STATS 701 – Theory of Reinforcement Learning Thompson/Posterior Sampling in MDPs

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#### 2 Posterior Sampling for Reinforcement Learning



## Finite Horizon (or episodic) MDP

- A finite horizon MDP M consists of
  - $\bullet~\mathcal{S},$  state space and  $\mathcal{A},$  action space
  - $\mu_0$ , the initial state distribution
  - Horizon H: every episode terminates in exactly H steps
  - Transition dynamics  $s_{t+1} \sim P_{s_t,a_t}$
  - Reward distributions  $r_t \sim R_{s_t,a_t}$
- Need to consider non-stationary policy  $\pi$

$$\boldsymbol{\pi} = (\pi_1, \ldots, \pi_H)$$

Trajectory

$$s_1 \sim \mu_0, a_1 \sim \pi_1(s_1), r_1 \sim R_{s_1,a_1},$$
  
 $s_2 \sim P_{s_1,a_1}, a_2 \sim \pi_2(s_2), r_2 \sim R_{s_2,a_2},$   
:

$$s_H \sim P_{s_{H-1},a_{H-1}}, a_H \sim \pi_H(s_{H-1}), r_H \sim R_{s_H,a_H}$$

# **Optimal policy**

• Value functions are now also indexed by time step within episode:

$$V_M^{\pi,h}(s) = \mathbb{E}_M^{\pi}\left[\sum_{t=h}^H r_t \middle| s_h = s
ight]$$

• Optimal policy  $\pi_M^{\star}$  satisfies, for all  $s \in S, h \in \{1, \dots, H\}$ :

$$V^{{m \pi}^\star_M,h}_M(s) = \max_{m \pi} V^{{m \pi},h}_M(s)$$

• Will omit MDP *M* if it is fixed and clear from context

#### DP equation for value functions of a policy

• DP equations for finite horizon case

$$V_{M}^{{m \pi},h} = T_{M}^{{m \pi}_{h}} V_{M}^{{m \pi},h+1}, \quad h = \{1,2,\ldots,H\}$$

• Base case is 
$$V^{\pi,H+1} = 0$$

• Here the operator  $T_M^{\pi}$  for a single stationary  $\pi$  is defined as usual:

$$T_M^{\pi}V = R_M^{\pi} + P_M^{\pi}V$$

#### Regret

- Let's say the agent interacts with a fixed but unknown finite horizon MDP *M* for *T* steps
- There are K = T/H episodes each of length H
- Agent chooses policy  $\pi^{(k)}$  at the start of episode k (based on available data at that moment)
- Regret in episode k

$$\Delta_k = \sum_{s \in \mathcal{S}} \mu_0(s) (V^{\pi^{\star},1}(s) - V^{\pi^{(k)},1}(s))$$

Overall regret

Regret(
$$T$$
; agent,  $M$ ) =  $\sum_{k=1}^{K} \Delta_k$ 

#### Posterior Sampling: Per Episode Version

- Also called Thompson Sampling because of [Tho33]
- Tends to perform better than optimism based algorithms
- Start with a prior distribution over MDPs
- In every episode:
  - Use collected statistics to create a posterior distribution over MDPs
  - Sample an MDP from this posterior
  - Compute optimal policy for the sampled MDP
  - For time steps within the episode:
    - Choose actions according to the optimal policy for sampled MDP

#### Posterior Sampling: Per Time Step Version

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## Per Episode vs Per Time Step

- Per time step version does worse, sometimes much worse, than per episode version
- Difference in performance increases as MDP size increases
- Per episode version is also computationally more efficient
- See [RVRK<sup>+</sup>18], Section 7.5 for details

#### **Bayesian Regret**

• Note that worst-case (or frequentist) regret bounds are of the form

 $\sup_{M \in \mathcal{M}} \operatorname{Regret}(T; \operatorname{agent}, M)$ 

for some class  ${\mathcal M}$  of MDPs

• It is easier to analyze Bayesian regret of posterior sampling

 $\mathbb{E}_{M \sim f} \left[ \text{Regret} (T; \text{agent}, M) \right]$ 

• Here f is the prior distribution over MDPs

# Posterior Sampling for RL (PSRL)

- Input: Prior distribution f
- $t \leftarrow 1$
- For episodes  $k = 1, 2, \ldots$  do
  - sample  $ilde{M}_k \sim f(\cdot | \mathcal{H}_{< k})$
  - compute  $ilde{\pi}^{(k)} = \pi^{\star}_{ ilde{M}_{k}}$
  - For timesteps  $h = 1, \ldots, H$  do
    - choose action  $a_t = \tilde{\pi}_h^{(k)}(s_t)$
    - observe  $r_t$  and  $s_{t+1}$

• 
$$t \leftarrow t+1$$

For more details see original paper [ORR13]

## A Crucial Observation

- (Bayesian) regret analysis of PS rests on a simple but crucial observation
- Let H<sub><k</sub> be the history of all observations available at the start of episode k

$$\mathbb{E}\left[g(\tilde{M}_k)|\mathcal{H}_{< k}\right] = \mathbb{E}\left[g(M)|\mathcal{H}_{< k}\right]$$

for any  $g(\cdot)$  measurable w.r.t.  $\mathcal{H}_{< k}$ 

• The sampled MDP  $\tilde{M}_k$  (observed) has the same distribution as the true MDP M (unobserved)!

## Regret Equivalence

• Recall per-episode regret

$$\Delta_k = \sum_{s \in \mathcal{S}} \mu_0(s) (V_M^{\pi^*,1}(s) - V_M^{\pi^{(k)},1}(s))$$

• Consider its proxy

$$ilde{\Delta}_k = \sum_{s\in\mathcal{S}} \mu_0(s) (V^{\boldsymbol{\pi}^{(k)},1}_{ ilde{\mathcal{M}}}(s) - V^{\boldsymbol{\pi}^{(k)},1}_{\mathcal{M}}(s))$$

• Note that by our crucial observation

$$\mathbb{E}\left[\Delta_k - ilde{\Delta}_k \Big| \mathcal{H}_{< k}
ight] = \mathbb{E}\left[\sum_{s \in \mathcal{S}} \mu_0(s) (V_M^{\pi^{\star}, 1}(s) - V_{ ilde{M}}^{\pi^{(k)}, 1}(s)) \Big| \mathcal{H}_{< k}
ight] = 0$$

#### Bounding the Proxy Regret

• So we will focus on bounding

$$egin{aligned} \mathbb{E}[ ilde{\Delta}_k] &= \mathbb{E}[\sum_{s\in\mathcal{S}} \mu_0(s)(V_{ ilde{\mathcal{M}}}^{\pi^{(k)},1}(s) - V_{\mathcal{M}}^{\pi^{(k)},1}(s))] \ &= \mathbb{E}[V_{ ilde{\mathcal{M}}}^{\pi^{(k)},1}(s_{t_k+1}) - V_{\mathcal{M}}^{\pi^{(k)},1}(s_{t_k+1})] \end{aligned}$$

Recall DP equations for finite horizon case (with V<sup>π,H+1</sup> = 0 as base case)

$$V_M^{\pi,h} = T_M^{\pi_h} V_M^{\pi,h+1}, \quad h = \{1, 2, \dots, H\}$$

where the operator  $T_M^{\pi}$  for a single stationary  $\pi$  is defined as usual:

$$T_M^{\pi}V = R_M^{\pi} + P_M^{\pi}V$$

#### Towards the Key Recursion

refer to states within the episodes as  $s_1, s_2, \ldots$  instead of  $s_{t_k+1}, s_{t_k+2}, \ldots$ denote the non-stationary policy  $\pi^{(k)}$  in episode k as  $\tilde{\pi}$ 

$$\begin{split} V_{\tilde{M}}^{\tilde{\pi},1} - V_{M}^{\tilde{\pi},1} &= T_{\tilde{M}}^{\tilde{\pi}_{1}} V_{\tilde{M}}^{\tilde{\pi},2} - T_{M}^{\tilde{\pi}_{1}} V_{M}^{\tilde{\pi},2} \\ &= T_{\tilde{M}}^{\tilde{\pi}_{1}} V_{\tilde{M}}^{\tilde{\pi},2} - T_{M}^{\tilde{\pi}_{1}} V_{\tilde{M}}^{\tilde{\pi},2} + T_{M}^{\tilde{\pi}_{1}} V_{\tilde{M}}^{\tilde{\pi},2} - T_{M}^{\tilde{\pi}_{1}} V_{M}^{\tilde{\pi},2} \\ &= (T_{\tilde{M}}^{\tilde{\pi}_{1}} - T_{M}^{\tilde{\pi}_{1}}) V_{\tilde{M}}^{\tilde{\pi},2} + T_{M}^{\tilde{\pi}_{1}} (V_{\tilde{M}}^{\tilde{\pi},2} - V_{M}^{\tilde{\pi},2}) \\ &= (T_{\tilde{M}}^{\tilde{\pi}_{1}} - T_{M}^{\tilde{\pi}_{1}}) V_{\tilde{M}}^{\tilde{\pi},2} + P_{M}^{\tilde{\pi}_{1}} (V_{\tilde{M}}^{\tilde{\pi},2} - V_{M}^{\tilde{\pi},2}) \end{split}$$

Therefore,

$$\mathbf{e}_{s_1}^\top (\boldsymbol{V}_{\tilde{M}}^{\tilde{\pi},1}-\boldsymbol{V}_{M}^{\tilde{\pi},1})=\mathbf{e}_{s_1}^\top (\boldsymbol{T}_{\tilde{M}}^{\tilde{\pi}_1}-\boldsymbol{T}_{M}^{\tilde{\pi}_1})\boldsymbol{V}_{\tilde{M}}^{\tilde{\pi},2}+\mathbf{e}_{s_1}^\top \boldsymbol{P}_{M}^{\tilde{\pi}_1} (\boldsymbol{V}_{\tilde{M}}^{\tilde{\pi},2}-\boldsymbol{V}_{M}^{\tilde{\pi},2})$$

## Key Recursion

$$\mathbf{e}_{s_{1}}^{\top}(V_{\tilde{M}}^{\tilde{\pi},1}-V_{M}^{\tilde{\pi},1}) = \mathbf{e}_{s_{1}}^{\top}(T_{\tilde{M}}^{\tilde{\pi}_{1}}-T_{M}^{\tilde{\pi}_{1}})V_{\tilde{M}}^{\tilde{\pi},2} + \mathbf{e}_{s_{1}}^{\top}P_{M}^{\tilde{\pi}_{1}}(V_{\tilde{M}}^{\tilde{\pi},2}-V_{M}^{\tilde{\pi},2}) \\ = \mathbf{e}_{s_{1}}^{\top}(T_{\tilde{M}}^{\tilde{\pi}_{1}}-T_{M}^{\tilde{\pi}_{1}})V_{\tilde{M}}^{\tilde{\pi},2} + \mathbf{e}_{s_{2}}^{\top}(V_{\tilde{M}}^{\tilde{\pi},2}-V_{M}^{\tilde{\pi},2}) \\ + \underbrace{(\mathbf{e}_{s_{1}}^{\top}P_{M}^{\tilde{\pi}_{1}}-\mathbf{e}_{s_{2}}^{\top})(V_{\tilde{M}}^{\tilde{\pi},2}-V_{M}^{\tilde{\pi},2})}_{\text{mean zero given } M,\tilde{M}}$$

We have therefore set up the key recursion

$$\mathbb{E}\left[\mathbf{e}_{s_{1}}^{\top}(V_{\tilde{M}}^{\tilde{\pi},1}-V_{M}^{\tilde{\pi},1})\Big|M,\tilde{M}\right] = \mathbb{E}\left[\mathbf{e}_{s_{1}}^{\top}(T_{\tilde{M}}^{\tilde{\pi}_{1}}-T_{M}^{\tilde{\pi}_{1}})V_{\tilde{M}}^{\tilde{\pi},2}\Big|M,\tilde{M}\right] \\ + \mathbb{E}\left[\mathbf{e}_{s_{2}}^{\top}(V_{\tilde{M}}^{\tilde{\pi},2}-V_{M}^{\tilde{\pi},2})\Big|M,\tilde{M}\right]$$

### Unrolling the Recursion

Unrolling the key recursion gives

$$\mathbb{E}\left[\tilde{\Delta}_{k}\middle|M,\tilde{M}\right] = \mathbb{E}\left[\mathbf{e}_{s_{1}}^{\top}(V_{\tilde{M}}^{\tilde{\pi},1} - V_{M}^{\tilde{\pi},1})\middle|M,\tilde{M}\right]$$
$$= \mathbb{E}\left[\sum_{h=1}^{H}\mathbf{e}_{s_{h}}^{\top}(T_{\tilde{M}}^{\tilde{\pi}_{h}} - T_{M}^{\tilde{\pi}_{h}})V_{\tilde{M}}^{\tilde{\pi},h+1}\middle|M,\tilde{M}\right]$$

#### Enter Confidence Sets

Let  $\hat{P}_k$  and  $\hat{R}_k$  be empirical estimates of the transition and reward function at the start of episode k Similar to UCRL2 analysis (but now confidence sets are only in the analysis, not in the algorithm!), define  $\mathcal{M}_k$  as the set of all MDPs M' such

that ∀*s*, *a*,

$$\begin{split} \|P_{M'}(\cdot|s,a) - \hat{P}_k(\cdot|s,a)\|_1 &\leq \beta_k(s,a) \\ |R_{M'}(s,a) - \hat{R}_k(s,a)| &\leq \beta_k(s,a) \end{split}$$

where

$$eta_k(s, \mathsf{a}) = O\left(\sqrt{rac{S\log(SAK)}{1 \lor \mathsf{N}_{t_k}(s, \mathsf{a})}}
ight)$$

## Confidence Set Failure Probability

Can easily show that

$$\mathbb{E}[\mathbf{1}_{(M \notin \mathcal{M}_k)}] \leq 1/K$$

Note that  $\mathcal{M}_k$  is  $\mathcal{H}_{< k}\text{-measurable}$  which, using the crucial observation again, gives

$$\mathbb{E}[\mathbf{1}_{\left( ilde{\mathcal{M}}_k 
otin \mathcal{M}_k
ight)}] \leq 1/K$$

### Sum up Regret over Episodes

Now we sum up regrets over all episodes

$$\mathbb{E}\left[\sum_{k=1}^{K} \tilde{\Delta}_{k}\right] = \mathbb{E}\left[\sum_{k=1}^{K} \tilde{\Delta}_{k} \mathbf{1}_{\left(M,\tilde{M}_{k}\in\mathcal{M}_{k}\right)}\right] + \mathbb{E}\left[\sum_{k=1}^{K} \tilde{\Delta}_{k} \mathbf{1}_{\left(M \text{ or } \tilde{M}_{k}\notin\mathcal{M}_{k}\right)}\right]$$
$$\leq \mathbb{E}\left[\sum_{k=1}^{K} \tilde{\Delta}_{k} \mathbf{1}_{\left(M,\tilde{M}_{k}\in\mathcal{M}_{k}\right)}\right] + H \sum_{k=1}^{K} 2\mathbb{E}[\mathbf{1}_{\left(M\notin\mathcal{M}_{k}\right)}]$$
$$= \mathbb{E}\left[\sum_{k=1}^{K} \mathbb{E}\left[\tilde{\Delta}_{k} \middle| M, \tilde{M}\right] \mathbf{1}_{\left(M,\tilde{M}_{k}\in\mathcal{M}_{k}\right)}\right] + 2H$$

Recall that we proved that

$$\mathbb{E}\left[\tilde{\Delta}_{k}\middle|M,\tilde{M}\right] = \mathbb{E}\left[\sum_{h=1}^{H}\mathbf{e}_{s_{t_{k}+h}}^{\top}(T_{\tilde{M}_{k}}^{\tilde{\pi}_{h}^{(k)}} - T_{M}^{\tilde{\pi}_{h}^{(k)}})V_{\tilde{M}_{k}}^{\tilde{\pi}^{(k)},h+1}\middle|M,\tilde{M}_{k}\right]$$

## **DP** Operators Concentrate

On the event  $M, \tilde{M}_k \in \mathcal{M}_k$ , the two MDPs are close Therefore  $\mathcal{T}_{\tilde{M}_k}^{\tilde{\pi}_h^{(k)}}$  and  $\mathcal{T}_M^{\tilde{\pi}_h^{(k)}}$  are also close Also, value function cannot exceed H (rewards are bounded)

$$\mathbb{E}\left[\sum_{k}\tilde{\Delta}_{k}\right] \leq \mathbb{E}\left[\sum_{k}\sum_{h=1}^{H}|\mathbf{e}_{s_{t_{k}+h}}^{\top}(\mathcal{T}_{\tilde{M}_{k}}^{\tilde{\pi}_{h}^{(k)}}-\mathcal{T}_{M}^{\tilde{\pi}_{h}^{(k)}})V_{\tilde{M}_{k}}^{\tilde{\pi}^{(k)},h+1}|\mathbf{1}_{\left(M,\tilde{M}_{k}\in\mathcal{M}_{k}\right)}\right]$$
$$+2H$$
$$\leq H\underbrace{\sum_{k}\sum_{h=1}^{H}\beta_{k}(s_{t_{k}+h},a_{t_{k}+h})}_{\text{contributes }\tilde{O}(\sqrt{S}\cdot\sqrt{SAT})}$$

## Bayesian Regret Bound for Posterior Sampling

#### Theorem (from [ORR13])

The Bayesian regret of PSRL in an H horizon problem with bounded rewards is at most  $\tilde{O}(HS\sqrt{AT})$ .

#### Regret Analysis of Posterior Sampling: Non-episodic case

- There is a subtlety in the extension of this analysis to the non-episodic case (where we compete against the average reward optimal policy)
- At the start of the episode

$$\mathbb{E}\left[\tilde{\rho}_{k}|\mathcal{H}_{< k}\right] = \mathbb{E}\left[\rho^{\star}|\mathcal{H}_{< k}\right]$$

- However, the length of episode k may not be measurable w.r.t. H<sub><k</sub> (see [OVR16] for explanation of this subtlety)
- Redefining the stopping criterion in posterior sampling allows us to prove Bayesian regret bounds [OGNJ17]
- Frequentist aka worst-case regret analysis more difficult and still not fully resolved in the non-episodic setting

## Summary

- Posterior sampling replaces optimism with sampling (from the posterior)
- Bayesian regret analysis relies on the equality of the distributions of the true and the sampled MDPs
- Confidence intervals still needed but only in the analysis
- Worst-case/frequentist analysis is technically more challenging
- Works better than optimism in practice (see [OVR17] for more discussion)

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