_{1}=1$$

$$v_{2}-v_{1}\leq\epsilon$$

$$\mu_{k}\geq\mu_{vB}^{k}-\epsilon$$

$$\mu_{k}'\leq\mu_{vB}^{k'}\leq\mu_{vB}^{k}$$

$$s_{0}\quad\mu_{k'}-\mu_{k'}\leq\epsilon$$

A Practical Problem: Video Recommendation

- You need to recommend videos to a user
- Each arm corresponds to a video
- Pull an arm: recommend the video to the user
- Reward: whether user clicks/likes the video
- Q: Can we use UCB1 to decide which video to recommend? What are the issues with this approach if we want to deploy it on Youtube?

Discussion

In food rescue domain that we have discussed, is there any problem that can be formulated as a MAB problem?

Contextual Bandits

- K arms
- In round $t \in \{1 \dots T\}$, we observe context $\mathbf{x}_{k,t}$ for all arms $k \in \{1 \dots K\}$, then choose an arm I_t , and receive reward r_t which depends on I_t and $\mathbf{x}_{I_t,t}$
- In video recommendation, x_{k,t} can be features of the user-video pair
- In food rescue, x_{k,t} can be features of the rescuevolunteer pair

LinUCB Overview (Disjoint linear models)

- Assume reward is a arm-dependent linear function of context vector + noise
 - $\succ r_t = \mathbf{x}_{I_t,t}^T \boldsymbol{\theta}_{I_t}^* + \epsilon_t$
 - $\blacktriangleright \mathbb{E}[r_t] = \mathbf{x}_{I_t,t}^T \boldsymbol{\theta}_{I_t}^*$
 - > θ_k^* are unknown coefficient vector associated with each arm
- After a number of rounds, for each arm k, apply linear regression on existing data $(\mathbf{x}_{I_t,t}, r_t)$ where $I_t = k$ to get estimated $\widehat{\boldsymbol{\theta}}_k^*$
- For a new round t, calculate the UCB for each arm k based on $\mathbf{x}_{k,t}^T \widehat{\boldsymbol{\theta}}_k^*$
- Choose the arm with the highest UCB

LinUCB Overview (Hybrid linear models)

$$\mathbf{E}[r_t] = \mathbf{z}_{I_t,t}^T \boldsymbol{\beta}^* + \mathbf{x}_{I_t,t}^T \boldsymbol{\theta}_{I_t}^*$$

- $\boldsymbol{\beta}^*$ is a shared coefficient vector across all arms
- Can still apply linear regression to get estimated $\widehat{\pmb{eta}}^*$ and $\widehat{\pmb{ heta}}^*_k$
- For a new round *t*, calculate the UCB for each arm *k* based on $\mathbf{z}_{k,t}^T \widehat{\boldsymbol{\beta}}^* + \mathbf{x}_{k,t}^T \widehat{\boldsymbol{\theta}}_k^*$
- Choose the arm with the highest UCB
- Q:What if we already have some data, but we don't believe the reward is a linear function of context?

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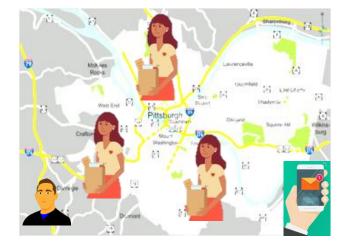


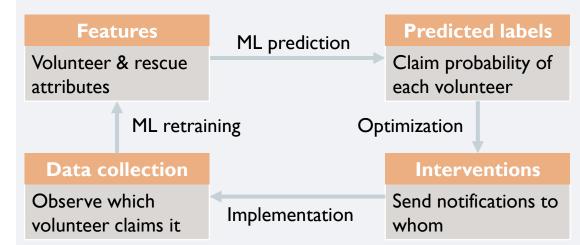
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Multi-Armed Bandit (MAB) Problems

- Bandit Data-Driven Optimization in Food Rescue
 (Optional)
- Markov Decision Process
- Restless Multi-Armed Bandits

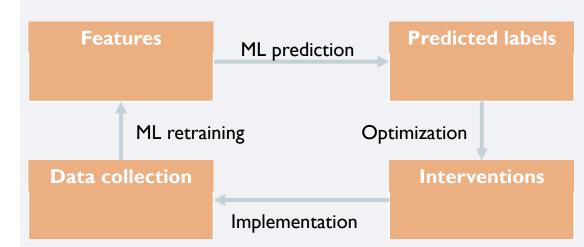
Volunteer engagement as iterative prediction-prescription



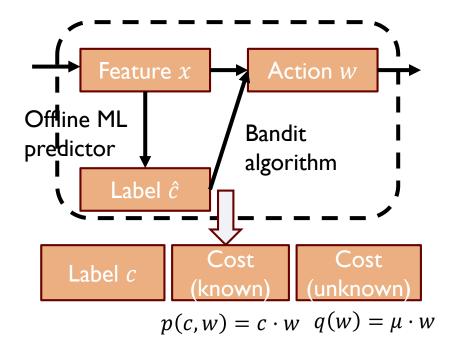


Application-independent iterative prediction-prescription

- Data-driven optimization
 [Bertsimas and Kallus, 2020;
 Elmachtoub and Grigas, 2017]
- Decision-focused learning [Donti et al., 2017]
- Contextual/linear bandit [Dani et al., 2008; Lai and Robbins, 1985]



Bandit data-driven optimization



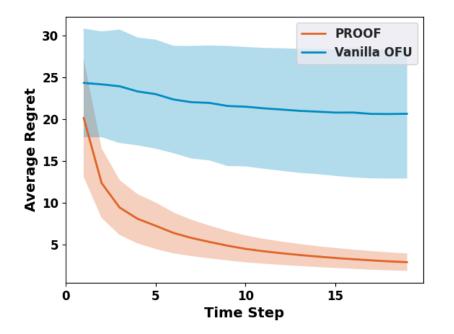
Optimal policy: $\pi(\mathbf{x}) = \arg\min_{\mathbf{w}} \mathbb{E}_{\mathbf{c},\eta|\mathbf{x}}[u(\mathbf{c},\mathbf{w})]$

Regret:
$$R_T = \mathbb{E}_{x,c,\eta} \left[\sum_{t=1}^T \left(u(\mathbf{c}^t, \mathbf{w}^t) - u(\mathbf{c}^t, \pi(\mathbf{x}^t)) \right) \right]$$

PROOF: PRedict-then-Optimize with Optimism in Face of uncertainty

Algorithm 2: PROOF: Predict-then-optimize with optimism in face of uncertainty		
1 Initialize:		
Find a barycentric spanner b_1, \ldots, b_d for W		
3 Set $A_i^1 = \sum_{j=1}^d b_j b_j^{\dagger}$ and $\hat{\mu}_i^1 = 0$ for all $i = 1, 2,, n$		
4 Receive initial dataset $\mathcal{D} = \{(x_i^0, c_i^0; w_i^0)_{i=1,,n}\}$ from distribution D on (X, C) .		
5 for $t = 1, 2,, T$ do		
Train the ML model & use it to make a prediction	Theorem.	
	Assuming ordinary	
8		
, Set the confidence radius for UCB	least squares	
10	regression, the	
¹¹ Select action by integrating UCB with offline ML model	PROOF algorithm has	
12	regret $ ilde{O}(n\sqrt{dmT})$	
13 Receive the true labels and cost		
	with probability $1 - \delta$.	
14		
Update the bandit cost estimate		

Numerical simulations



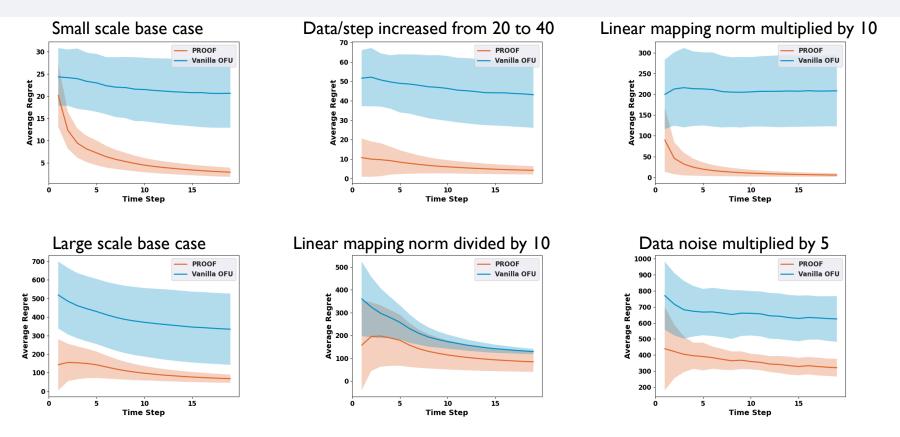
PROOF converges

- much faster, and
- with smaller variance

than vanilla bandit.

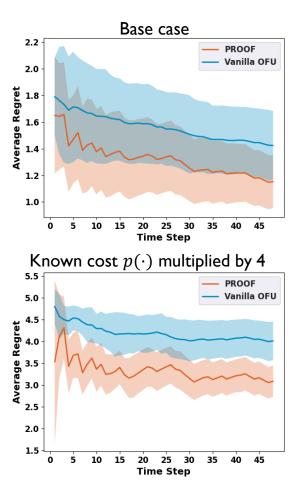
Numerical simulations

PROOF outperforms vanilla bandit in both convergence speed and variance.



PROOF for food rescue volunteer recommendation

Feature x	Volunteer-rescue pair features
Label $c \in \{0, 1\}^d$	whether volunteer claimed the rescue
Action $w \in \{0, 1\}^d$	whether to send push notifications to each volunteer
Known cost $p(c, w)$	whether we send push notifications to the "right" volunteer
Unknown cost $q(w)$	how volunteers might react to notifications





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General Sequential Decision Making Problems

- The agent move from state to state
- At each time step, the agent choose an action
- Action bring the agent to a successor state
- Actions and / or states lead to reward
- A rational agent acts so as to maximize the expected utility in total (which is some function of the reward)







Markov Decision Process (MDP)

- Special case of sequential decision problems
- MDP = (S, A, T, R, γ)
 - ▶ S: set of states, $s_t \in S$ (where can agent be?)
 - ▶ A: set of actions, $a_t \in A$
- (where can agent be?) (what can agent do?)
- > T: transition function $T(s_t, a_t, s_{t+1}) = \mathbb{P}(s_{t+1}|s_t, a_t)$

(what happens next?)

Next state only depends on the current state, not previous states! (Markovian)

 R: reward function r_t = R(s_t) or R(s_t, a_t) or R(s_t, a_t, s_{t+1}) (what do I gain?)
 γ ∈ [0, 1] (discount factor)

Markov Decision Process (MDP)

- Assume an agent starts at s_0 , takes action a_0 , gets reward r_0 , arrives at s_1 , takes action a_1 , ...
- Agent's utility = accumulated reward with discount = $\sum_t \gamma^t r_t$





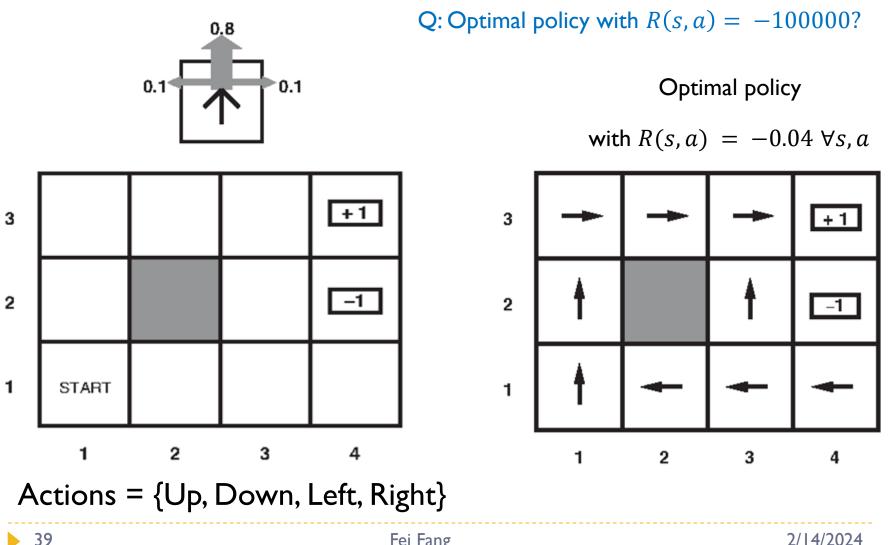


Markov Decision Process (MDP)

$$\mathsf{MDP} = (S, A, T, R, \gamma)$$

- (Deterministic) Policy π: S → A
 Maps state to action, defines a plan
- Given a policy π , we can sample history $h = \{s_0, a_0, s_1, a_1, ...\}$
- Goal: find π to maximize utility
 - Expected
 - $\pi^* = \operatorname{argmax}_{\pi} \mathbb{E}_{h \sim \pi} \left[\sum_t \gamma^t R(s_t, \pi(s_t)) \right]$
- Myopic strategy does not work: a_t affects future states

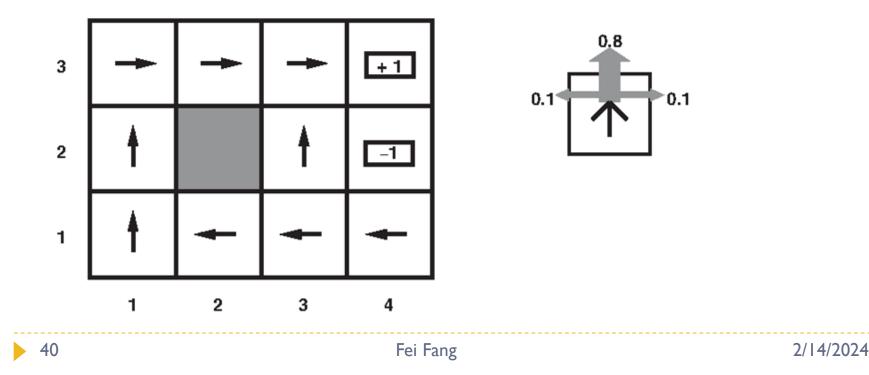
Example



Fei Fang

Example

- If we want to find optimal policy through brute force search: Enumerate all possible policies and compare expected utility
- How to compute/estimate the expected utility?



Value Function

The value function of a given policy π describes the expected accumulated reward with discount starting from a state

$$V^{\pi}(s) = \mathbb{E}\left[\sum_{t=0}^{\infty} \gamma^{t} R(s_{t}, \pi(s_{t}))\right]$$

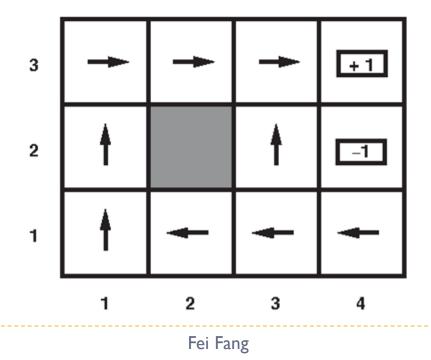
Where $s_0 = s$

Sometimes called state value function or V-value function

Value Function

The goal can be restated as finding the policy π that lead to the optimal V^π(s), i.e., argmax V^π(s)

$$V(s) = V^*(s) = \max_{\pi} V^{\pi}(s) = V^{\pi^*}(s)$$

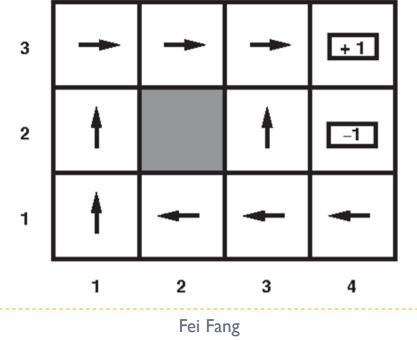


Value Function

Q: Given $V^*(s)$, how to find the optimal policy?

Pick the action which maximizes *current* + *future reward* (assuming continued optimal behavior)

$$\pi^*(s) = \operatorname*{argmax}_{a \in A} \left[R(s, a) + \gamma \sum_{s'} \mathbb{P}(s'|s, a) V^*(s') \right], \forall s$$



Bellman Equation

• $V^*(s)$ satisfy the following Bellman Equation

$$V^{*}(s) = \max_{a \in A} \left[R(s, a) + \gamma \sum_{s'} \mathbb{P}(s'|s, a) V^{*}(s') \right]$$

Necessary and sufficient condition for optimality!

Q-Value Function

- Similar to state value function $V^{\pi}(s)$, but defined on state-action pair
- Q^π(s, a): expected total reward from state s onward if taking action a in state s, and follow policy π afterward

That is
$$Q^{\pi}(s, a) = R(s) + \gamma \sum_{s'} P(s'|s, a) V^{\pi}(s')$$

Obviously $V^{\pi}(s) = Q^{\pi}(s, \pi(s))$

So $Q^{\pi}(s, a) = R(s) + \gamma \sum_{s'} P(s'|s, a) Q^{\pi}(s', \pi(s'))$

Optimal Q-Value

Recall $V^{\pi}(s) = R(s) + \gamma \sum_{s'} P(s'|s, \pi(s)) V^{\pi}(s')$ And $Q^{\pi}(s, a) = R(s) + \gamma \sum_{s'} P(s'|s, a) V^{\pi}(s')$ And $V^{\pi}(s) = Q^{\pi}(s, \pi(s))$

• When using optimal policy π^* , we will take the action that leads to maximum total utility at each state

$$\pi^*(s) = \operatorname*{argmax}_a Q^*(s, a)$$

Therefore

$$V^*(s) = Q^*(s, \pi^*(s)) = \max_a Q^*(s, a)$$
$$Q^*(s, a) = R(s) + \gamma \sum_{s'} P(s'|s, a) V^*(s')$$
$$= R(s) + \gamma \sum_{s'} P(s'|s, a) \max_{a'} Q^*(s', a')$$
Bellman Equation

Again, necessary and sufficient condition for optimality!

How to Solve MDPs (Non-Exhaustive List)

Exact

- Value Iteration
- Policy Iteration
- Linear Programming

Approximate

- Sampling-based
- Function approximation

How to Solve MDPs in Practice

- Call MDP solvers
 - E.g., MDP toolbox in python

>>> import mdptoolbox, mdptoolbox.example
>>> P, R = mdptoolbox.example.rand(10, 3)
>>> pi = mdptoolbox.mdp.PolicyIteration(P, R, 0.9)
>>> pi.run()



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Restless Multi-Armed Bandit

- N arms
- Each arm is a 2-action MDP
 - In time t, an arm is in some state
 - Two possible actions: active (pull the arm), or passive (not pull the arm)
 - Action brings the planner reward and brings the arm into a successor state in time t + 1
 - "Restless": state transition happens even if the arm is not pulled
- Planner can observe the state of each arm, and pull αN arms in each time step





 $\mathsf{MDP} = (S, A, T, R, \gamma)$

Example

- You take 5 courses this semester
- Each arm is a course
- Everyday, you choose two courses and spend 4 hours on each of them
- The state of each arm is your level of understanding of the course material
- If you choose a course A in one day, your level of understanding for course A ↑
- If you do not choose A in one day, your level of understanding for course A ↓ (we forget things ☺)

Discussion

- What real-world problems can be viewed / modeled as a restless MAB problem?
- Can you design a heuristic way of choosing the arms to pull?

Restless Multi-Armed Bandit

- Assuming you know the MDP associated with each arm, how to choose the arms to pull in each time step given the observed states of the arms?
- Whittle solution approach:
 - Key idea: "passive subsidy" a hypothetical reward offered to the planner, in addition to the original reward function, for choosing the passive action
 - Whittle Index: Infimum subsidy that makes the planner indifferent between the "active" and the "passive" actions

$$W(s) = \inf_{\lambda} \{\lambda: Q_{\lambda}(s, passive) = Q_{\lambda}(s, active)\}$$

• Choose the arms with highest W(s)

Backup Slides

Value Iteration

Value Iteration

Initialize $V_0^*(s) \leftarrow 0$ Typical termination condition: difference< ϵ Iterate $V_{i+1}^*(s) \leftarrow \max_{a \in A} [R(s,a) + \gamma \sum_{s'} \mathbb{P}(s'|s,a)V_i^*(s')]$

Based on state-value Bellman Equations

$$V^{*}(s) = \max_{a \in A} \left[R(s, a) + \gamma \sum_{s'} \mathbb{P}(s'|s, a) V^{*}(s') \right]$$

- Consider the finite horizon view: Pretend we have a really long horizon
- aka 'Value update', 'Bellman backups/updates'
- Guaranteed to converge to $V^*(s)$

What is the optimal policy π^* ?

Policy Iteration

Not necessary to get an accurate estimate of V^* to induce π^*

Policy iteration

- Compute optimal policy π^* directly
- Iterate between 2 steps
 - Policy Evaluation (check how good current policy is)
 - Policy Improvement (get a 'better' policy)

Policy Iteration

- Policy Evaluation
 - Method I: Iterative approach
 - $\blacktriangleright V_{i+1}^{\pi}(s) \leftarrow R(s,\pi(s)) + \gamma \sum_{s'} \mathbb{P}(s'|s,a) V_i^{\pi}(s'), V_0^{\pi}(s) \leftarrow 0$
 - Method 2: Solve system of linear equations
 - $V^{\pi}(s) = R(s, \pi(s)) + \gamma \sum_{s'} \mathbb{P}(s'|s, a) V^{\pi}(s')$
- Policy Improvement

 $\pi^{new}(s) \leftarrow \operatorname*{argmax}_{a \in A} \left[R(s,a) + \gamma \sum_{s'} \mathbb{P}(s'|s,a) V^{\pi}(s') \right]$

- Note that when π is optimal, π^{new} is the same as π
- Policy iteration converges to the optimal policy in a finite number of steps
- Often converge faster than value iteration

LinUCB

- Assume reward is a arm-dependent linear function of context vector + noise
 - $\succ r_t = \mathbf{x}_{I_t,t}^T \theta_{I_t}^* + \epsilon_t$
 - $\mathbf{E}[r_t] = \mathbf{x}_{I_t,t}^T \theta_{I_t}^*$
 - $\blacktriangleright \ \theta^*$ are unknown coefficient vector associated with each arm