Lecture 9: Exploration and Exploitation

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Outline

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 decisions

Examples

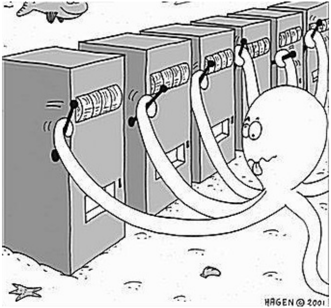
- Restaurant Selection
  - **Exploitation** Go to your favourite restaurant
  - **Exploration** Try a new restaurant
- Online Banner Advertisements
  - **Exploitation** Show the most successful advert
  - **Exploration** Show a different advert
- Oil Drilling
  - **Exploitation** Drill at the best known location
  - **Exploration** Drill at a new location
- Game Playing
  - **Exploitation** Play the move you believe is best
  - **Exploration** Play an experimental move

Principles

- Naive Exploration
  - Add noise to greedy policy (e.g. ϵ-greedy)
- Optimistic Initialisation
  - 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

The Multi-Armed Bandit

- A multi-armed bandit is a tuple $\langle \mathcal{A}, \mathcal{R} \rangle$
- $\mathcal{A}$ is a known set of m actions (or "arms")
- $\mathcal{R}^a(r) = \mathbb{P}\left[r | a\right]$ 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 $r_t \sim \mathcal{R}^{a_t}$
- The goal is to maximise cumulative reward $\sum_{\tau=1}^{t} r_\tau$



Regret

- The *action-value* is the mean reward for action a,

$$Q(a) = \mathbb{E}\left[r | a\right]$$

- The *optimal value* V^* is

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

- The *regret* is the opportunity loss for one step

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

- The *total regret* is the total opportunity loss

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

- Maximise cumulative reward $\equiv$ minimise total regret

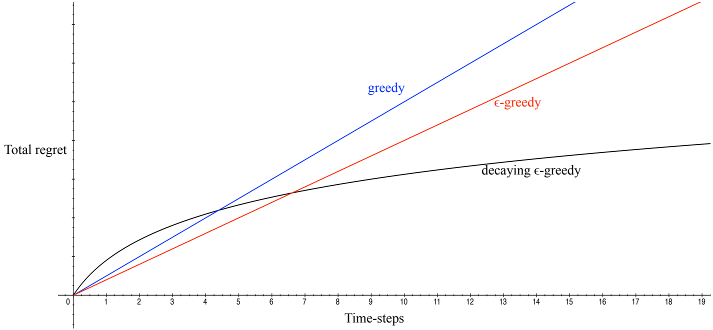
Counting Regret

- The *count* $N_t(a)$ is expected number of selections for action a
- The *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 the counts

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

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

Linear or Sublinear Regret



- If an algorithm forever explores it will have linear total regret
- If an algorithm never explores it will have linear total regret
- Is it possible to achieve sublinear total regret?

Greedy Algorithm

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

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

- The *greedy* algorithm selects action with highest value

$$a_t^* = \underset{a \in \mathcal{A}}{\operatorname{argmax}} \ \hat{Q}_t(a)$$

- Greedy can lock onto a suboptimal action forever
- $\Rightarrow$ Greedy has linear total regret

ϵ-Greedy Algorithm

- The ϵ-*greedy* algorithm continues to explore forever
  - With probability $1 - \epsilon$ select $a = \underset{a \in \mathcal{A}}{\operatorname{argmax}} \hat{Q}(a)$
  - With probability ϵ select a random action
- Constant ϵ ensures minimum regret

$$l_t \geq \frac{\epsilon}{\mathcal{A}} \sum_{a \in \mathcal{A}} \Delta_a$$

- $\Rightarrow$ ϵ-greedy has linear total regret

Optimistic Initialisation

- Simple and practical idea: initialise $Q(a)$ 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
- $\Rightarrow$ greedy + optimistic initialisation has linear total regret
- $\Rightarrow$ ϵ-greedy + optimistic initialisation has linear total regret

Decaying ϵ_t-Greedy Algorithm

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

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

- Decaying ϵ_t-greedy has *logarithmic* asymptotic total regret!
- Unfortunately, schedule requires advance knowledge of gaps
- Goal: find an algorithm with sublinear regret for any multi-armed bandit (without knowledge of $\mathcal{R}$)

Lower Bound

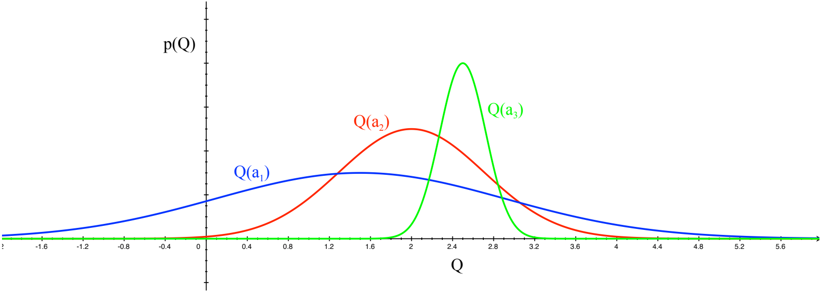
- The performance of any algorithm is determined by similarity between optimal arm and other arms
- Hard problems have similar-looking arms with different means
- This is described formally by the gap Δ_a and the similarity in distributions $KL(\mathcal{R}^a||\mathcal{R}^a*)$

Theorem (Lai and Robbins)

Asymptotic total regret is at least logarithmic in number of steps

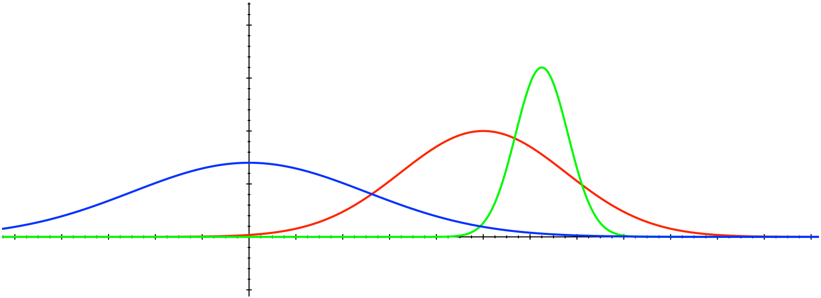
$$\lim_{t\to\infty} L_t \geq \log t \sum_{a|\Delta_a>0} \frac{\Delta_a}{KL(\mathcal{R}^a||\mathcal{R}^{a^*})}$$

Optimism in the Face of Uncertainty



- Which action should we pick?
- The more uncertain we are about an action-value
- The more important it is to explore that action
- It could turn out to be the best action

Optimism in the Face of Uncertainty (2)



- After picking blue action
- We are less uncertain about the value
- And more likely to pick another action
- Until we home in on best action

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 $\hat{U}_t(a)$ (estimated value is uncertain)
  - Large $N_t(a) \Rightarrow$ small $\hat{U}_t(a)$ (estimated value is accurate)
- Select action maximising Upper Confidence Bound (UCB)

$$a_t = \underset{a \in \mathcal{A}}{\operatorname{argmax}} \; \hat{Q}_t(a) + \hat{U}_t(a)$$

Hoeffding's Inequality

Theorem (Hoeffding's Inequality)

Let $X_1, ..., X_t$ be i.i.d. random variables in [0,1], and let $\overline{X}_t = \frac{1}{\tau}\sum_{\tau=1}^{t} X_\tau$ be the sample mean. Then

$$\mathbb{P}\left[\mathbb{E}\left[X\right] > \overline{X}_t + u\right] \leq e^{-2tu^2}$$

- We will apply Hoeffding's Inequality to rewards of the bandit
- conditioned on selecting action a

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

Calculating Upper Confidence Bounds

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

$$e^{-2N_t(a)U_t(a)^2} = p$$

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

- Reduce p as we observe more rewards, e.g. $p = t^{-4}$
- 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

$$a_t = \underset{a \in \mathcal{A}}{\operatorname{argmax}}\; Q(a) + \sqrt{\frac{2 \log t}{N_t(a)}}$$

Theorem

The UCB algorithm achieves logarithmic asymptotic total regret

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

Example: UCB vs. ϵ-Greedy On 10-armed Bandit

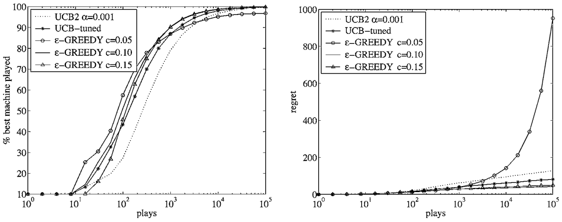


Figure 9. Comparison on distribution 11 (10 machines with parameters 0.9, 0.6, . . . , 0.6).

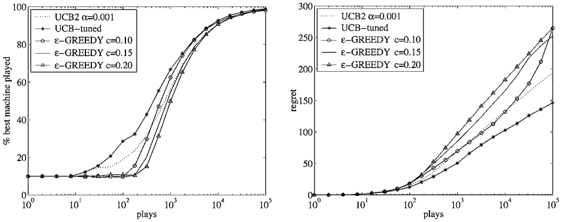


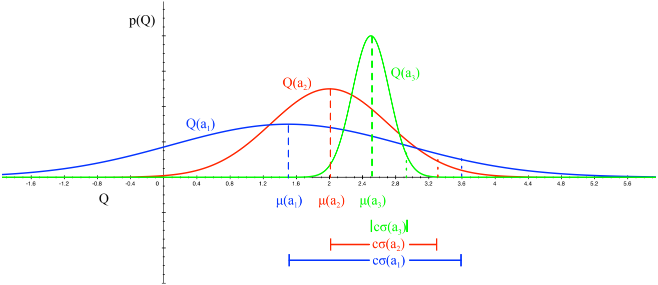
Figure 10. Comparison on distribution 12 (10 machines with parameters 0.9, 0.8, 0.8, 0.8, 0.7, 0.7, 0.7, 0.6, 0.6, 0.6).

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 $h_t = a_1, r_1, ..., a_{t-1}, r_{t-1}$ is the history
- Use posterior to guide exploration
  - 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)

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

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

$$a_t = \operatorname{argmax} \mu_a + c\sigma_a / \sqrt{N(a)}$$

Probability Matching

- Probability matching selects action a according to probability that a is the optimal action

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

- 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

- Thompson sampling implements probability matching

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

- Use Bayes law to compute posterior distribution $p\left[\mathcal{R} \mid h_t\right]$
- Sample a reward distribution $\mathcal{R}$ from posterior
- Compute action-value function $Q(a) = \mathbb{E}\left[\mathcal{R}_a\right]$
- Select action maximising value on sample, $a_t = \operatorname*{argmax}_{a \in \mathcal{A}} Q(a)$
- Thompson sampling achieves Lai and Robbins lower bound!

Value of Information

- Exploration is useful because it gains information
- Can we quantify the value of information?
  - 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
- Information gain is higher in uncertain situations
- Therefore it makes sense to explore uncertain situations more
- If we know value of information, we can trade-off exploration and exploitation *optimally*

Information State Space

- We have viewed bandits as *one-step* decision-making problems
- Can also view as *sequential* decision-making problems
- At each step there is an *information state* $\tilde{s}$
  - $\tilde{s}$ is a statistic of the history, $\tilde{s}_t = f(h_t)$
  - summarising all information accumulated so far
- Each action a causes a transition to a new information state $\tilde{s}'$ (by adding information), with probability $\tilde{\mathcal{P}}^a_{\tilde{s},\tilde{s}'}$
- This defines MDP $\tilde{\mathcal{M}}$ in augmented information state space

$$\tilde{\mathcal{M}} = \langle \tilde{\mathcal{S}}, \mathcal{A}, \tilde{\mathcal{P}}, \mathcal{R}, \gamma \rangle$$

Example: Bernoulli Bandits

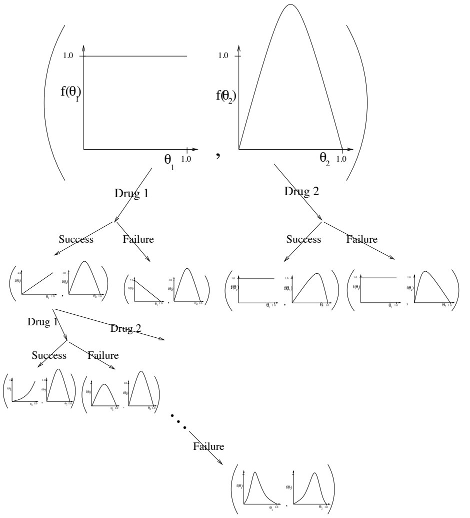
- Consider a Bernoulli bandit, such that $\mathcal{R}^a = \mathcal{B}(\mu_a)$
- e.g. Win or lose a game with probability μ_a
- Want to find which arm has the highest μ_a
- The information state is $\tilde{s} = \langle \alpha, \beta \rangle$
  - α_a counts the pulls of arm a where reward was 0
  - β_a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

Solving Information State Space Bandits

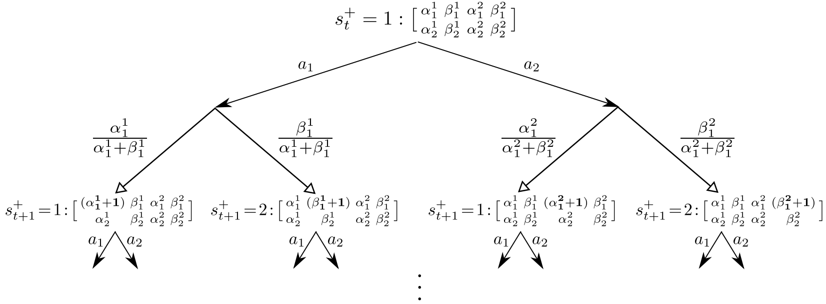
- We now have an infinite MDP over information states
- This MDP can be solved by reinforcement learning
- Model-free reinforcement learning
  - e.g. Q-learning (Duff, 1994)
- Bayesian model-based reinforcement learning
  - e.g. Gittins indices (Gittins, 1979)
  - This approach is known as *Bayes-adaptive* RL
  - Finds Bayes-optimal exploration/exploitation trade-off with respect to prior distribution

Bayes-Adaptive Bernoulli Bandits

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



Bayes-Adaptive MDP for Bernoulli Bandits



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

Contextual Bandits

- A contextual bandit is a tuple $\langle \mathcal{A}, \mathcal{S}, \mathcal{R} \rangle$
- $\mathcal{A}$ is a known set of actions (or "arms")
- $\mathcal{S} = \mathbb{P}[s]$ is an unknown distribution over states (or "contexts")
- $\mathcal{R}_s^a(r) = \mathbb{P}[r | s, a]$ is an unknown probability distribution over rewards
- At each step t
  - Environment generates state $s_t \sim \mathcal{S}$
  - Agent selects action $a_t \in \mathcal{A}$
  - Environment generates reward $r_t \sim \mathcal{R}_{s_t}^{a_t}$
- Goal is to maximise cumulative reward $\sum_{\tau=1}^{t} r_\tau$

Linear Regression

- Action-value function is expected reward for state s and action a

$$Q(s, a) = \mathbb{E}\left[r | s, a\right]$$

- Estimate value function with a linear function approximator

$$Q_\theta(s, a) = \phi(s, a)^\top \theta \approx Q(s, a)$$

- Estimate parameters by least squares regression

$$A_t = \sum_{\tau=1}^{t} \phi(s_\tau, a_\tau)\phi(s_\tau, a_\tau)^\top$$

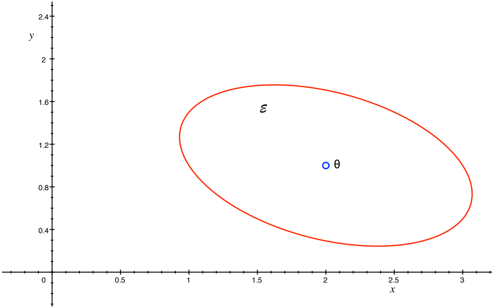
$$b_t = \sum_{\tau=1}^{t} \phi(s_\tau, a_\tau) r_\tau$$

$$\theta_t = A_t^{-1} b_t$$

Linear Upper Confidence Bounds

- Least squares regression estimates the mean action-value $Q_\theta(s, a)$
- But it can also estimate the variance of the action-value $\sigma^2_\theta(s, a)$
- i.e. the uncertainty due to parameter estimation error
- Add on a bonus for uncertainty, $U_\theta(s, a) = c\sigma$
- i.e. define UCB to be c standard deviations above the mean

Geometric Interpretation



- Define confidence ellipsoid $\mathcal{E}_t$ around parameters θ_t
- Such that $\mathcal{E}_t$ includes true parameters θ^* with high probability
- Use this ellipsoid to estimate the uncertainty of action values
- Pick parameters within ellipsoid that maximise action value

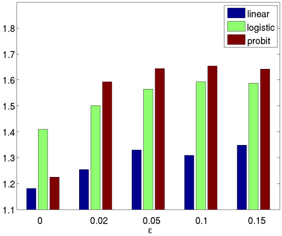
$$\underset{\theta \in \mathcal{E}}{\operatorname{argmax}} \; Q_\theta(s, a)$$

Calculating Linear Upper Confidence Bounds

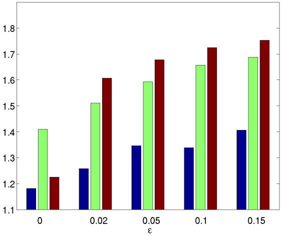
- For least squares regression, parameter covariance is A^{-1}
- Action-value is linear in features, $Q_\theta(s, a) = \phi(s, a)^\top \theta$
- So action-value variance is quadratic, $\sigma_\theta^2(s, a) = \phi(s, a)^\top A^{-1} \phi(s, a)$
- Upper confidence bound is $Q_\theta(s, a) + c\sqrt{\phi(s, a)^\top A^{-1} \phi(s, a)}$
- Select action maximising upper confidence bound

$$a_t = \underset{a \in \mathcal{A}}{\operatorname{argmax}}\ Q_\theta(s_t, a) + c\sqrt{\phi(s_t, a)^\top A_t^{-1} \phi(s_t, a)}$$

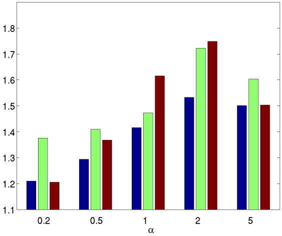
Example: Linear UCB for Selecting Front Page News



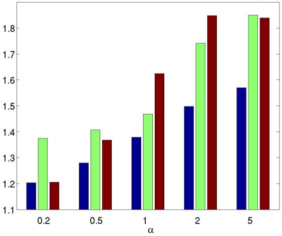
(a)



(b)



(c)



(d)

Exploration/Exploitation Principles to MDPs

The same principles for exploration/exploitation apply to MDPs

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

Optimistic Initialisation: Model-Free RL

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

Optimistic Initialisation: Model-Based RL

- Construct an optimistic model of the MDP
- Initialise transitions to go to heaven
  - (i.e. transition to terminal state with r_{max} reward)
- Solve optimistic MDP by favourite planning algorithm
  - policy iteration
  - value iteration
  - tree search
  - ...
- Encourages systematic exploration of states and actions
- e.g. RMax algorithm (Brafman and Tennenholtz)

Upper Confidence Bounds: Model-Free RL

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

$$a_t = \underset{a \in \mathcal{A}}{\operatorname{argmax}}\, Q(s_t, a) + U(s_t, a)$$

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

$$a_t = \underset{a \in \mathcal{A}}{\operatorname{argmax}}\, Q(s_t, a) + U_1(s_t, a) + U_2(s_t, a)$$

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

Bayesian Model-Based RL

- Maintain posterior distribution over MDP models
- Estimate both transitions and rewards, $p\left[\mathcal{P}, \mathcal{R} \mid h_t\right]$
  - where $h_t = s_1, a_1, r_2, ..., s_t$ 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

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

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

Information State Search in MDPs

- MDPs can be augmented to include information state
- Now the augmented state is $\langle s, \tilde{s} \rangle$
  - 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

$$\tilde{\mathcal{M}} = \langle \tilde{\mathcal{S}}, \mathcal{A}, \tilde{\mathcal{P}}, \mathcal{R}, \gamma \rangle$$

Bayes Adaptive MDPs

- Posterior distribution over MDP model is an information state

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

- Augmented MDP over $\langle s, \tilde{s} \rangle$ 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.)

Conclusion

- Have covered several principles for exploration/exploitation
  - Naive methods such as ϵ-greedy
  - Optimistic initialisation
  - Upper confidence bounds
  - Probability matching
  - Information state search
- Each principle was developed in bandit setting
- But same principles also apply to MDP setting