Lecture 2: Exploration and Exploitation

Hado van Hasselt

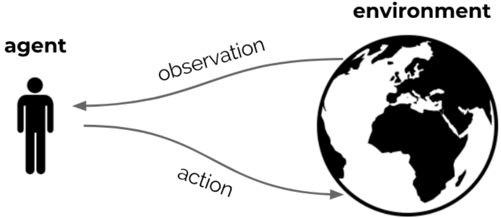
Reinforcement learning, 2021

Background

Recommended reading:
Sutton & Barto 2018, Chapter 2

Further background material:
Bandit Algorithms, Lattimore & Szepesvári, 2020
Finite-time analysis of the multiarmed bandit problem, Auer, Cesa-Bianchi, Fischer, 2002

Recap



- Reinforcement learning is the science of learning to make decisions
- Agents can learn a **policy**, **value function** and/or a **model**
- The general problem involves taking into account **time** and **consequences**
- Decisions affect the **reward**, the **agent state**, and **environment state**
- Learning is **active**: decisions impact data

This Lecture

In this lecture, we simplify the setting

- The environment is assumed to have only a **single state**
- $\implies$ actions no longer have long-term consequences in the environment
- $\implies$ actions still do impact **immediate reward**
- $\implies$ other observations can be ignored
- We discuss how to learn a policy in this setting

Blackboard: Example

Exploration vs. Exploitation

- Learning agents need to trade off two things
  - **Exploitation**: Maximise performance based on current knowledge
  - **Exploration**: Increase knowledge
- We need to gather information to make the best overall decisions
- The best long-term strategy may involve short-term sacrifices

Formalising the problem

The Multi-Armed Bandit

- A multi-armed bandit is a set of distributions $\{\mathcal{R}_a | a \in \mathcal{A}\}$
- $\mathcal{A}$ is a (known) set of actions (or “arms")
- $\mathcal{R}_a$ is a distribution on rewards, given action a
- 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 $\sum_{i=1}^{t} R_i$
- We do this by learning a **policy**: a distribution on $\mathcal{A}$

Values and Regret

- The **action value** for action a is the expected reward

$$q(a) = \mathbb{E}\left[R_t | A_t = a\right]$$

- The **optimal value** is

$$v_* \quad = \quad \max_{a \in \mathcal{A}} q(a) \quad = \quad \max_a \mathbb{E}\left[R_t \mid A_t = a\right]$$

- **Regret** of an action a is

$$\Delta_a = v_* - q(a)$$

- The regret for the optimal action is zero

Regret

- We want to minimise **total regret**:

$$L_t = \sum_{n=1}^{t} v_* - q(A_n) = \sum_{n=1}^{t} \Delta_{A_n}$$

- Maximise cumulative reward ≡ minimise total regret
- The summation spans over the full 'lifetime of learning'

Algorithms

Algorithms

- We will discuss several algorithms:
  - Greedy
  - ϵ-greedy
  - UCB
  - Thompson sampling
  - Policy gradients
- The first three all use **action value estimates** $Q_t(a) \approx q(a)$

Action values

- The **action value** for action a is the expected reward

$$q(a) = \mathbb{E}\left[R_t | A_t = a\right]$$

- A simple estimate is the average of the sampled rewards:

$$Q_t(a) = \frac{\sum_{n=1}^{t} \mathcal{I}(A_n = a)\ R_n}{\sum_{n=1}^{t} \mathcal{I}(A_n = a)}$$

  $\mathcal{I}(\cdot)$ is the **indicator** function: $\mathcal{I}(\text{True}) = 1$ and $\mathcal{I}(\text{False}) = 0$

- The **count** for action a is

$$N_t(a) = \sum_{n=1}^{t} \mathcal{I}(A_n = a)$$

Action values

- This can also be updated incrementally:

$$Q_t(A_t) = Q_{t-1}(A_t) + \alpha_t \underbrace{\left(R_t - Q_{t-1}(A_t)\right)}_{\text{error}},$$

$$\forall a \neq A_t : Q_t(a) = Q_{t-1}(a)$$

with

$$\alpha_t = \frac{1}{N_t(A_t)} \qquad \text{and} \qquad N_t(A_t) = N_{t-1}(A_t) + 1,$$

where $N_0(a) = 0$.

- We will later consider other **step sizes** α
- For instance, constant α would lead to **tracking**, rather than averaging

Algorithms: greedy

The greedy policy

- One of the simplest policies is **greedy**:
  - Select action with highest value: $A_t = \operatorname*{argmax}_a Q_t(a)$
  - Equivalently: $\pi_t(a) = \mathcal{I}(A_t = \operatorname*{argmax}_a Q_t(a))$ (assuming no ties are possible)

Example:
Regret of the greedy policy

Algorithms: ϵ-greedy

ϵ-Greedy Algorithm

- Greedy can get stuck on a suboptimal action forever
  $\implies$ linear expected total regret
- The **ϵ-greedy** algorithm:
  - With probability $1 - \epsilon$ select greedy action: $a = \underset{a \in \mathcal{A}}{\operatorname{argmax}}\, Q_t(a)$
  - With probability ϵ select a random action
  - Equivalently:

$$\pi_t(a) = \begin{cases} (1-\epsilon) + \epsilon/|\mathcal{A}| & \text{if } Q_t(a) = \max_b Q_t(b) \\ \epsilon/|\mathcal{A}| & \text{otherwise} \end{cases}$$

- ϵ-greedy continues to explore
  $\Rightarrow$ ϵ-greedy with constant ϵ has linear expected total regret

Algorithms: Policy gradients

Policy search

- Can we learn policies $\pi(a)$ directly, instead of learning values?
- For instance, define **action preferences** $H_t(a)$ and a policy

$$\pi(a) = \frac{e^{H_t(a)}}{\sum_b e^{H_t(b)}} \qquad \text{(\textbf{softmax})}$$

- The preferences are not values: they are just learnable policy parameters
- Goal: learn by optimising the preferences

Policy gradients

- Idea: update policy parameters such that expected value increases
- We can use **gradient ascent**
- In the bandit case, we want to update:

$$\theta_{t+1} = \theta_t + \alpha \nabla_\theta \mathbb{E}[R_t | \pi_{\theta_t}] ,$$

  where θ_t are the current policy parameters
- Can we compute this gradient?

Gradient bandits

- Log-likelihood trick (also known as REINFORCE trick, Williams 1992):

$$
\begin{aligned}
\nabla_\theta \, \mathbb{E}[R_t|\pi_\theta] &= \nabla_\theta \sum_a \pi_\theta(a) \, \overbrace{\mathbb{E}[R_t|A_t = a]}^{=\, q(a)} \\
&= \sum_a q(a) \, \nabla_\theta \pi_\theta(a) \\
&= \sum_a q(a) \, \frac{\pi_\theta(a)}{\pi_\theta(a)} \, \nabla_\theta \pi_\theta(a) \\
&= \sum_a \pi_\theta(a) \, q(a) \, \frac{\nabla_\theta \pi_\theta(a)}{\pi_\theta(a)} \\
&= \mathbb{E}\left[R_t \, \frac{\nabla_\theta \pi_\theta(A_t)}{\pi_\theta(A_t)} \right] \qquad = \mathbb{E}\left[R_t \nabla_\theta \log \pi_\theta(A_t) \right]
\end{aligned}
$$

Gradient bandits

- Log-likelihood trick (also known as REINFORCE trick, Williams 1992):

$$\nabla_\theta \mathbb{E}[R_t|\theta] = \mathbb{E}\left[R_t \nabla_\theta \log \pi_\theta(A_t)\right]$$

- We can sample this!
- So

$$\theta = \theta + \alpha R_t \nabla_\theta \log \pi_\theta(A_t)\,,$$

  this is **stochastic gradient ascent** on the (true) value of the policy
- Can use **sampled** rewards — does not need value estimates

Gradient bandits

- For soft max:

$$
\begin{aligned}
H_{t+1}(a) &= H_t(a) + \alpha R_t \frac{\partial \log \pi_t(A_t)}{\partial H_t(a)} \\
&= H_t(a) + \alpha R_t (\mathcal{I}(a = A_t) - \pi_t(a))
\end{aligned}
$$

- $\Rightarrow$

$$
\begin{aligned}
H_{t+1}(A_t) &= H_t(A_t) + \alpha R_t (1 - \pi_t(A_t)) \\
H_{t+1}(a) &= H_t(a) - \alpha R_t \pi_t(a) && \text{if } a \neq A_t
\end{aligned}
$$

- Preferences for actions with higher rewards increase more (or decrease less), making them more likely to be selected again

Theory: what is possible?

How well can we do?

Theorem (Lai and Robbins)

Asymptotic total regret is at least logarithmic in number of steps

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

(Note: $\mathrm{KL}(\mathcal{R}_a||\mathcal{R}_{a*}) \propto \Delta_a^2$)

- Note that **regret grows at least logarithmically**
- That's still a whole lot better than linear growth! Can we get it in practice?
- Are there algorithms for which the **upper bound** is logarithmic as well?

Counting Regret

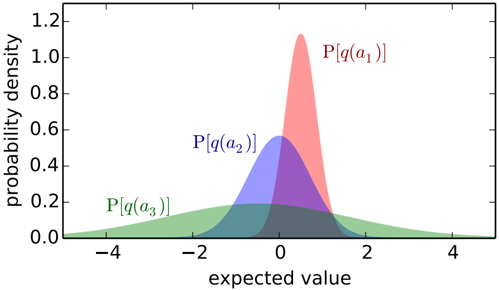
- Recall $\Delta_a = v_* - q(a)$
- Total regret depends on action regrets Δ_a and action counts

$$L_t = \sum_{n=1}^{t} \Delta_{A_n} = \sum_{a \in \mathcal{A}} N_t(a) \Delta_a$$

- A good algorithm ensures small counts for large action regrets

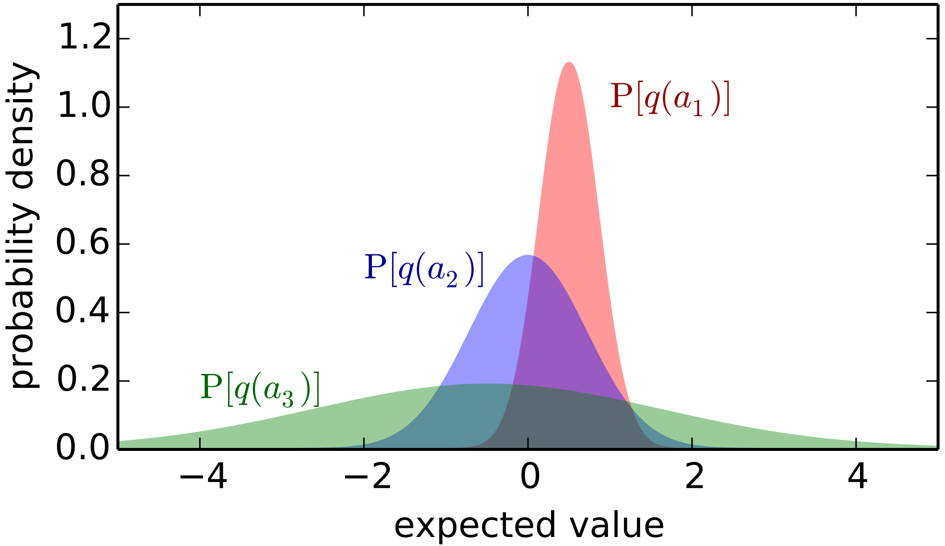
Optimism in the face of uncertainty

Optimism in the Face of Uncertainty



- Which action should we pick?
- More uncertainty about its value: more important to explore that action

Optimism in the Face of Uncertainty



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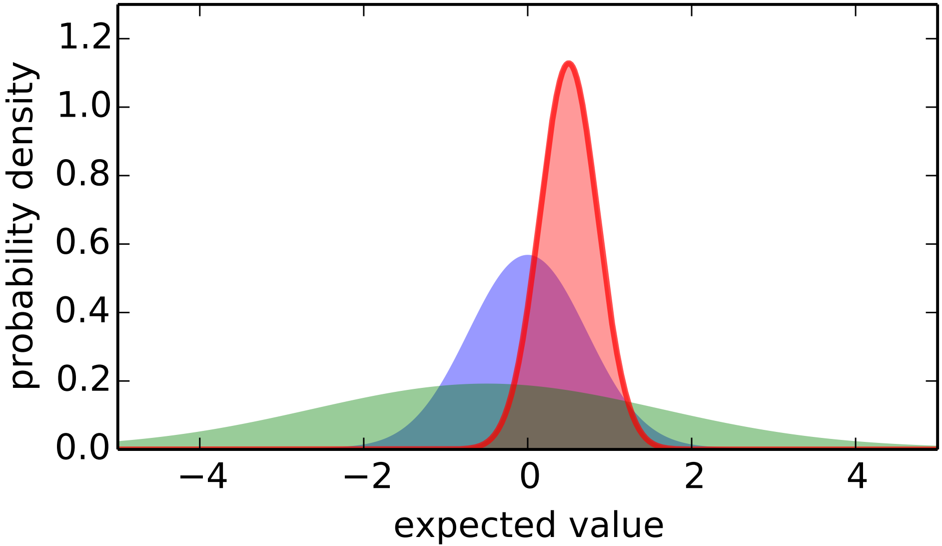

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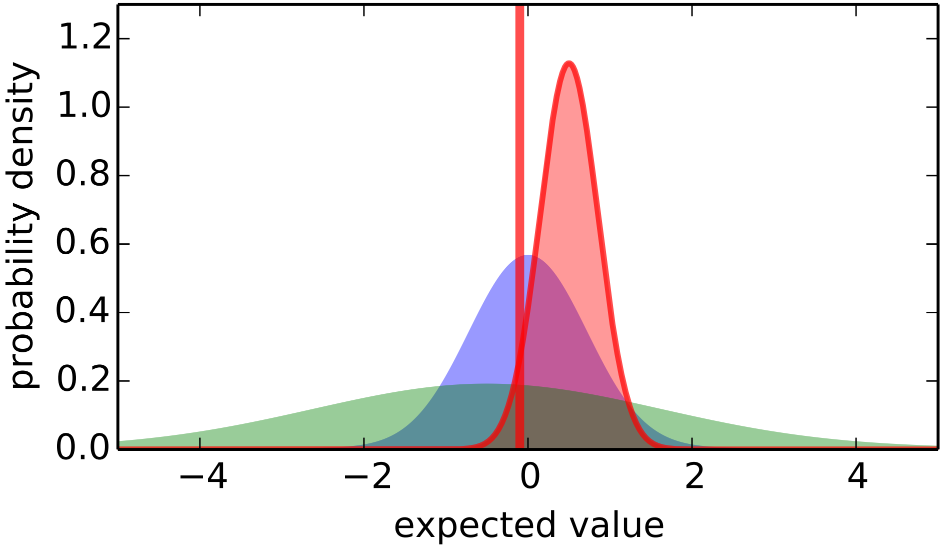

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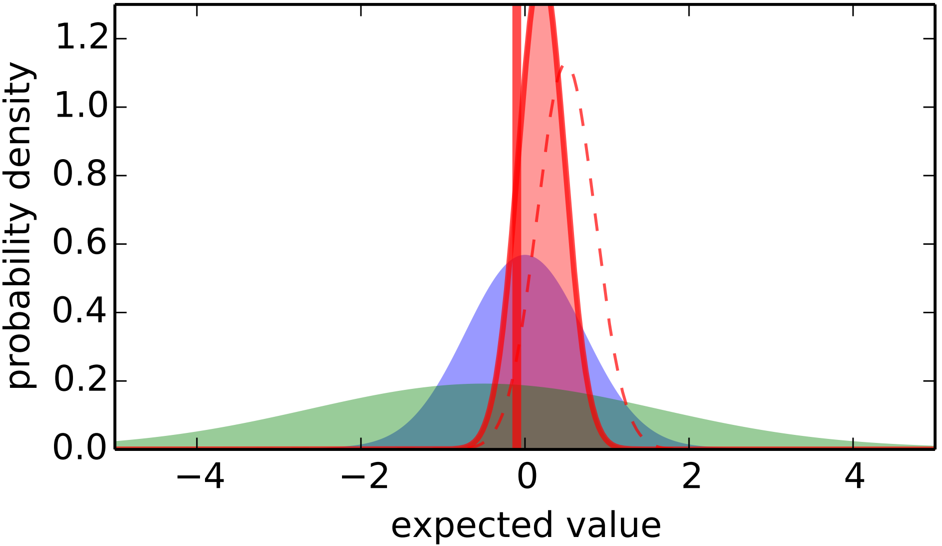

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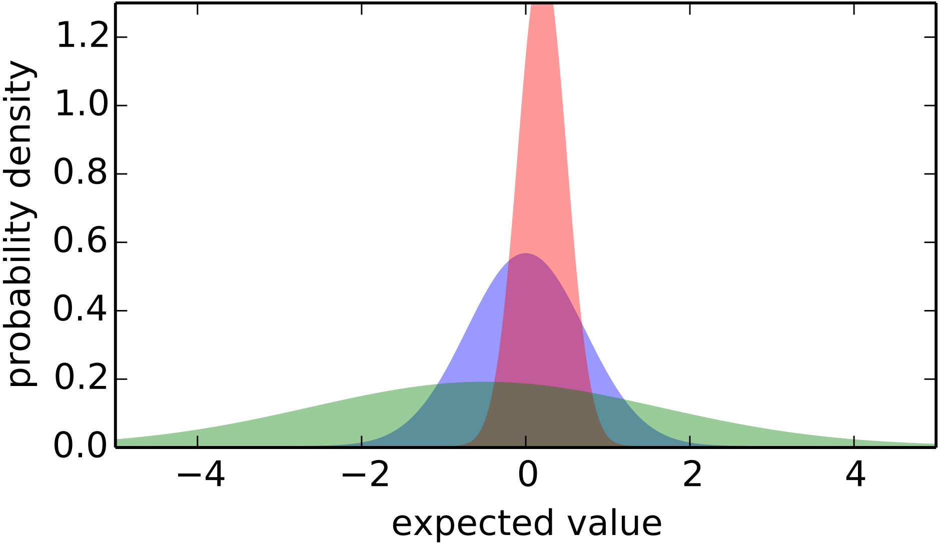

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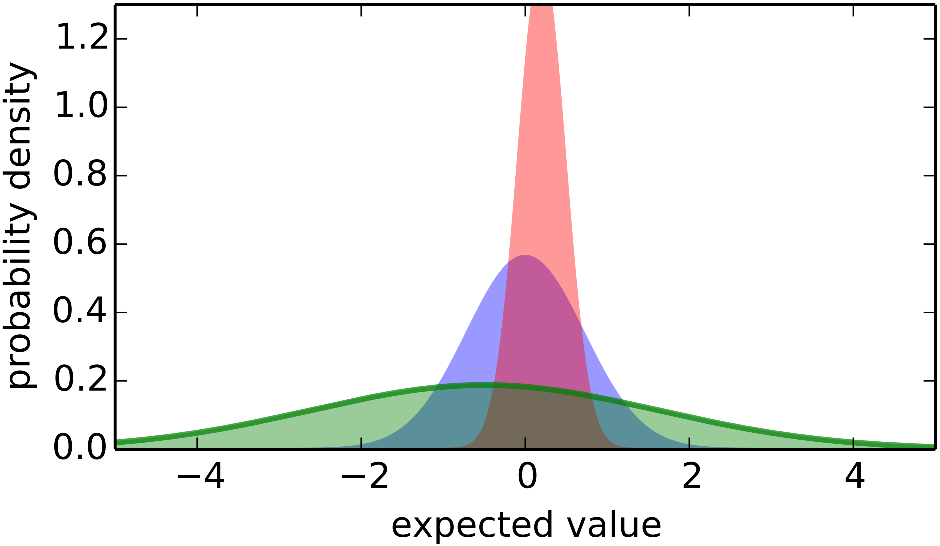

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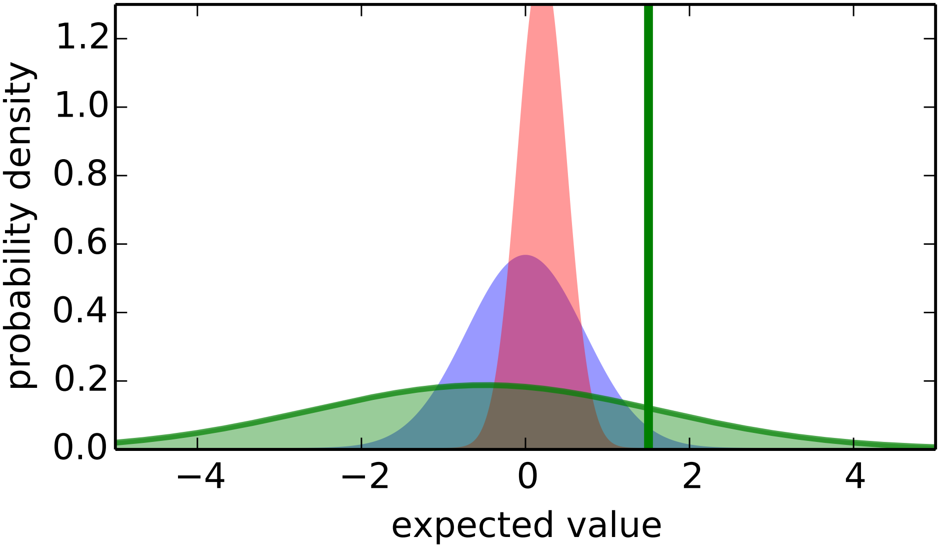
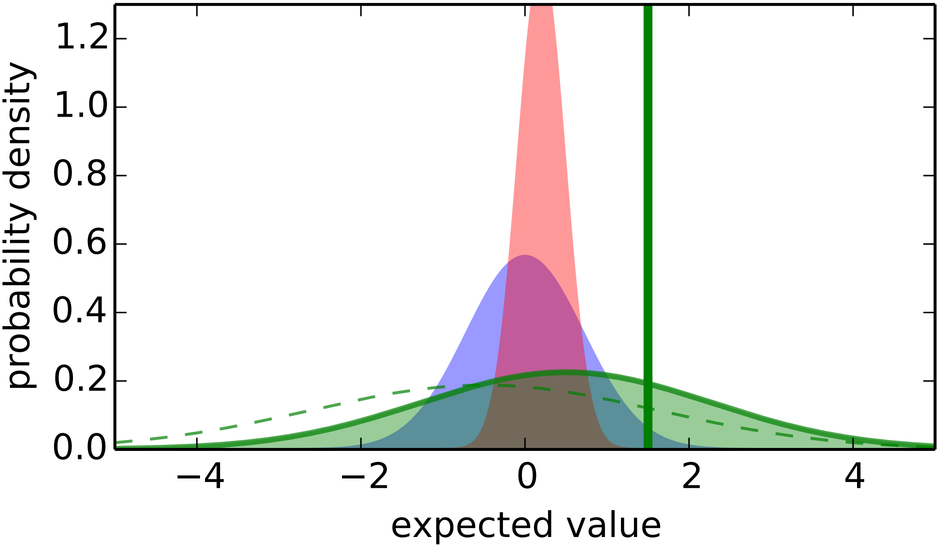


Optimism in the Face of Uncertainty



Algorithms: UCB

Upper Confidence Bounds

- Estimate an upper confidence $U_t(a)$ for each action value, such that $q(a) \leq Q_t(a) + U_t(a)$ with high probability
- Select action maximizing **upper confidence bound** (UCB)

$$a_t = \underset{a \in \mathcal{A}}{\operatorname{argmax}} \; Q_t(a) + U_t(a)$$

- The uncertainty should depend on the number of times $N_t(a)$ action a has been selected
  - Small $N_t(a) \Rightarrow$ large $U_t(a)$ (estimated value is uncertain)
  - Large $N_t(a) \Rightarrow$ small $U_t(a)$ (estimated value is accurate)
- Then a is only selected if either...
  - ...$Q_t(a)$ is large (=good action), or
  - ...$U_t(a)$ is large (=high uncertainty) (or both)
- Can we **derive** an optimal bound?

Theory: the optimality of UCB

Hoeffding's Inequality

Theorem (Hoeffding's Inequality)

Let $X_1, \ldots, X_n$ be i.i.d. random variables in [0,1] with true mean $\mu = \mathbb{E}[X]$, and let $\overline{X}_t = \frac{1}{n}\sum_{i=1}^n X_i$ be the sample mean. Then

$$p\left(\overline{X}_n + u \le \mu\right) \le e^{-2nu^2}$$

- We can apply Hoeffding's Inequality to bandits with bounded rewards
- If $R_t \in [0, 1]$, then

$$p\left(Q_t(a) + U_t(a) \le q(a)\right) \le e^{-2N_t(a)U_t(a)^2}$$

- By symmetry, we can also flip it around

$$p\left(Q_t(a) - U_t(a) \ge q(a)\right) \le e^{-2N_t(a)U_t(a)^2}$$

Calculating Upper Confidence Bounds

- We can pick a maximal desired probability p that the true value exceeds an upper bound and solve for this bound $U_t(a)$

$$
\begin{aligned}
&& e^{-2N_t(a)U_t(a)^2} &= p \\
\implies && U_t(a) &= \sqrt{\frac{-\log p}{2N_t(a)}}
\end{aligned}
$$

  We then know the probability that this happens is smaller than p

- Idea: reduce p as we observe more rewards, e.g., $p = 1/t$

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

- This ensures that we always keep exploring, but not too much

UCB

- UCB:

$$a_t = \operatorname*{argmax}_{a \in \mathcal{A}} Q_t(a) + c\sqrt{\frac{\log t}{N_t(a)}}$$

- Intuition:
  - If Δ_a is large, then $N_t(a)$ is small, because $Q_t(a)$ is likely to be small
  - So either Δ_a is small or $N_t(a)$ is small
  - In fact, we can prove $\Delta_a N_t(a) \leq O(\log t)$, for all a

UCB

- UCB:

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

where c is a hyper-parameter

Theorem (Auer et al., 2002)

UCB with $c = \sqrt{2}$ achieves logarithmic expected total regret

$$L_t \leq 8 \sum_{a|\Delta_a > 0} \frac{\log t}{\Delta_a} + O(\sum_a \Delta_a), \qquad \forall t\,.$$

Blackboard:
UCB derivation

Bayesian approaches

Bayesian Bandits

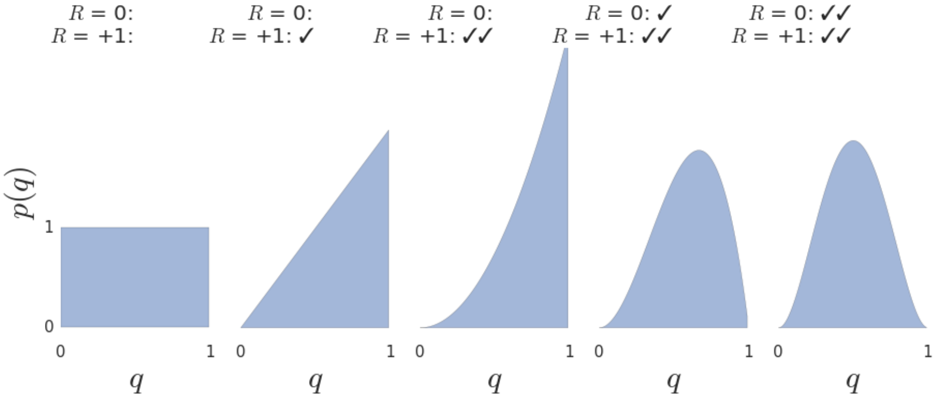
- We could adopt **Bayesian** approach and model distributions over values $p(q(a) \mid \theta_t)$
- This is interpreted as our **belief** that, e.g., $q(a) = x$ for all $x \in \mathbb{R}$
- E.g., θ_t could contain the means and variances of Gaussian belief distributions
- Allows us to inject rich prior knowledge θ_0
- We can then use posterior belief to guide exploration

Bayesian Bandits: Example

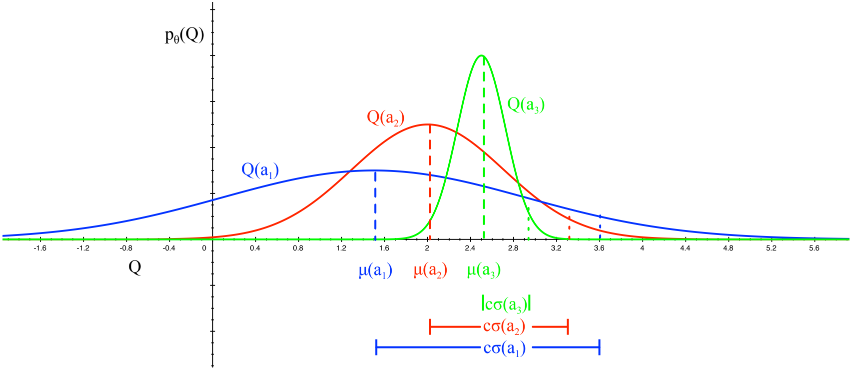
- Consider bandits with **Bernoulli** reward distribution: rewards are 0 or +1
- For each action, the prior could be a **uniform distribution** on $[0, 1]$
- This means we think each value in $[0, 1]$ is equally likely
- The posterior is a Beta distribution $\text{Beta}(x_a, y_a)$ with initial parameters $x_a = 1$ and $y_a = 1$ for each action a
- Updating the posterior:
  - $x_{A_t} \leftarrow x_{A_t} + 1$ when $R_t = 0$
  - $y_{A_t} \leftarrow y_{A_t} + 1$ when $R_t = 1$

Bayesian Bandits: Example

Suppose: $R_1 = +1$, $R_2 = +1$, $R_3 = 0$, $R_4 = 0$



Bayesian Bandits with Upper Confidence Bounds



- We can estimate upper confidences from the posterior
  - e.g., $U_t(a) = c\sigma_t(a)$ where $\sigma(a)$ is std dev of $p_t(q(a))$
- Then, pick an action that maximises $Q_t(a) + c\sigma(a)$

Algorithms: Thompson sampling

Probability Matching

- A different option is to use **probability matching**:
  Select action a according to the probability (belief) that a is optimal

$$\pi_t(a) = p\left(q(a) = \max_{a'} q(a') \mid \mathcal{H}_{t-1}\right)$$

- Probability matching is optimistic in the face of uncertainty:
  Actions have higher probability when either the estimated value is high, or the uncertainty is high
- Can be difficult to compute $\pi(a)$ analytically from posterior (but can be done numerically)

Thompson Sampling

- Thompson sampling (Thompson 1933):
  - Sample $Q_t(a) \sim p_t(q(a)), \forall a$
  - Select action maximising sample, $A_t = \underset{a \in \mathcal{A}}{\operatorname{argmax}}\ Q_t(a)$
- **Thompson sampling** is sample-based probability matching

$$\pi_t(a) = \mathbb{E}\left[\mathcal{I}(Q_t(a) = \max_{a'} Q_t(a'))\right]$$
$$= p\left(q(a) = \max_{a'} q(a')\right)$$

- For Bernoulli bandits, Thompson sampling achieves Lai and Robbins lower bound on regret, and therefore is **optimal**

Planning to explore

Information State Space

- We have viewed bandits as **one-step** decision-making problems
- Can also view as **sequential** decision-making problems
- Each step the agent updates state S_t to summarise the past
- Each action A_t causes a transition to a new **information state** S_{t+1} (by adding information), with probability $p(S_{t+1} \mid A_t, S_t)$
- We now have a Markov decision problem
- The state is fully internal to the agent
- State transitions are random due to rewards & actions
- Even in bandits actions affect the future after all, via learning

Example: Bernoulli Bandits

- Consider a Bernoulli bandit, such that

$$p(R_t = 1 \mid A_t = a) = \mu_a$$
$$p(R_t = 0 \mid A_t = a) = 1 - \mu_a$$

- 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 $I = (\boldsymbol{\alpha}, \boldsymbol{\beta})$
  - 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 formulated the bandit as an infinite MDP over information states
- This can be solved by reinforcement learning
- E.g., learn a Bayesian reward distribution, plan into the future
- This is known as **Bayes-adaptive** RL:
  optimally trades off exploration with respect to the prior distribution
- Can be extended to full RL, by also learning a transition model
- Can be unwieldy... unclear how to scale effectively

Example

End of lecture