Exploration-Exploitation

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Outline

- ✓Introduction
- ✓Exploration and Exploitation
  - ✓ Simple naïve exploration (ϵ-greedy)
  - ✓ Optimistic approaches
  - ✓ Probability matching & Information Value
- ✓Bandits
  - ✓Multi-armed
  - ✓Contextual
- ✓Back to MDPs

Introduction

Exploration-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
- ✓ Holiday planning
  - ✓ Exploitation – The camping site you go to since you are born
  - ✓ Exploration – Hitchhike and follow the flow
- ✓ Game Playing
  - ✓ Exploitation - Play the move you believe is best
  - ✓ Exploration - Play an experimental move

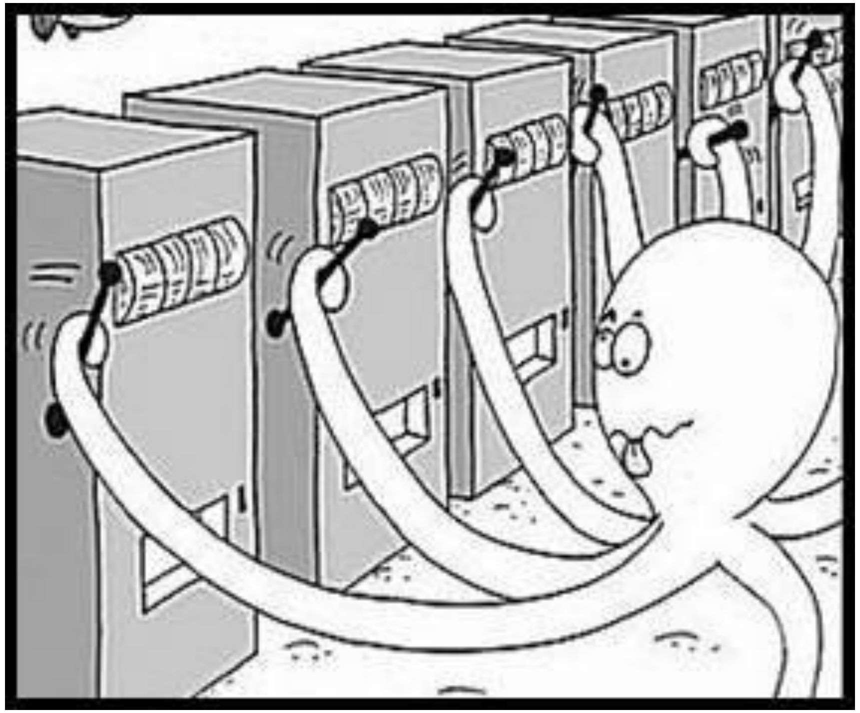
Principles

- ✓ Random Exploration
  - ✓ Add noise to greedy policy (e.g. -greedy)
- ✓ Optimism in the Face of Uncertainty
  - ✓ Estimate uncertainty on value
  - ✓ Prefer to explore states/actions with highest uncertainty
- ✓ Information State Search
  - ✓ Consider agent’s information as part of its state
  - ✓ Lookahead to see how information helps rewards

Bandits

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”)
  - $\mathcal{R}^a(r) = P(r|a)$ is an unknown probability distribution over rewards
- At each step t the agent selects an action $\mathrm{a}_t \in \mathcal{A}$
- 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

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

- ✓The optimal value V^* is

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

- ✓The regret is the opportunity loss for one step

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

- ✓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 ≡ minimise total regret

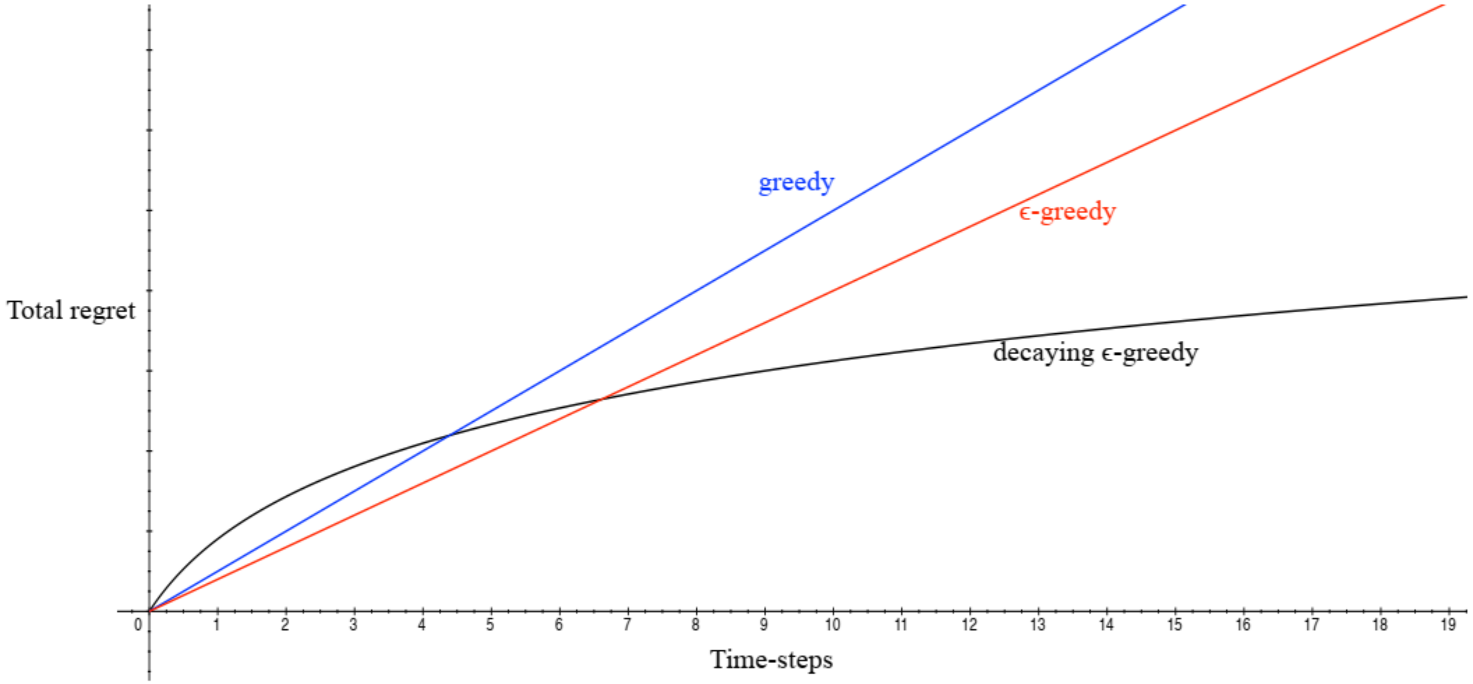
Counting Regret

- ✓The count $N_t(a)$ is expected number of selections for action a
- ✓The gap $\Delta_a = V^* - Q(a)$ is the difference in value between action a and optimal action a^*
- ✓Regret is a function of gaps and the counts

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

- ✓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?

Exploration Strategies

Greedy Algorithms

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

$$\hat{Q}_t(a) = \frac{1}{N_t(a)} \sum_{\tau} r_\tau \mathbf{1}(a_\tau; a)$$

- ✓The greedy algorithm selects action with highest value

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

- ✓Greedy can lock onto a suboptimal action forever

Greedy has linear total regret

ϵ-greedy Algorithms

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

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

ϵ-greedy has linear total regret

Decaying ϵ_t-greedy Algorithms

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

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

- ✓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 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 $KL(\mathcal{R}^a || \mathcal{R}^{a^*})$

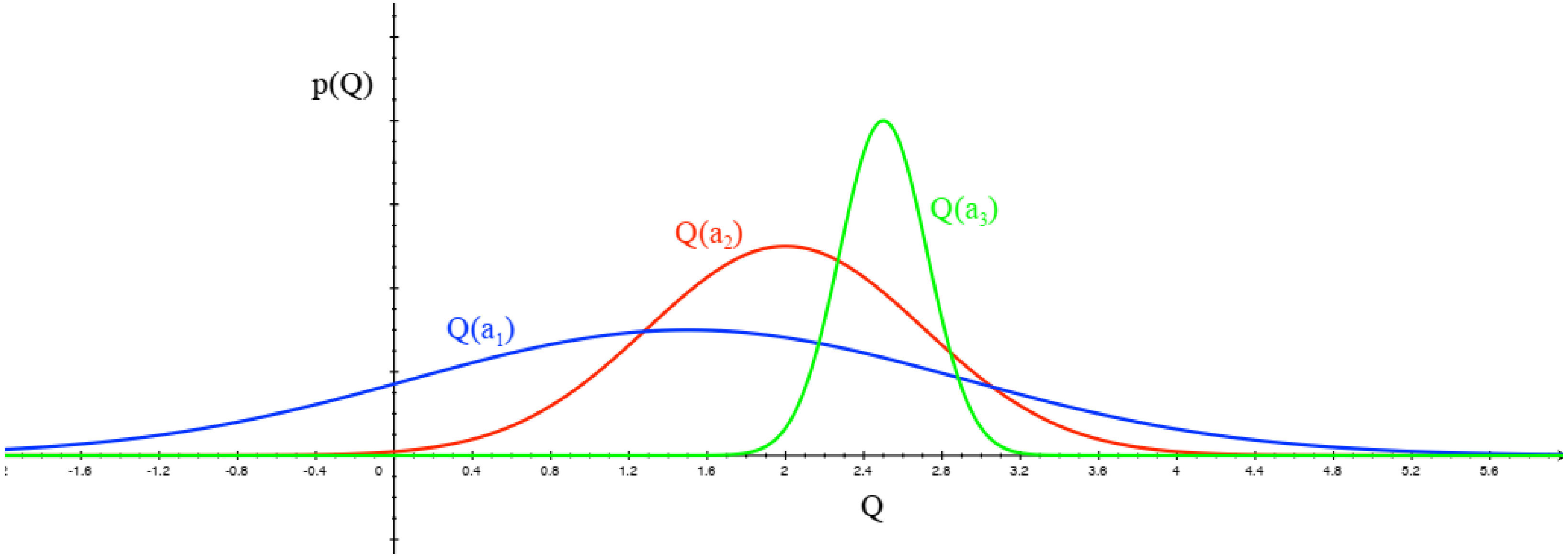
Theorem (Lai and Robbins)

Asymptotic total regret is at least logarithmic in the number of steps

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

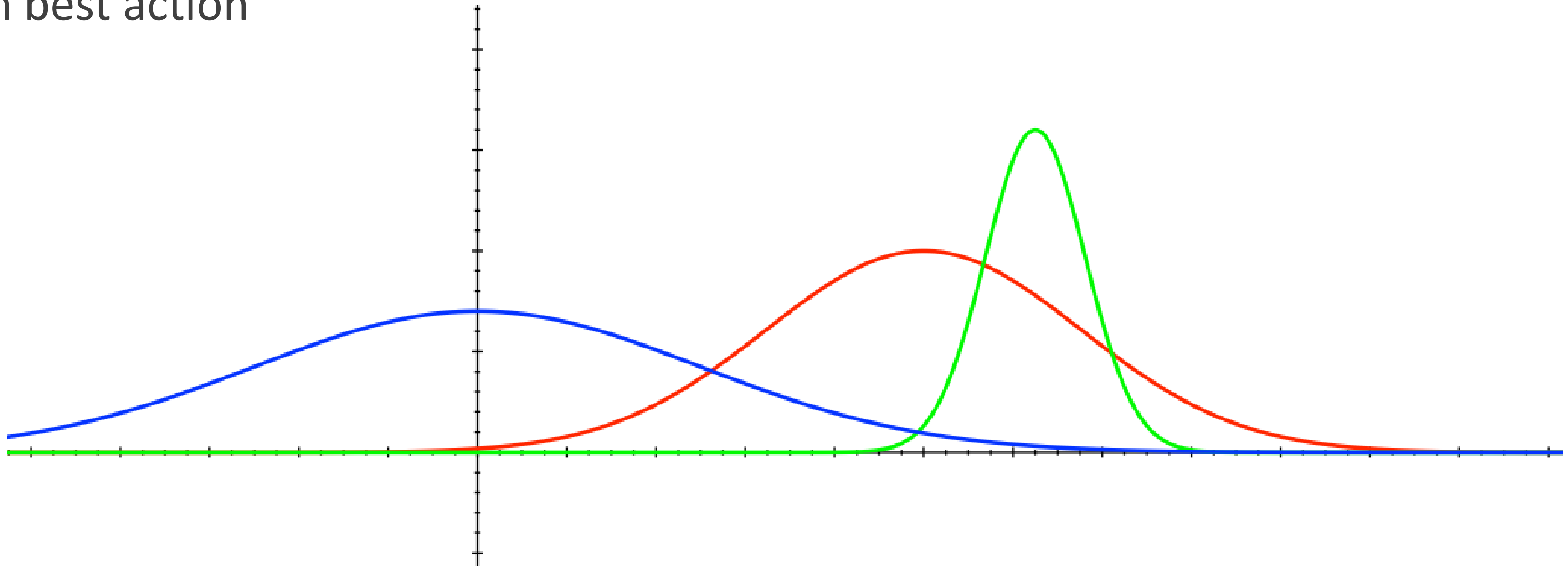
Optimism in the Face of Uncertainty (I)

- ✓ 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 (II)

- ✓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 $\mathrm{Q(a)} \leq \hat{Q}_t(a) + \hat{U}_t(a)$ with high probability
- ✓This depends on the number of times $N(a)$ has been selected
  - ✓Small $N_t(a)$ ⇒large $\hat{U}_t(a)$ (estimated value is uncertain)
  - ✓Large $N_t(a)$ ⇒ small $\hat{U}_t(a)$ (estimated value is accurate)
- ✓Select action maximising 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 $X_1, \dots, X_t$ *be i.i.d random variables in* $[0,1]$ *and let* $\bar{X}_t = \frac{1}{\tau}\sum_{\tau=1}^{t} x_t$ *be the sample mean. Then*

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

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

$$P\left(\mathrm{Q(a)} \leq \hat{Q}_t(a) + \hat{U}_t(a)\right) \leq e^{-2N_t(a)\hat{U}_t(a)^2}$$

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

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

- ✓The UCB algorithm achieves logarithmic asymptotic total regret

UCB vs. ϵ-greedy on 10-armed Bandit

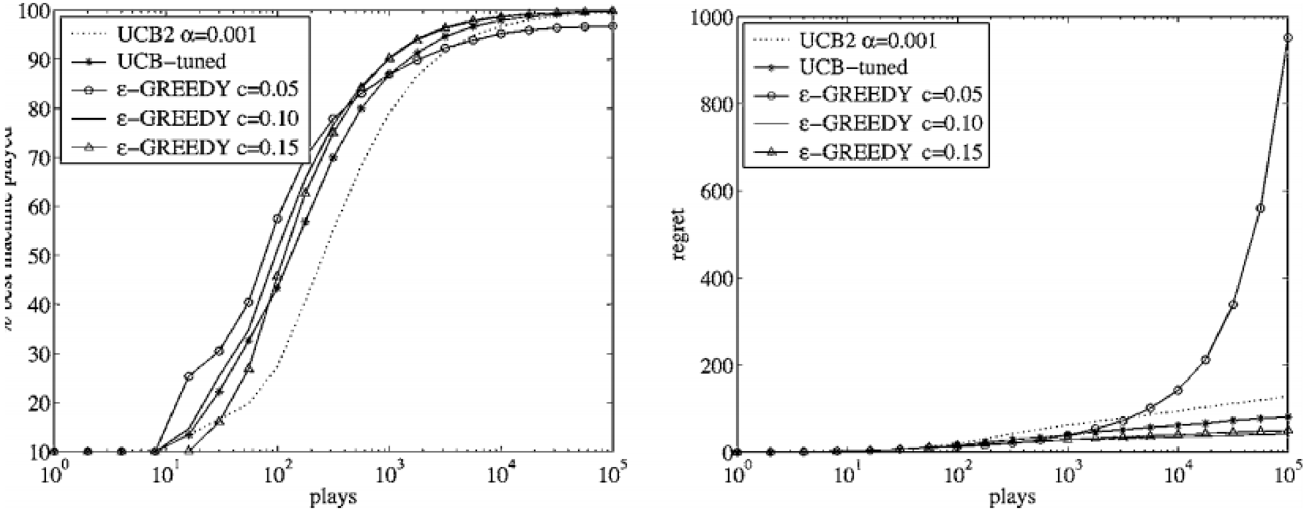
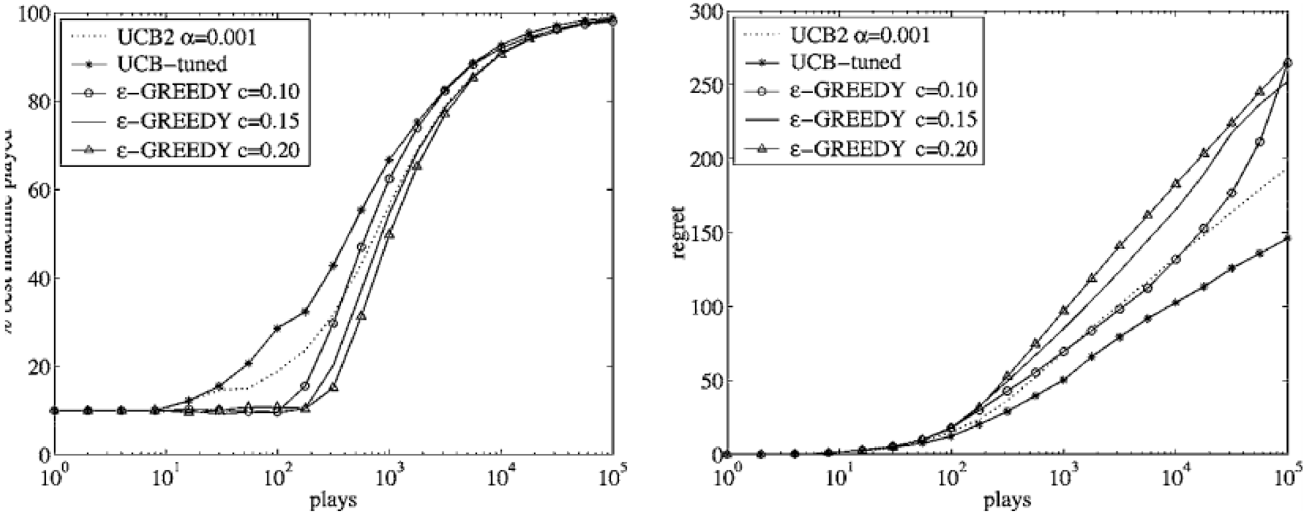


Figure 9. Comparison on distribution 11 (10 machines with parameters 0.9, 0.6, . . . , 0.6).



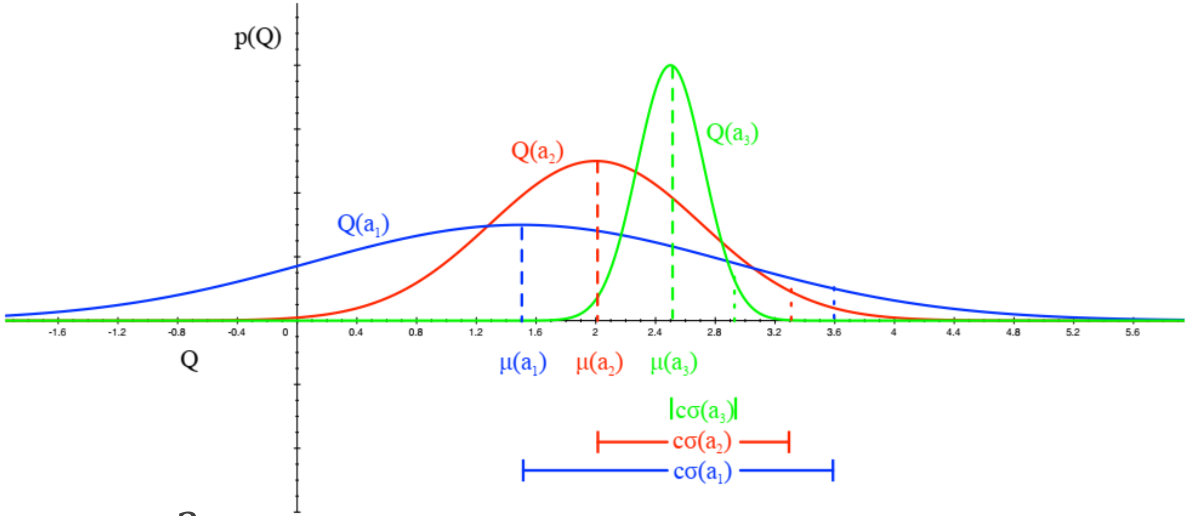
Bayesian Bandits

- So far, no assumptions about the reward distribution $\mathcal{R}$
  - Except bounds on rewards
- Bayesian bandits exploit prior knowledge of rewards $\mathrm{P}(\mathcal{R})$
- They compute posterior distribution of rewards $\mathrm{P}(\mathcal{R}|h_t)$
  - where $h_t = a_1, r_1; \ldots; a_{t-1} r_{t-1}$ 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 (Bayes)

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

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

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

Probability Matching

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

$$\pi(a|h_t) = P\left(Q(a) = \max_{a'} Q(a')\,|h_t\right)$$

- ✓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

$$\pi(a|h_t) = \mathbb{E}_{\mathcal{R}|h_t}\left[\mathbf{1}\left(Q(a); \arg\max_{a' \in \mathcal{A}} Q(a')\right)|h_t\right]$$

- ✓Use Bayes law to compute posterior distribution $P(\mathcal{R}|h_t)$
- ✓Sample a reward distribution $\mathcal{R}$ from posterior
- ✓Compute action-value function $\mathrm{Q(a)} = \mathbb{E}[\mathcal{R}_a]$
- ✓Select action maximising value on sample $a_t = \arg\max_{a \in \mathcal{A}} Q(a)$
- ✓Thompson sampling achieves Lai and Robbins lower bound!

Information State

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, i.e. $\tilde{s} = f(h_t)$
  - ✓summarizes all information accumulated so far
- ✓Each action a causes a transition to a new information state $\tilde{s}$' (and adds information) with probability $\tilde{P}^{a}_{\tilde{s},\tilde{s}'}$
- ✓Defines an MDP $\widetilde{\mathcal{M}}$ in augmented information state space

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

Example - Bernoulli Bandits

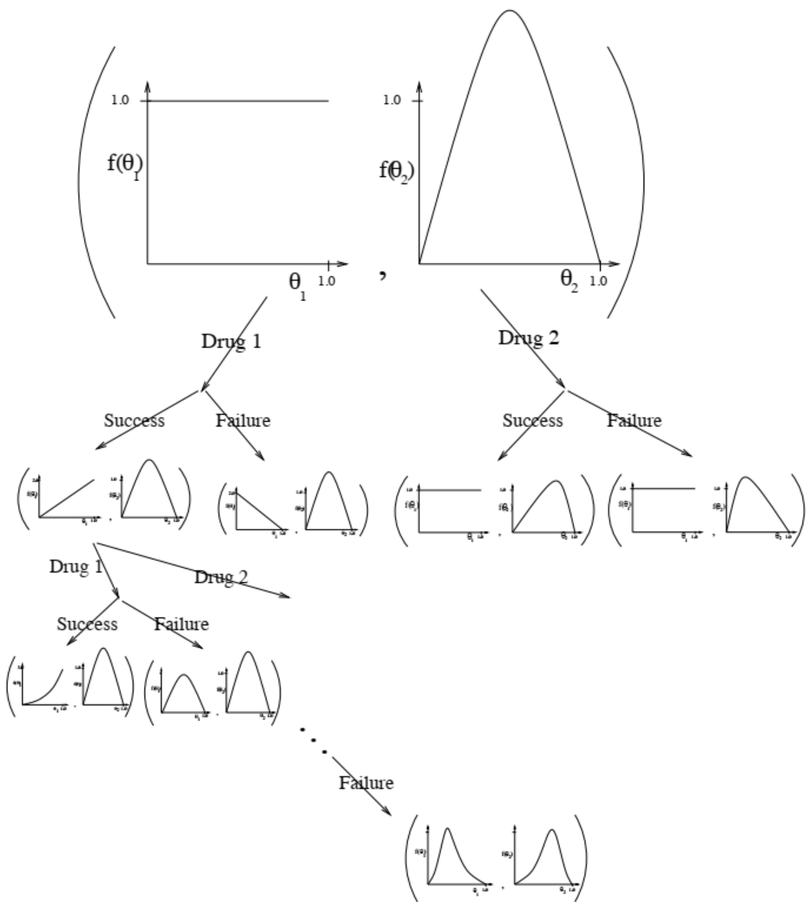
- Consider a Bernoulli bandit, such that $\mathcal{R}_a = \mathcal{B}(\mu_a)$ (e.g. win or lose a game with probability μ_a)
- Want to find which arm has the highest μ_a
- The information state is $\tilde{s} = \langle \alpha, \beta \rangle$
  - α_a counts the pulls of arm a where reward was 0
  - β_a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

Solving Information State Space Bandits

- ✓We now have an infinite MDP over information states that 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 $\tilde{P}$ 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



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
- ✓ More recent idea: apply simulation-based search (Guez et al. 2012)
  - ✓ Forward search in information state space
  - ✓ Using simulations from current information state

Contextual Bandits

Contextual Bandits

- ✓A contextual bandit is a tuple $\langle \mathcal{A}, \mathcal{S}, \mathcal{R} \rangle$
- ✓$\mathcal{S} = P(s)$ is an unknown distribution over states (contexts)
- ✓$\mathcal{R}_s^a(r) = P(r|s,a)$ 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 $r_t \sim \mathcal{R}_{s_t}^{a_t}$

Linear Regression

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

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

✓Estimate value function with a linear function approximator

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

✓Estimate parameters by least squares regression

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

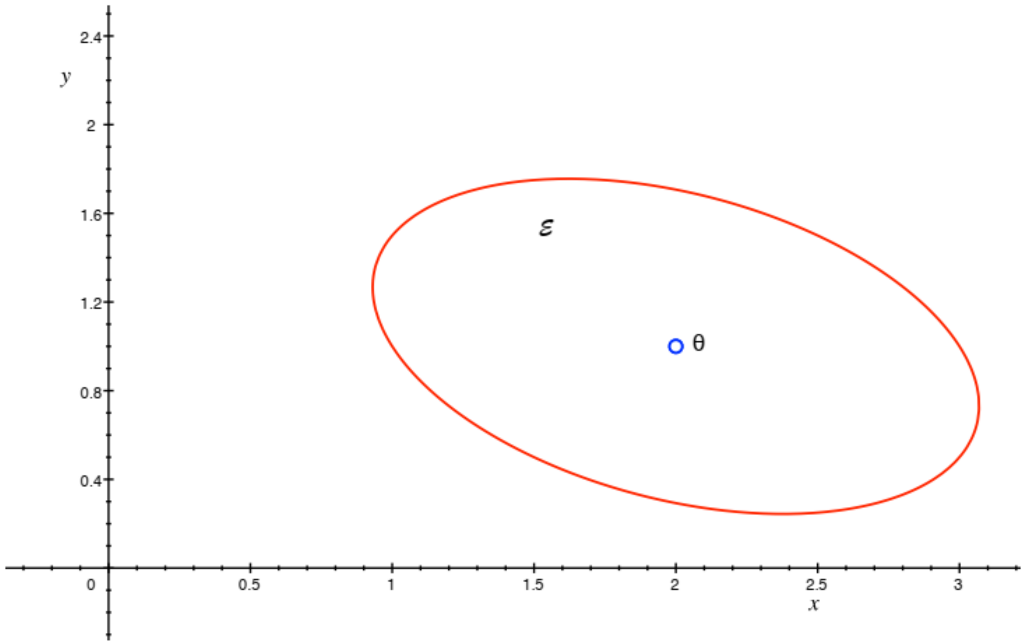
$$b_t = \sum_{\tau=1}^{t} \phi(s_\tau, a_\tau) r_\tau$$

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

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 $\sigma_\theta^2(s,a)$
  - ✓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 ε_t around parameters θ_t
- Such that ε_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

$$\arg\max_{\theta \in \epsilon} Q_\theta(s, a)$$

Calculating Linear Upper Confidence Bounds (LinUCB)

- ✓For least squares regression, parameter covariance is A^{-1}
- ✓Action-value is linear in features

$$Q_\theta(s,a) = \phi(s,a)^T\theta$$

- ✓So action-value variance is quadratic

$$\sigma_\theta^2(s,a) = \phi(s,a)^T A^{-1}\phi(s,a)$$

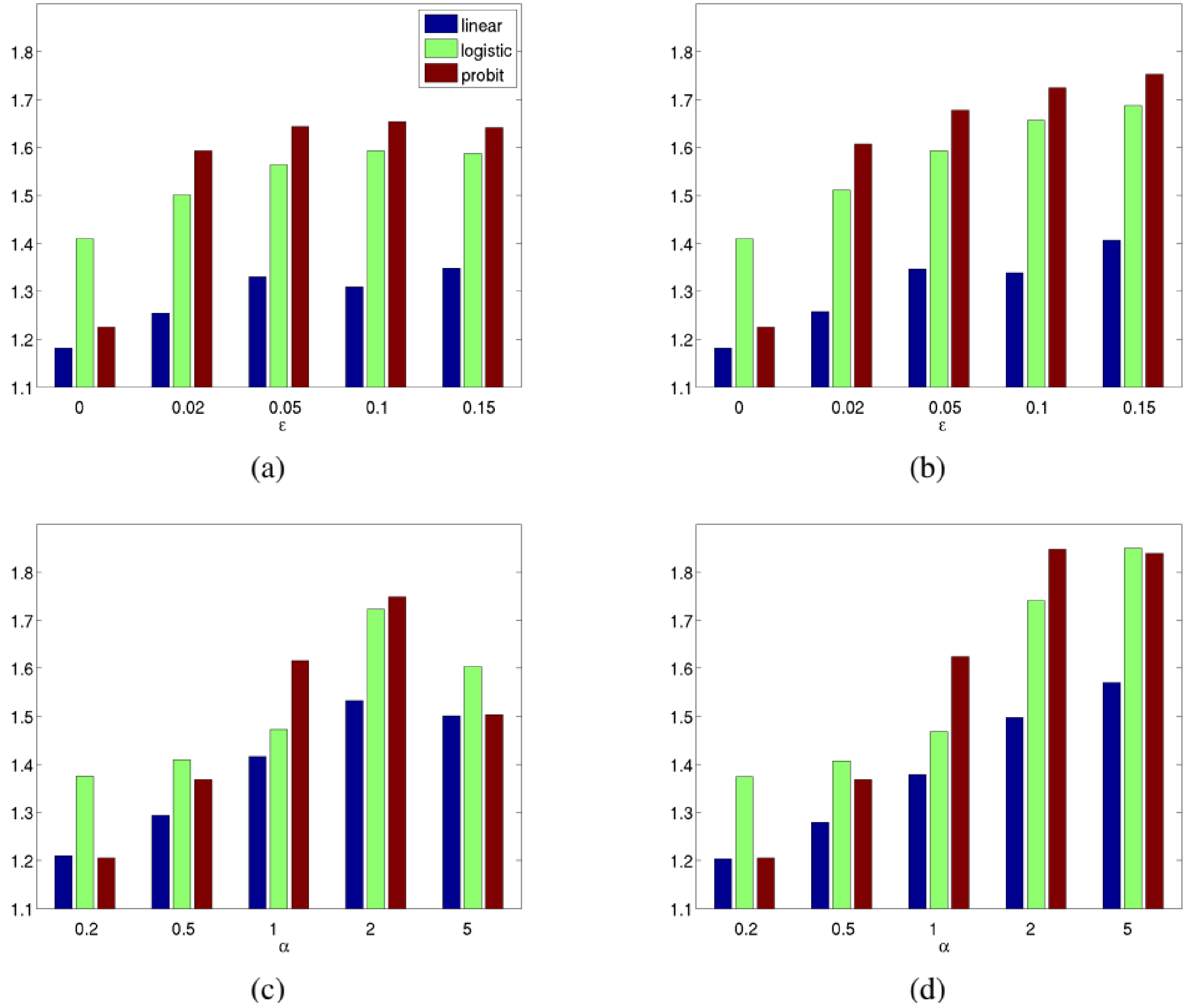
- ✓Upper confidence bound is

$$Q_\theta(s,a) + c\sqrt{\phi(s,a)^T A^{-1}\phi(s,a)}$$

- ✓Select action maximising upper confidence bound

$$a_t = \arg\max_{a\in\mathcal{A}} Q_\theta(s_t,a) + c\sqrt{\phi(s_t,a)^T A^{-1}\phi(s_t,a)}$$

Linear UCB for Selecting Front Page News



Exploration-Exploitation in MDPs

Applying Exploration/Exploitation to MDPs

The same principles for exploration/exploitation apply to MDPs

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

Upper Confidence Bounds - Model-Free RL

- Maximise 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
  - Ignore uncertainty from policy improvement

- Maximise 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
  - Estimate uncertainty from policy improvement

Information State Search in MDPs

- ✓MDPs can be augmented to include information state
- ✓Now the augmented state is $\langle s, \tilde{s} \rangle$
  - ✓ s is original state within MDP
  - ✓ $\tilde{s}$ is a statistic of the history
- ✓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 $\widetilde{\mathcal{M}}$ in augmented information state space

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

- ✓Posterior distribution over MDP model is an information state

$$\tilde{s} = P(\mathcal{P}, \mathcal{R} | h_t)$$

- ✓Solve this MDP to find optimal exploration/exploitation trade-off (with respect to prior)

Wrap-up

Take (stay) home messages

- ✓A selection of principles for exploration/exploitation
  - ✓Naive methods (ϵ-greedy)
  - ✓Upper confidence bounds
  - ✓Probability matching
  - ✓Information state search
- ✓Principles developed in bandit setting but also apply to MDP setting

Coming up

Imitation Learning

- ✓Demonstration techniques
- ✓Inverse reinforcement learning
- ✓Reinforcement learning with generative models