Exploration in MDPs

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We have addressed all 3 main challenges in online RL

Data + Function approximation

Generalization

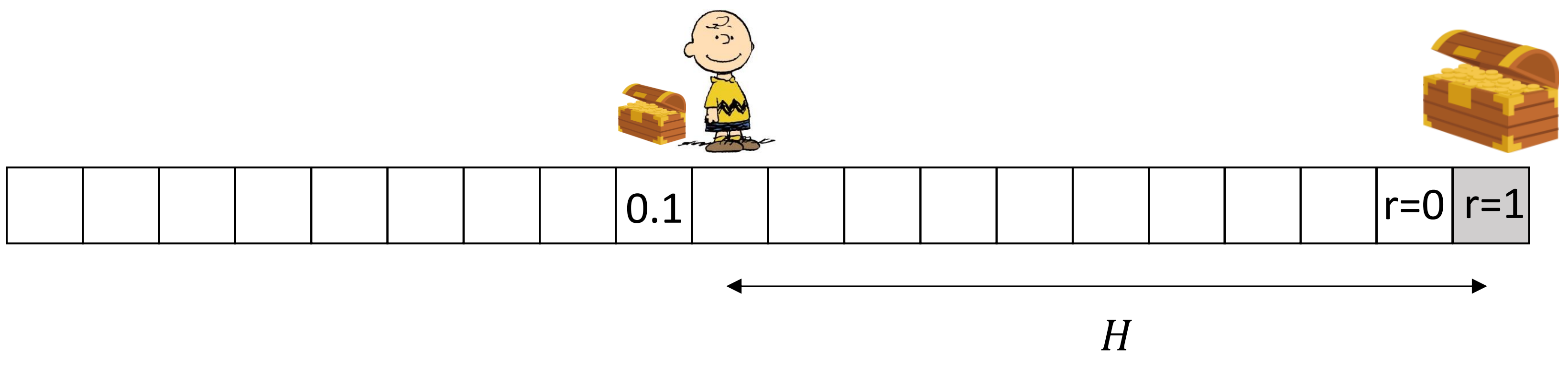
EG
BE
IGW
UCB
TS

Exploration

Credit Assignment

VI
PI

We have addressed all 3 main challenges in online RL (?)



Environment:

- Fixed-horizon MDP with episode length H
- Initial state at 0
- A single rewarding state at state H
- Actions: Go LEFT or RIGHT

Suppose we perform DQN with ϵ-greedy with random initialization
⇒ On average, we need 2^H episodes to see the reward
(before that, we won't make any meaningful update and will just do random walk around state 0)

Regret Analysis for MDPs?

- We have done regret analysis for several bandit algorithms:
  - Regression oracle + (ϵ-greedy or inverse gap weighting)
  - UCB
  - EXP3

- We did not really establish regret bounds for MDPs
  - Partially – DQN under 2 assumptions: the data in replay buffer is exploratory and Bellman completeness
  - Not for policy-iteration-based algorithms

Regret Analysis for MDPs?

$$\mathbb{E}_{s\sim\rho}\left[V^{\pi^\star}(s)\right] - \mathbb{E}_{s\sim\rho}\left[V^{\pi}(s)\right]$$

1

$$= \sum_{s,a} d_\rho^\pi(s)\left(\pi^\star(a|s) - \pi(a|s)\right)\underline{Q^\star(s,a)} = \sum_{s,a} d_\rho^\pi(s,a)\left(V^\star(s) - Q^\star(s,a)\right)$$

For VI-based algorithm (approximating $Q^\star$)

Approximating $Q^\star(s,a)$ requires the replay buffer to cover **wide range of** state-actions.

2

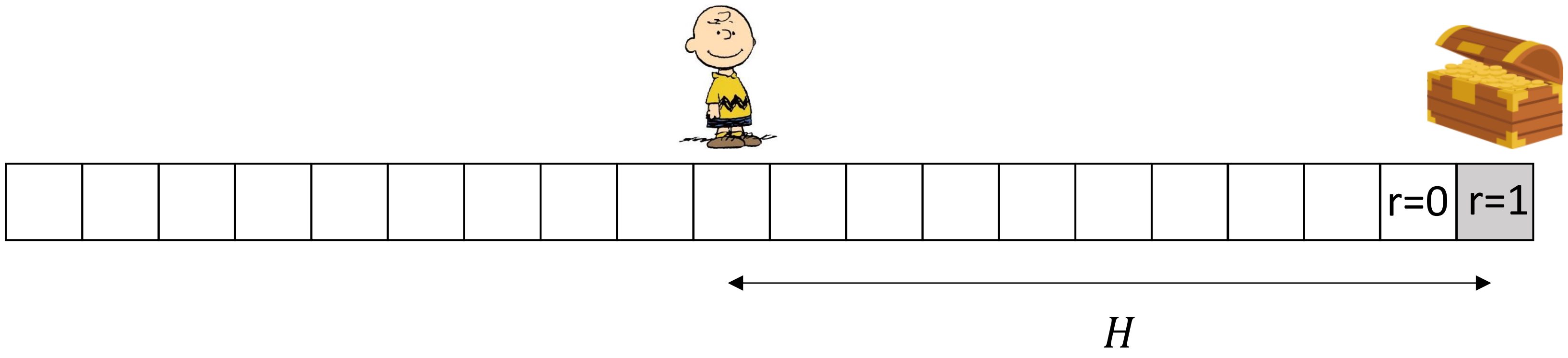
$$= \sum_{s,a} \boxed{d_\rho^{\pi^\star}(s)}\left(\pi^\star(a|s) - \pi(a|s)\right)\underline{Q^\pi(s,a)} = \sum_{s,a} \boxed{d_\rho^{\pi^\star}(s,a)}\left(Q^\pi(s,a) - V^\pi(s)\right)$$

For PI-based algorithm (approximating Q^π)

Approximating $Q^\pi(s,a)$ only requires state-actions generated from current policy

But…

Regret Analysis for MDPs?



$$\sum_{s,a} d_\rho^\pi(s,a)\,(V^\star(s) - Q^\star(s,a))$$

$\exists s,a$. $\quad d_\rho^{\pi^*}(s,a)$ large $\quad Q^\pi(s,a) - V^\pi(s,a)$ large

$d_\rho^{\pi_k}(s,a)$

$$\sum_{s,a} d_\rho^{\pi^\star}(s,a)\,(Q^\pi(s,a) - V^\pi(s))$$

large

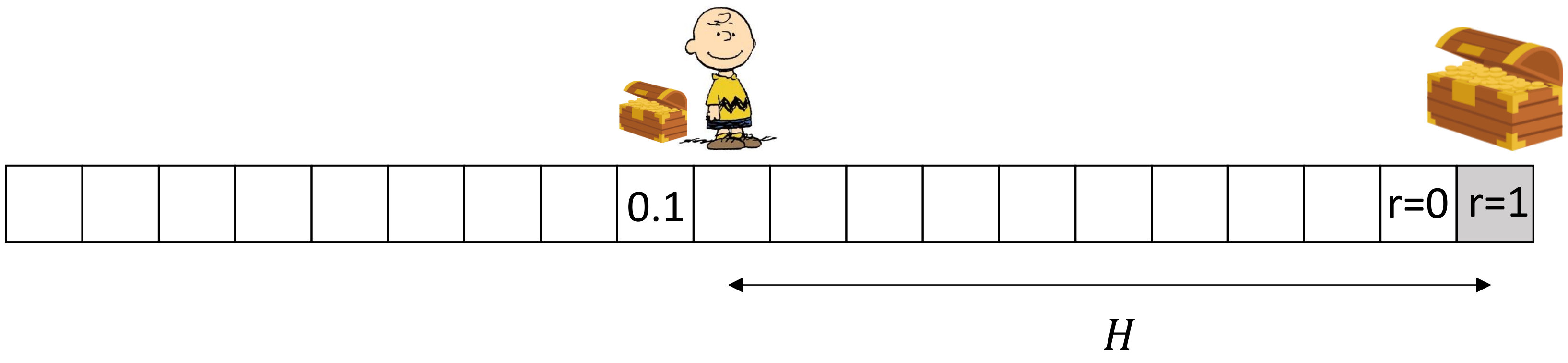
small

PI-based algorithm only tries to make $\boxed{\sum_{s,a} d_\rho^{\pi_k}(s,a)\,(Q^\pi(s,a) - V^\pi(s))}$ small.

It can only quickly find optimal policy when $d_\rho^{\pi_k} \approx d_\rho^{\pi^\star}$

Insufficiency of algorithms we have discussed for MDPs

- Lack of **exploration over the state space** (we need **deep exploration**)
- This issue is particular critical if
  - Local reward does not provide any information (Sparse reward)
  - Local reward provide misleading information



- Solution
  - Try to make the data (i.e., state-action) distribution close to $d^{\pi^\star}$
  - Try to visit as many states as possible

Exploration Bonus (Optimism Principle)

- We have discussed this idea for action exploration – UCB.

Upper Confidence Bound

$$a_t = \operatorname{argmax}_a \;\; \hat{R}_t(a) + \sqrt{\frac{2\log(2/\delta)}{N_t(a)}}$$

$\hat{R}_t(a)$ = the empirical mean of arm a up to time $t-1$.
$N_t(a)$ = the number of times we draw arm a up to time $t-1$.

Exploration Bonus (Optimism Principle)

$$\boxed{a_t = \text{argmax}_a \quad \hat{R}_t(a) + \sqrt{\frac{2\log(2/\delta)}{N_t(a)}}} \overset{\delta}{=} \boxed{\tilde{R}_t(a)}$$

$$\underline{\sum_t \sqrt{\frac{1}{N_t(a_t)}} \leq \sqrt{AT}}$$

$$\text{Regret} = \sum_t \left(R(a^*) - R(a_t)\right)$$

$$= \sum_t \underbrace{\left(\tilde{R}(a^*) - \tilde{R}(a_t)\right)}_{\leq 0} + \sum_t \underbrace{\left(R(a^*) - \tilde{R}(a^*)\right)}_{\leq 0} + \sum_t \underbrace{\left(\tilde{R}(a_t) - R(a_t)\right)}_{\lesssim \sqrt{\frac{1}{N_t(a_t)}}}$$

bonus

① $\tilde{R}_t(a) + b_t(a) \geq R(a)$

② $\sum_t b_t(a_t) \leq \text{sub-linear}(T)$

Exploration Bonus for MDPs

UCB Value Iteration (UCBVI) (finite state - action)

For episode $1, 2, \ldots, T$:

$\tilde{Q}_{H+1}(s, a) = 0 \quad \forall s, a$

For step $H, H-1, \ldots, 1$:

$$\tilde{Q}_h(s, a) \triangleq \hat{R}(s, a) + \sum_{s'} \hat{P}(s'|s, a) \max_{a'} \tilde{Q}_{h+1}(s', a') + H\sqrt{\frac{2\log(2/\delta)}{N_t(s, a)}} \quad \forall s, a$$

Receive $s_1 \sim \rho$

For step $1, 2, \ldots, H$:

Take action $a_h = \mathrm{argmax}_a \, \tilde{Q}_h(s_h, a)$

Receive $r_h = R(s_h, a_h) + \text{noise}, \qquad s_{h+1} \sim P(\cdot\,|s_h, a_h)$

Exploration Bonus for MDPs

$$\tilde{Q}_h(s,a) \triangleq \hat{R}(s,a) + \sum_{s'} \hat{P}(s'|s,a) \max_{a'} \tilde{Q}_{h+1}(s',a') + H\sqrt{\frac{2\log(2/\delta)}{N_t(s,a)}} \quad \forall s,a$$

$$\tilde{Q}_h(s,a) \geq Q^*_h(s,a) \quad \forall s,a,h \quad \text{w.h.p.}$$

$$\tilde{Q}_H(s,a) = \hat{R}(s,a) + H\sqrt{\frac{2\log(2/\delta)}{N_t(s,a)}} \geq Q^*_H(s,a) = R(s,a)$$

for $h<H$

$$\tilde{Q}_h(s,a) = \hat{R}(s,a) + \sum_{s'} \hat{P}(s'|s,a)\,\tilde{V}_{h+1}(s') + H\sqrt{\frac{2\log(4/\delta)}{N_t(s,a)}} \geq \hat{R}(s,a) + \sum_{s'} \hat{P}(s'|s,a)\,V^*_{h+1}(s') + H\sqrt{\frac{2\log(4/\delta)}{N_t(s,a)}}$$

$$\geq R(s,a) + \sum_{s'} P(s'|s,a)\,V^{\pi}_{h+1}(s') = Q^*_h(s,a)$$

Exploration Bonus for MDPs

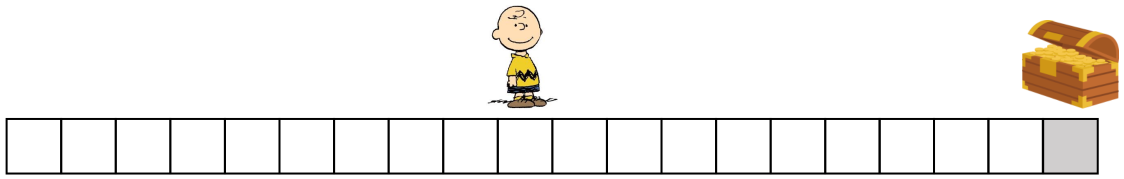
Theorem. Regret Bound of UCBVI

UCBVI ensures with high probability,

$$\text{Regret} = \sum_{t=1}^{T}\left(V^\star\left(s_{t,1}\right) - V^{\pi_t}\left(s_{t,1}\right)\right) \lesssim H\sqrt{SAT}.$$

$$\frac{1}{T}\sum_{t=1}^{T}\left(V^\star(s_{t,1}) - V^{\pi_t}(s_{t,1})\right) \lesssim H\sqrt{\frac{SA}{T}} \le \varepsilon$$

$$\Rightarrow T \gtrsim \frac{H^2 SA}{\varepsilon^2}$$



Improving the required number of episodes from 2^H to $\text{poly}(H)$

Jaksch, Ortner, Auer. Near-Optimal Regret Bounds for Reinforcement Learning. 2010.
Azar, Osband, Munos. Minimax Regret Bounds for Reinforcement Learning. 2017.

Thompson Sampling
(Posterior Sampling)

$\mathcal{H}_t = (a_1, r_1, a_2, r_2, \cdots, a_{t-1}, r_{t-1})$

Bayesian interpretation:
Assume the reward mean $(\theta(1), \dots, \theta(A))$ is drawn from a Gaussian distribution (prior distribution).
Then the **posterior distribution** is

$$P(\theta(a)|\mathcal{H}_t) = \mathcal{N}\left(\hat{R}_t(a), \frac{1}{N_t(a)}\right)$$

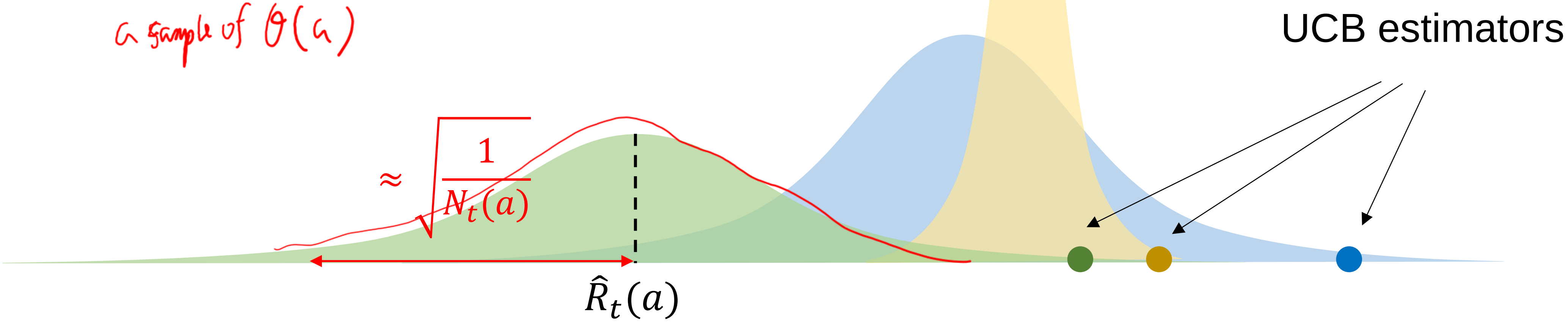
we want to find $\underset{a}{\operatorname{argmax}}\ \theta(a)$

TS: sample $\theta \sim P(\cdot|\mathcal{H}_t)$
pick $a_t = \underset{a}{\operatorname{argmax}}\ \theta(a)$

UCB: $a_t \approx \operatorname{argmax}_a\ \hat{R}_t(a) + c\sqrt{\frac{1}{N_t(a)}}$

TS: $a_t \approx \operatorname{argmax}_a\ \hat{R}_t(a) + c\sqrt{\frac{1}{N_t(a)}}\,n_t(a)$ with $n_t(a) \sim \mathcal{N}(0,1)$

a sample of $\theta(a)$



Randomized Exploration for MDPs

Randomized Value Iteration

For episode $1, 2, \dots, T$:

$\tilde{V}_{H+1}(s) = 0$

For step $H, H-1, \dots, 1$:

$$\tilde{Q}_h(s,a) \triangleq \hat{R}(s,a) + \sum_{s'} \hat{P}(s'|s,a) \max_{a'} \tilde{Q}_{h+1}(s',a') + H\sqrt{\frac{2\log(2/\delta)}{N_t(s,a)}}\, \underbrace{n_t(s,a)}_{\sim \mathcal{N}(0,1)}$$

Receive $s_1 \sim \rho$

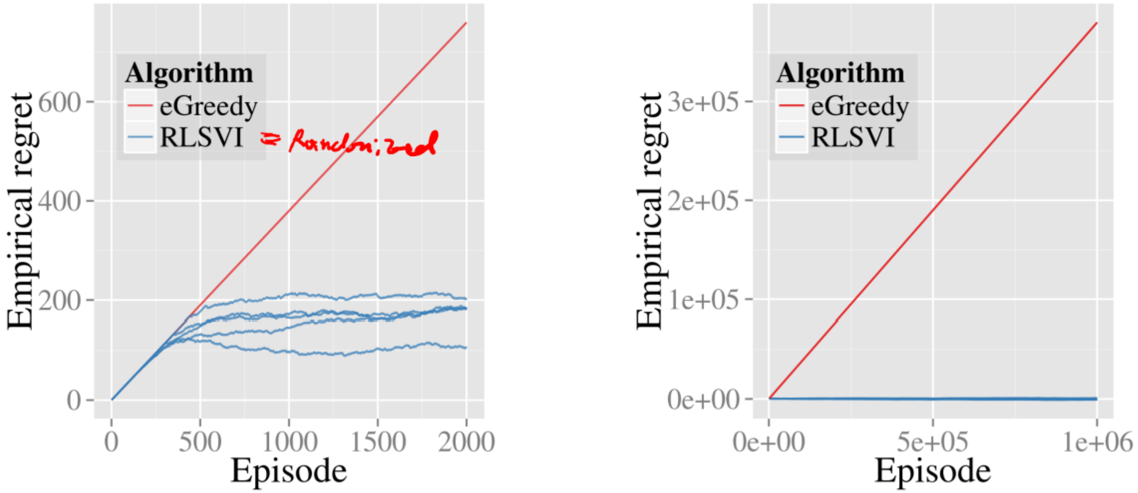
For step $1, 2, \dots, H$:

Take action $a_h = \operatorname{argmax}_a \tilde{Q}_h(s_h, a)$

Receive $r_h = R(s_h, a_h) + \text{noise}, \quad s_{h+1} \sim P(\cdot\,|s_h, a_h)$

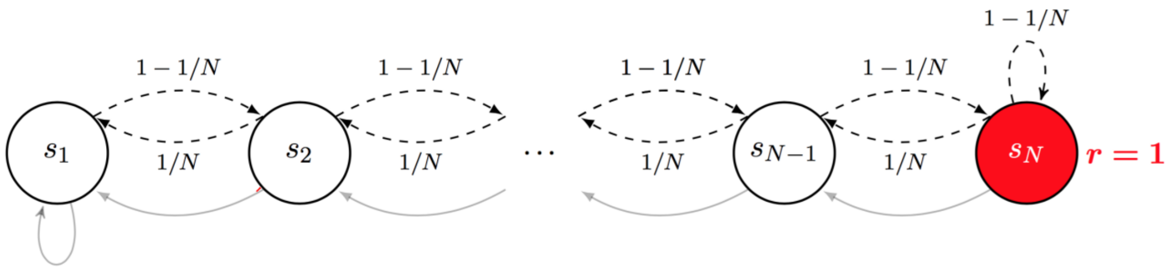
Osband, Van Roy, Wen. Generalization and Exploration via Randomized Value Functions. 2014.

Randomized Exploration for MDPs



(a) First 2000 episodes (b) First 10^6 episodes

Figure 2. Efficient exploration on a 50-chain



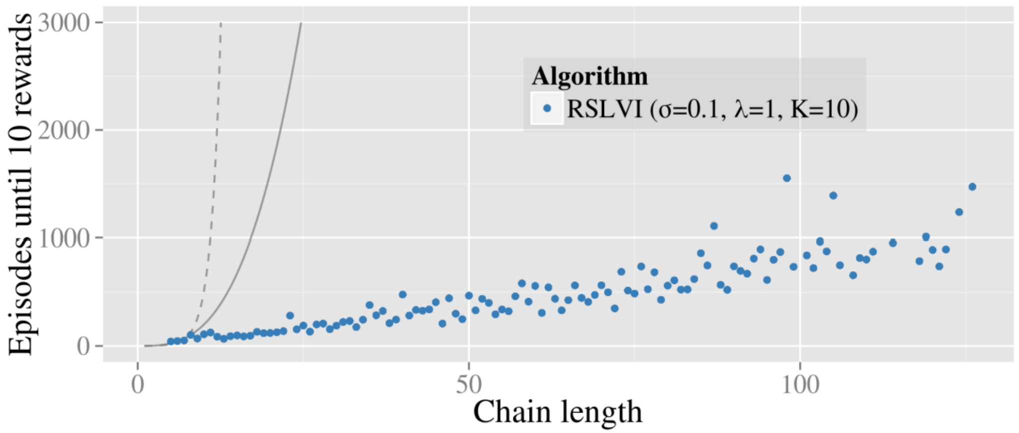


Figure 3. RLSVI learning time against chain length.

Osband, Van Roy, Wen. Generalization and Exploration via Randomized Value Functions. 2014.

Common Approaches of Exploration

- Optimistic-Value Exploration
  - Upper Confidence Bound
- Randomized-Value Exploration
  - Thompson Sampling (Posterior Sampling)
- Information-Directed Exploration

Information-Directed Exploration (1/3)

Another Bayesian approach – like Thompson sampling.

Assume the parameter of the world (e.g., the mean reward of the arms) is drawn as $\theta \sim P_{\text{prior}}$

After observing history $\mathcal{H}_t = (a_1, r_1, a_2, r_2, \dots, a_{t-1}, r_{t-1})$, we can calculate the posterior distribution of θ:

$$P(\theta|\mathcal{H}_t) = \frac{P(\mathcal{H}_t, \theta)}{P(\mathcal{H}_t)} = \frac{P(\mathcal{H}_t|\theta)P_{\text{prior}}(\theta)}{P(\mathcal{H}_t)} \propto P(\mathcal{H}_t|\theta)P_{\text{prior}}(\theta)$$

Key question: Based on the posterior estimation of the world $P(\theta|\mathcal{H}_t)$, what action should we pick next?

Information-Directed Exploration (2/3)

Thompson Sampling: Sample $\theta_t \sim P(\cdot \mid \mathcal{H}_t)$ and choose $a_t = a^\star(\theta_t) = \operatorname{argmax}_a \theta_t(a)$

The optimal action in the world of θ_t

Equivalently, execute $\pi(a) = \operatorname{argmax}_\pi \mathbb{E}_{\theta \sim P(\cdot|\mathcal{H}_t)}[\mathbb{I}\{a^\star(\theta) = a\}]$

Information-directed Sampling: Select an arm that tradeoffs **regret** and **information gain**

$$\text{Regret}_\theta(\pi) = \max_{a^\star} \theta(a^\star) - \theta(\pi)$$

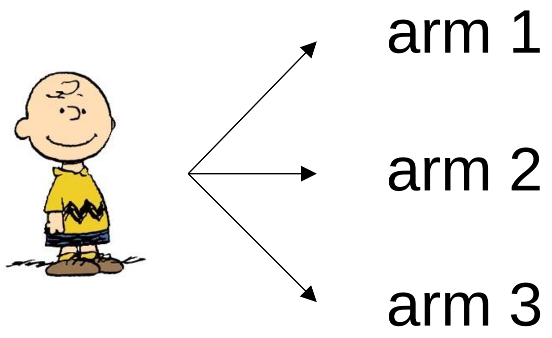
$$\text{InfoGain}_\theta(\pi) = \mathbb{E}_{r\sim\theta(\pi)}[\text{KL}(P(\cdot \mid \mathcal{H}_t, \pi, r), P(\cdot \mid \mathcal{H}_t))]$$

How much will the posterior change after obtaining a new sample from π?

Execute $\pi = \operatorname{argmin}_\pi \mathbb{E}_{\theta\sim P(\cdot|\mathcal{H}_t)} [\text{Regret}_\theta(\pi) - \lambda \, \text{InfoGain}_\theta(\pi)]$

Information-Directed Exploration (3/3)

When is information-directed exploration better than optimistic / posterior exploration?



Suppose we know there are two possible worlds, where the three arms follow

$\{\text{Bernoulli}(0.5), \text{Bernoulli}(0.6), {\color{red}0.1}\}$ or $\{\text{Bernoulli}(0.6), \text{Bernoulli}(0.5), {\color{red}0}\}$

$\Rightarrow$ Although we know arm 3 is definitely not the best arm, we still want to sample it (once), so we can easily tell which world we're in.

Next

We will see how to generalize

- Optimistic-Value Exploration
- Posterior-Value Exploration
- Information-Directed Exploration

to large state space by incorporating **function approximation**