Lecture 11: Fast Reinforcement Learning [2]

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CS234 Reinforcement Learning.

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[2] With many slides from or derived from David Silver

Class Structure

- Last time: Midterm!
- **This time: Exploration and Exploitation**
- Next time: Batch RL

Atari: Focus on the x-axis

- Last time: Midterm!
- **This time: Exploration and Exploitation**
- Next time: Batch RL

Other Areas: Health, Education, ...

- Asymptotic convergence to good/optimal is not enough

Table of Contents

Performance Criteria of RL Algorithms

- Empirical performance
- Convergence (to something ...)
- Asymptotic convergence to optimal policy
- Finite sample guarantees: probably approximately correct
- Regret (with respect to optimal decisions)
- Optimal decisions given information have available
- PAC uniform

Performance Criteria of RL Algorithms

- **Empirical performance**
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Strategic Exploration

- To get stronger guarantees on performance, need **strategic exploration**

Table of Contents

Exploration vs. Exploitation Dilemma

- Online decision-making involves a fundamental choice:
  - **Exploitation:** Make the best decision given current information
  - **Exploration:** Gather more information
- The best long-term strategy may involve short-term sacrifices
- Gather enough information to make the best overall decision

Examples

- Restaurant Selection
  - Go off-campus
  - Eat at Treehouse (again)
- Online advertisements
  - Show the most successful ad
  - Show a different ad
- Oil Drilling
  - Drill at best known location
  - Drill at new location
- Game Playing
  - Play the move you believe is best
  - Play an experimental move

Table of Contents

Principles

- Naive Exploration
- Optimistic Initialization
- Optimism in the Face of Uncertainty
- Probability Matching
- Information State Search

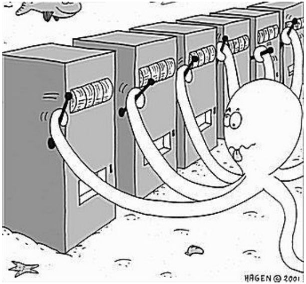
Table of Contents

MABs

- Will introduce various principles for multi-armed bandits (MABs) first instead of for generic reinforcement learning
- MABs are a subclass of reinforcement learning
- Simpler (as will see shortly)

Multiarmed Bandits

- Multi-armed bandit is a tuple of $(\mathcal{A}, \mathcal{R})$
- $\mathcal{A}$: known set of m actions
- $\mathcal{R}^a(r) = \mathbb{P}[r \mid a]$ is an unknown probability distribution over rewards
- At each step t the agent selects an action $a_t \in \mathcal{A}$
- The environment generates a reward $r_t \sim \mathcal{R}^{a_t}$
- Goal: Maximize cumulative reward $\sum_{\tau=1}^{t} r_\tau$



Greedy Algorithm

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

$$\hat{Q}_t(a) = \frac{1}{N_t(a)} \sum_{t=1}^{T} r_t \mathbb{1}(a_t = a)$$

- The **greedy** algorithm selects action with highest value

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

- Greedy can lock onto suboptimal action, forever

ϵ-Greedy Algorithm

- With probability $1 - \epsilon$ select $a = \arg\max_{a \in \mathcal{A}} \hat{Q}_t(a)$
- With probability ϵ select a random action

- Always will be making a sub-optimal decision ϵ fraction of the time
- Already used this in prior homeworks

Optimistic Initialization

- Simple and practical idea: initialize Q(a) to high value
- Update action value by incremental Monte-Carlo evaluation
- Starting with $N(a) > 0$

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

- Encourages systematic exploration early on
- But can still lock onto suboptimal action[21]

[21] Depends on how high initialize Q

Decaying ϵ_t-Greedy Algorithm

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

$$
\begin{aligned}
c &> 0 \\
d &= \min_{a|\Delta_a>0} \Delta_i \\
\epsilon_t &= \min\left\{1, \frac{c|\mathcal{A}|}{d^2 t}\right\}
\end{aligned}
$$

How to Compare these Methods?

- Empirical performance
- Convergence (to something ...)
- Asymptotic convergence to optimal policy
- Finite sample guarantees: probably approximately correct
- **Regret (with respect to optimal decisions)**
  - Very common criteria for bandit algorithms
  - Also frequently considered for reinforcement learning methods
- Optimal decisions given information have available
- PAC uniform

Regret

- **Action-value** is the mean reward for action a

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

- **Optimal value** V^*

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

- **Regret** is the opportunity loss for one step

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

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

$$L_t = \mathbb{E}[\sum_{\tau=1}^{t} V^* - Q(a_\tau)]$$

- Maximize cumulative reward $\iff$ minimize total regret

Evaluating Regret

- **Count** $N_t(a)$ is expected number of selections for action a
- **Gap** Δ_a is the difference in value between action a and optimal action a^*, $\Delta_a = V^* - Q(a)$
- Regret is a function of gaps and counts

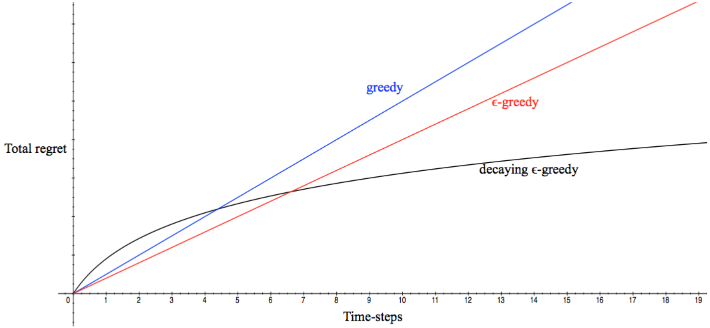
$$
\begin{aligned}
L_t &= \mathbb{E}\left[\sum_{\tau=1}^{t} V^* - Q(a_\tau)\right] \\
&= \sum_{a \in \mathcal{A}} \mathbb{E}[N_t(a)](V^* - Q(a)) \\
&= \sum_{a \in \mathcal{A}} \mathbb{E}[N_t(a)]\Delta_a
\end{aligned}
$$

- A good algorithm ensures small counts for large gaps
- But: gaps are not known

Types of Regret bounds

- **Problem independent**: Bound how regret grows as a function of T, the total number of time steps the algorithm operates for
- **Problem dependent**: Bound regret as a function of the number of times pull each arm and the gap between the reward for the pulled arm and the true optimal arm

"Good": Sublinear or below regret



- **Explore forever**: have linear total regret
- **Explore never**: have linear total regret
- Is it possible to achieve sublinear regret?

Greedy Bandit Algorithms and Optimistic Initialization

- **Greedy**: Linear total regret
- **Constant ϵ-greedy**: Linear total regret
- **Decaying ϵ-greedy**: Sublinear regret but schedule for decaying ϵ requires knowledge of gaps, which are unknown
- **Optimistic initialization**: Sublinear regret if initialize values sufficiently optimistically, else linear regret
- Check your understanding: why does fixed ϵ-greedy have linear regret? (Do a proof sketch)

Lower Bound

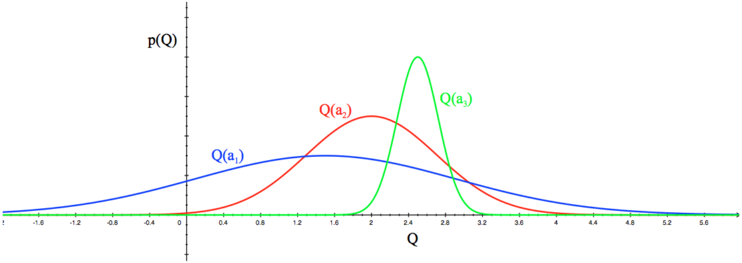
- Use lower bound to determine how hard this problem is
- The performance of any algorithm is determined by similarity between optimal arm and other arms
- Hard problems have similar looking arms with different means
- This is described formally by the gap Δ_a and the similarity in distributions $KL(\mathcal{R}^a \| \mathcal{R}^{a^*})$
- Theorem (Lai and Robbins): Asymptotic total regret is at least logarithmic in number of steps

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

Principles

- Naive Exploration
- Optimistic Initialization
- **Optimism in the Face of Uncertainty**
- Probability Matching
- Information State Search

Optimism in the Face of Uncertainty



- Which action should we pick?
- Choose arms that could be good
- Intuitively choosing an arm with potentially high mean reward will either lead to:
  - Getting high reward: if the arm really has a high mean reward
  - Learn something: if the arm really has a lower mean reward, pulling it will (in expectation) reduce its average reward and the uncertainty over its value

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 $N(a)$ has been selected
  - Small $N_t(a) \rightarrow$ large $\hat{U}_t(a)$ (estimate value is uncertain)
  - Large $N_t(a) \rightarrow$ small $\hat{U}_t(a)$ (estimate 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 $\bar{X}_t = \frac{1}{\tau}\sum_{\tau=1}^{t} X_\tau$ be the sample mean. Then

$$\mathbb{P}\left[\mathbb{E}\left[X\right] > \bar{X}_t + u\right] \leq \exp(-2tu^2)$$

- Applying Hoeffding's Inequality to the rewards of the bandit,

$$\mathbb{P}\left[Q(a) > \hat{Q}_t(a) + U_t(a)\right] \leq \exp(-2N_t(a)U_t(a)^2)$$

Calculating UCB

- Pick a probability p that true value exceeds UCB
- Now solve for $U_t(a)$

$$\exp(-2N_t(a)U_t(a)^2) = p$$
$$U_t(a) = \sqrt{\frac{-\log p}{2N_t(a)}}$$

- Reduce p as we observe more rewards, e.q. $p = t^{-4}$
- Ensures we select optimal action as $t \to \infty$

$$U_t(a) = \sqrt{\frac{2\log t}{N_t(a)}}$$

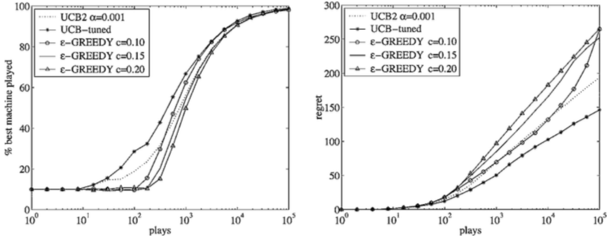
UCB1

- This leads to the UCB1 algorithm

$$a_t = \arg\max_{a \in \mathcal{A}} Q(a) + \sqrt{2 \log t} N_t(a)$$

- Theorem: The UCB algorithm achieves logarithmic asymptotic total regret

$$\lim_{t \to \infty} L_t \leq 8 \log t \sum_{a | \Delta_a > 0} \Delta_a$$



Check Your Understanding

- An alternative would be to always select the arm with the highest lower bound
- Why can this yield linear regret?

Bayesian Bandits

- So far we have made no assumptions about the reward distribution $\mathcal{R}$
  - Except bounds on rewards
- **Bayesian bandits** exploit prior knowledge of rewards, $p[\mathcal{R}]$
- They compute posterior distribution of rewards $p[\mathcal{R} \mid h_t$, where $h_t = (a_1, r_1, \dots, a_{t-1}, r_{t-1})$
- Use posterior to guide exporation
  - Upper confidence bounds (Bayesian UCB)
  - Probability matching (Thompson Sampling)
- Better performance if prior knowledge 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 and σ_a^2 (by Bayes law)

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

- Pick action that maximizes standard deviation of $Q(a)$

$$a_t = \arg\max_{a \in \mathcal{A}} \mu_a + c \frac{c\sigma_a}{\sqrt{N(a)}}$$

Principles

- Naive Exploration
- Optimistic Initialization
- Optimism in the Face of Uncertainty
- **Probability Matching**
- Information State Search

Probability Matching

- Again assume have a parametric distribution over rewards for each arm
- **Probability matching** selects action a according to probability that a is the optimal action

$$\pi(a \mid h_t) = \mathbb{P}[Q(a) > Q(a'), \forall a' \neq a \mid h_t]$$

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

- **Thompson sampling** implements probability matching

$$\pi(a \mid h_t) = \mathbb{P}[Q(a) > Q(a'), \forall a' \neq a \mid h_t]$$
$$= \mathbb{E}_{\mathcal{R}|h_t}\left[\mathbb{1}(a = \arg\max_{a \in \mathcal{A}} Q(a))\right]$$

- Use Bayes law to compute posterior distribution $p[\mathcal{R} \mid h_t]$
- **Sample** a reward distribution $\mathcal{R}$ from posterior
- Compute action-value function $Q(a) = \mathbb{E}[\mathcal{R}_a]$
- Select action maximizing value on sample, $a_t = \arg\max_{a \in \mathcal{A}} Q(a)$
- Thompson sampling achieves Lai and Robbins lower bound
- Last checked: bounds for optimism are tighter than for Thomspon sampling
- But empirically Thompson sampling can be extremely effective

Principles

- Naive Exploration
- Optimistic Initialization
- Optimism in the Face of Uncertainty
- Probability Matching
- **Information State Search**

Relevant Background: Value of Information

- Exploration is useful because it gains information
- Can we quantify the **value of information (VOI)**?
  - How much reward a decision-maker would be prepared to pay in order to have that information, prior to making a decision
  - Long-term reward after getting information - immediate reward

Relevant Background: Value of Information Example

- Consider bandit where only get to make a **single** decision
- Oil company considering buying rights to drill in 1 of 5 locations
- 1 of locations contains $10 million worth of oil, others 0
- Cost of buying rights to drill is $2 million
- Seismologist says for a fee will survey one of 5 locations and report back definitively whether that location does or does not contain oil
- What is the should consider paying seismologist?

Relevant Background: Value of Information Example

- 1 of locations contains \$10 million worth of oil, others 0
- Cost of buying rights to drill is \$2 million
- Seismologist says for a fee will survey one of 5 locations and report back definitively whether that location does or does not contain oil
- Value of information: expected profit if ask seismologist minus expected profit if don't ask
- Expected profit if don't ask:
  - Guess at random

$$= \frac{1}{5}(10-2) + \frac{4}{5}(0-2) = 0 \tag{1}$$

- Expected profit if ask:
  - If one surveyed has oil, expected profit is: $10 - 2 = 8$
  - If one surveyed doesn't have oil, expected profit: (guess at random from other locations) $\frac{1}{4}(10-2) - \frac{3}{4}(-2) = 0.5$
  - Weigh by probability will survey location with oil: $= \frac{1}{5}8 + \frac{4}{5}0.5 = 2$
- VOI: $2 - 0 = 2$

Relevant Background: Value of Information

- Back to making a sequence of decisions under uncertainty
- Information gain is higher in uncertain situations
- But need to consider value of that information
  - Would it change our decisions?
  - Expected utility benefit

Information State Space

- So far viewed bandits as a simple fully observable Markov decision process (where actions don't impact next state)
- Beautiful idea: frame bandits as a partially observable Markov decision process where the hidden state is the mean reward of each arm

Information State Space

- So far viewed bandits as a simple fully observable Markov decision process (where actions don't impact next state)
- Beautiful idea: frame bandits as a partially observable Markov decision process where the hidden state is the mean reward of each arm
- (Hidden) State is static
- Actions are same as before, pulling an arm
- Observations: Sample from reward model given hidden state
- POMDP planning = Optimal Bandit learning

Information State Space

- POMDP belief state / information state $\tilde{s}$ is posterior over hidden parameters (e.g. mean reward of each arm)
- $\tilde{s}$ is a statistic of the history, $\tilde{s} = f(h_t)$
- Each action a causes a transition to a new information state $\tilde{s}'$ (by adding information), with probability $\tilde{\mathcal{P}}^a_{\tilde{s},\tilde{s}'}$
- Equivalent to a POMDP
- Or a MDP $\tilde{\mathcal{M}} = (\tilde{\mathcal{S}}, \mathcal{A}, \tilde{\mathcal{P}}, \mathcal{R}, \gamma)$ in augmented information state space

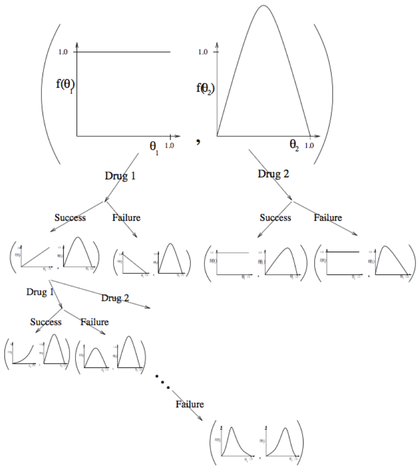
Bernoulli Bandits

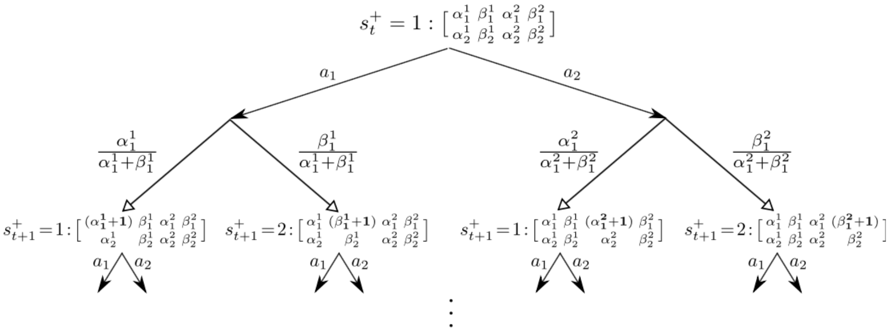
- Consider a Bernoulli bandit such that $\mathcal{R}^a = \mathcal{B}(\mu_a)$
- e.g. Win or lose a game with probability μ_a
- Want to find which arm has the highest μ_a
- The information state is $\tilde{s} = (\alpha, \beta)$
  - α_a counts the pulls of arm a where the reward was 0
  - β_a counts the pulls of arm a where the reward was 1

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 (e.g. Q-learning)
- Bayesian model-based RL (e.g. Gittins indices)
- This approach is known as Bayes-adaptive RL: Finds Bayes-optimal exploration/exploitation trade-off with respect to prior distribution
- In other words, selects actions that maximize expected reward given information have so far
- Check your understanding: Can an algorithm that optimally solves an information state bandit have a non-zero regret? Why or why not?

- Start with $\mathrm{Beta}(\alpha_a, \beta_a)$ prior over reward function $\mathcal{R}^a$
- Each time a is selected, update posterior for $\mathcal{R}^a$
  - $\mathrm{Beta}(\alpha_a + 1, \beta_a)$ if $r = 0$
  - $\mathrm{Beta}(\alpha_a, \beta_a + 1)$ if $r = 1$
- This defines transition function $\tilde{\mathcal{P}}$ for the Bayes-adaptive MDP
- Information state (α, β) corresponds to reward model $\mathrm{Beta}(\alpha, \beta)$
- Each state transition corresponds to a Bayesian model update




$s_t^+ = 1 : \begin{bmatrix} \alpha_1^1 & \beta_1^1 & \alpha_1^2 & \beta_1^2 \\ \alpha_2^1 & \beta_2^1 & \alpha_2^2 & \beta_2^2 \end{bmatrix}$
a_1
a_2
$\frac{\alpha_1^1}{\alpha_1^1+\beta_1^1}$
$\frac{\beta_1^1}{\alpha_1^1+\beta_1^1}$
$\frac{\alpha_1^2}{\alpha_1^2+\beta_1^2}$
$\frac{\beta_1^2}{\alpha_1^2+\beta_1^2}$
$s_{t+1}^+ = 1 : \begin{bmatrix} (\boldsymbol{\alpha_1^1+1}) & \beta_1^1 & \alpha_1^2 & \beta_1^2 \\ \alpha_2^1 & \beta_2^1 & \alpha_2^2 & \beta_2^2 \end{bmatrix}$
$s_{t+1}^+ = 2 : \begin{bmatrix} \alpha_1^1 & (\boldsymbol{\beta_1^1+1}) & \alpha_1^2 & \beta_1^2 \\ \alpha_2^1 & \beta_2^1 & \alpha_2^2 & \beta_2^2 \end{bmatrix}$
$s_{t+1}^+ = 1 : \begin{bmatrix} \alpha_1^1 & \beta_1^1 & (\boldsymbol{\alpha_1^2+1}) & \beta_1^2 \\ \alpha_2^1 & \beta_2^1 & \alpha_2^2 & \beta_2^2 \end{bmatrix}$
$s_{t+1}^+ = 2 : \begin{bmatrix} \alpha_1^1 & \beta_1^1 & \alpha_1^2 & (\boldsymbol{\beta_1^2+1}) \\ \alpha_2^1 & \beta_2^1 & \alpha_2^2 & \beta_2^2 \end{bmatrix}$
a_1 a_2
a_1 a_2
a_1 a_2
a_1 a_2

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-adaptiev MDP is typically intractable; information state space is too large
- Recent idea: apply simulation-based search (Guez et al. 2012, 2013)
  - Forward search in information state space
  - Using simulations from current information state

Table of Contents

- The sample principles for exploration/exploitation apply to MDPs
  - Naive Exploration
  - Optimistic Initialization
  - Optimism in the Face of Uncertainty
  - Probability Matching
  - Information State Search

Optimistic Initialization: Model-Free RL

- Initialize action-value function Q(s,a) to $\frac{r_{max}}{1-\gamma}$
- Run favorite model-free RL algorithm
  - Monte-Carlo control
  - Sarsa
  - Q-learning
  - etc.
- Encourages systematic exploration of states and actions

Optimistic Initialization: Model-Free RL

- Construct an **optimistic** model of the MDP
- Initialize transitions to go to terminal state with r_{max} reward
- Solve optimistic MDP by favorite planning algorithm
- Encourages systematic exploration of states and actions
- e.g. RMax algorithm (Brafman and Tennenholtz)

UCB: Model-Free RL

- Maximize UCB on action-value function $Q^\pi(s, a)$

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

  - Estimate uncertainty in policy evaluation (easy)
  - Ignores uncertainty from policy improvement
- Maximize UCB on optimal action-value function $Q^*(s, a)$

$$a_t = \arg\max_{a \in \mathcal{A}} Q(s_t, a) + U_1(s_t, a) + U_2(s_t, a)$$

  - Estimate uncertainty in policy evaluation (easy)
  - plus uncertainty from policy improvement (hard)

Bayesian Model-Based RL

- Maintain posterior distribution over MDP models
- Estimate both transition and rewards, $p[\mathcal{P}, \mathcal{R} \mid h_t]$, where $h_t = (s_1, a_1, r_1, \ldots, s_t)$ is the history
- Use posterior to guide exploration
  - Upper confidence bounds (Bayesian UCB)
  - Probability matching (Thompson sampling)

Thompson Sampling: Model-Based RL

- Thompson sampling implements probability matching

$$\begin{aligned}\pi(s, a \mid h_t) &= \mathbb{P}[Q(s,a) > Q(s,a'), \forall a' \neq a \mid h_t] \\ &= \mathbb{E}_{\mathcal{P},\mathcal{R}\mid h_t}\left[\mathbb{1}(a = \arg\max_{a\in\mathcal{A}} Q(s,a))\right]\end{aligned}$$

- Use Bayes law to compute posterior distribution $p[\mathcal{P}, \mathcal{R} \mid h_t]$
- **Sample** an MDP $\mathcal{P}, \mathcal{R}$ from posterior
- Solve MDP using favorite planning algorithm to get $Q^*(s,a)$
- Select optimal action for sample MDP, $a_t = \arg\max_{a\in\mathcal{A}} Q^*(s_t, a)$

Information State Search in MDPs

- MDPs can be augmented to include information state
- Now the augmented state is $(s, \tilde{s})$
  - where s is original state within MDP
  - and $\tilde{s}$ is a statistic of the history (accumulated information)
- Each action a causes a transition
  - to a new state s' with probability $\mathcal{P}^{a}_{s,s'}$
  - to a new information state $\tilde{s}'$
- Defines MDP $\tilde{\mathcal{M}}$ in augmented information state space

Bayes Adaptive MDP

- Posterior distribution over MDP model is an information state

$$\tilde{s}_t = \mathbb{P}[\mathcal{P}, \mathcal{R} \mid h_t]$$

- Augmented MDP over $(s, \tilde{s})$ is called **Bayes-adaptive MDP**
- Solve this MDP to find optimal exploration/exploitation trade-off (with respect to prior)
- However, Bayes-adaptive MDP is typically enormous
- Simulation-based search has proven effective (Guez et al, 2012, 2013)

Table of Contents

Principles

- Naive Exploration
  - Add noise to greedy policy (e.g. ϵ-greedy)
- Optimistic Initialization
  - Assume the best until proven otherwise
- Optimism in the Face of Uncertainty
  - Prefer actions with uncertain values
- Probability Matching
  - Select actions according to probability they are best
- Information State Search
  - Lookahead search incorporating value of information

Other evaluation criteria

- Probably approximately correct:
  - On all but N steps, algorithm will select an action whose value is near optimal $Q(s, a_t) - V(s) \geq -\epsilon$ with probability at least $1 - \delta$.
  - N is a polynomial function of the MDP parameters $(|S|, |A|, \frac{1}{1-\gamma}, \delta, \epsilon)$
- Bounded "mistakes"
- Many PAC RL algorithms use ideas of optimism under uncertainty

Generalization and Strategic Exploration

- Significant interest in combining generalization with strategic exploration
- Many approaches are grounded by the principles outlined in this lecture
- Some examples:
  - Optimism under uncertainty: Bellemare et al. NIPS 2016; Ostrovski et al. ICML 2017; Tang et al. NIPS 2017
  - Probability matching: Osband et al. NIPS 2016; Mandel et al. IJCAI 2016

Class Structure

- Last time: Midterm!
- **This time: Exploration and Exploitation**
- Next time: Batch RL