Lecture 2: Exploration and Exploitation

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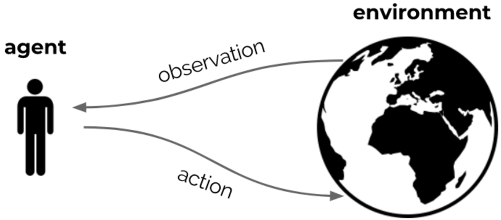
Background

Sutton & Barto 2018, Chapter 2

Recap

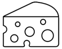


- Reinforcement learning is the science of learning to make decisions
- Agents can learn a policy, value function and/or a model
- The general problem involves taking into account time and consequences
- Decisions affect the reward, the agent state, and environment state

This Lecture

- Consider simple case: multiple actions, but only one state
- No sequential structure — past actions do not influence the future
- Formally: the distribution of R_t given A_t is identical and independent across time

Rat Example

	action	reward
Monday		
Tuesday		
Wednesday	?	

Rat Example

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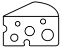
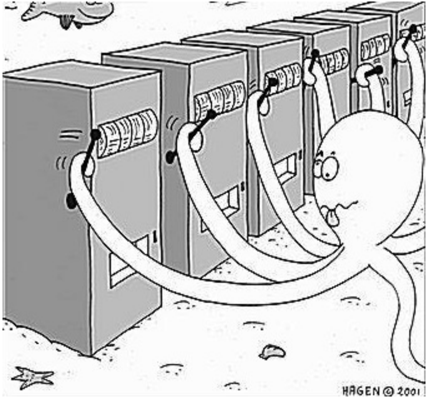
Tuesday		
Wednesday		
Thursday	?	

Exploration vs. Exploitation

- Online decision-making involves a fundamental choice:
  - Exploitation: Maximize performance based on current knowledge
  - Exploration: Increase knowledge
- The best long-term strategy may involve short-term sacrifices
- We want to gather enough information to make the best overall decisions

The Multi-Armed Bandit

- We formalise the simplest setting
- $\mathcal{A}$ is a known set of actions (or "arms")
- At each step t the agent selects an action $A_t \in \mathcal{A}$
- The environment generates a reward R_t
- The distribution $p(r \mid a)$ is fixed, but unknown
- The goal is to maximize cumulative reward $\sum_{i=1}^{t} R_i$
- Note: we sum over the whole lifetime of the agent
- Repeated 'game against nature'



Action values

- The true 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:

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

where $\mathcal{I}(\text{True}) = 1$ and $\mathcal{I}(\text{False}) = 0$

Action values

- This can be updated incrementally:

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

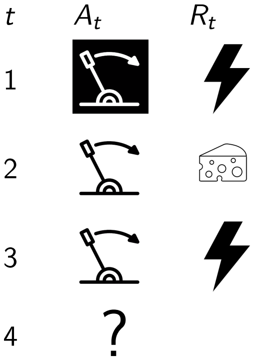
$$\forall a \neq A_t \; : Q_t(a) = Q_{t-1}(a)$$

  with

$$\alpha_t = \frac{1}{N_t(A_t)}, \qquad N_t(A_t) = N_{t-1}(A_t) + 1, \qquad \text{and} \qquad N_t(a) = 0\,, \forall a$$

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

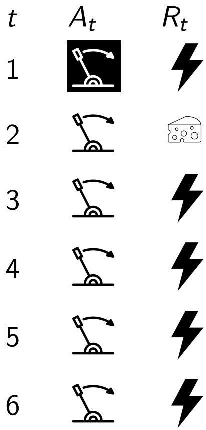
Rat Example



- Cheese: $R = +1$
- Shock: $R = -1$
- Then:

$$Q_3(\text{white lever}) = 0$$
$$Q_3(\text{black lever}) = -1$$

Rat Example



- Cheese: $R = +1$
- Shock: $R = -1$
- Then:

$$Q_6(\text{white lever}) = -\mathbf{0.6}$$
$$Q_6(\text{black lever}) = -1$$

- When to stop being greedy?

Regret

- How can we reason about the exploration trade off?
- Seems natural to somehow take into account that estimates can be uncertain
- Can we reason about this formally?
- Can we trade off exploration and exploitation optimally?

Regret

- The optimal value is

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

- Regret is the opportunity loss for one step

$$v_* - q(A_t)$$

  - In hindsight, I might 'regret' taking the tube rather than cycling
  - I might have regretted taking a bus even more
- The agent cannot observe, or even sample, the real regret directly
- But we can use it to analyze different learning algorithms

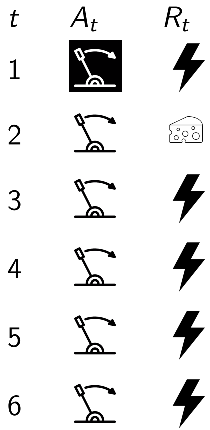
Regret

- Goal: Trade-off exploration and exploitation by minimizing total regret:

$$L_t = \sum_{i=1}^{t} (v_* - q(a_i))$$

- Maximise cumulative reward $\equiv$ minimise total regret
- Note: the sum extends beyond (single step) episodes
- View extends over 'lifetime of learning', rather than over 'current episode'

Regret of greedy



- Regret can grow unbounded
- More interesting is how fast it grows
- The greedy policy has linear regret
- This means that, in expectation, the regret grows as a function that is linear in t
  - Suppose $p(\text{cheese} \mid \text{white}) = 0.1$ and $p(\text{cheese} \mid \text{black}) = 0.9$
  - Then $v_* = q(\text{black}) = 0.8$ and $q(\text{white}) = -0.8$
  - The greedy rat incurs regret of $1.6t$ (If the first two actions and rewards are as shown on the left)

Counting Regret

- The action regret Δ_a for a given action is the difference between the optimal value and the true value of a:

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

- Total regret then depends on action regrets and action counts

$$L_t = \sum_{i=1}^{t} v_* - q(a_i) = \sum_{a \in \mathcal{A}} N_t(a)(v_* - q(a)) = \sum_{a \in \mathcal{A}} N_t(a)\Delta_a$$

- A good algorithm ensures small counts for large action regrets
- But, action regrets are not known...

Exploration

- We need to explore to learn the values
- One common solution: ϵ-greedy
  - Select greedy action (exploit) w.p. $1 - \epsilon$
  - Select random action (explore) w.p. ϵ
- Is this enough?
- How to pick ϵ?

ϵ-Greedy Algorithm

- Greedy can lock onto a suboptimal action forever
  $\Rightarrow$ Greedy has linear expected total regret
- The ϵ-greedy algorithm continues to explore forever
  - With probability $1 - \epsilon$ select $a = \underset{a \in \mathcal{A}}{\operatorname{argmax}}\, Q_t(a)$
  - With probability ϵ select a random action
- Will continue to select all suboptimal actions with, at least, probability $\epsilon / |\mathcal{A}|$
  $\Rightarrow$ ϵ-greedy, with constant ϵ, has linear expected total regret

Lower Bound

- The performance of any algorithm is determined by similarity between optimal arm and other arms
- Hard problems have arms with similar distributions but different means
- This is described formally by the gap Δ_a and the similarity in distributions $KL(p(r|a)||p(r|a_*))$

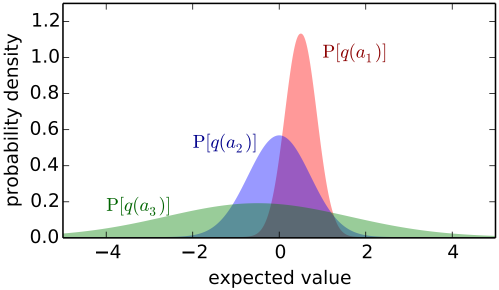
Theorem (Lai and Robbins)

Asymptotic total regret is at least logarithmic in number of steps

$$\lim_{t\to\infty} L_t \geq \log t \sum_{a|\Delta_a>0} \frac{\Delta_a}{KL(p(r|a)||p(r|a_*))}$$

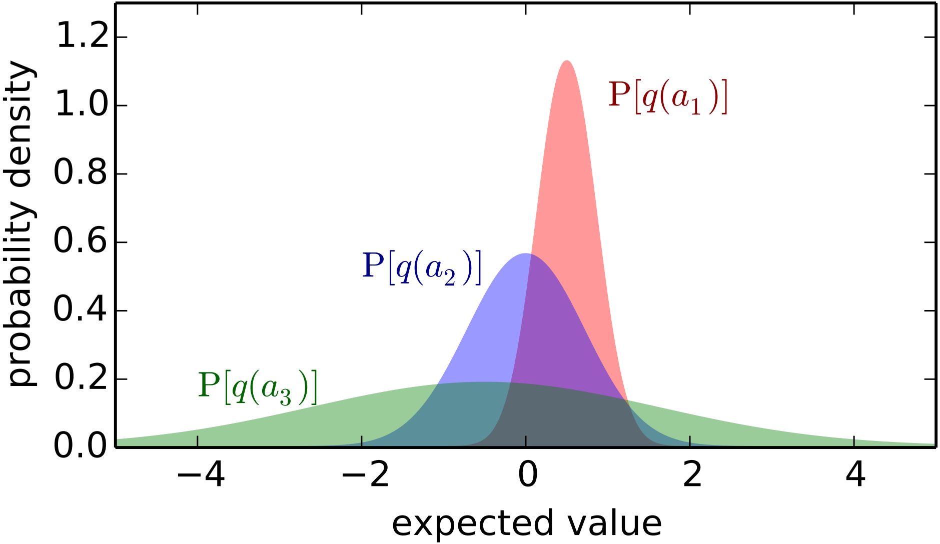
Note: logarithmic is a whole lot better than linear!

Optimism in the Face of Uncertainty

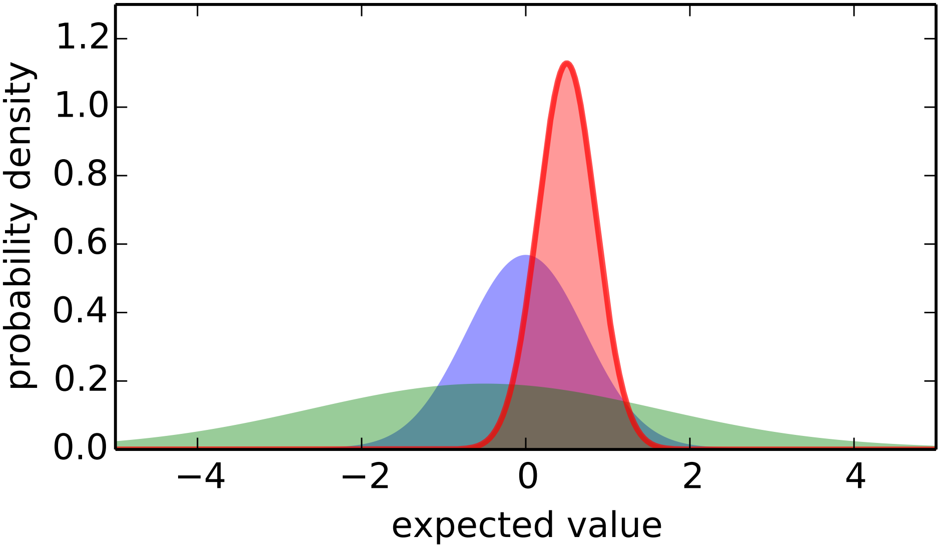


- Which action should we pick?
- More uncertainty about its value: more important to explore that action

Optimism in the Face of Uncertainty



Optimism in the Face of Uncertainty



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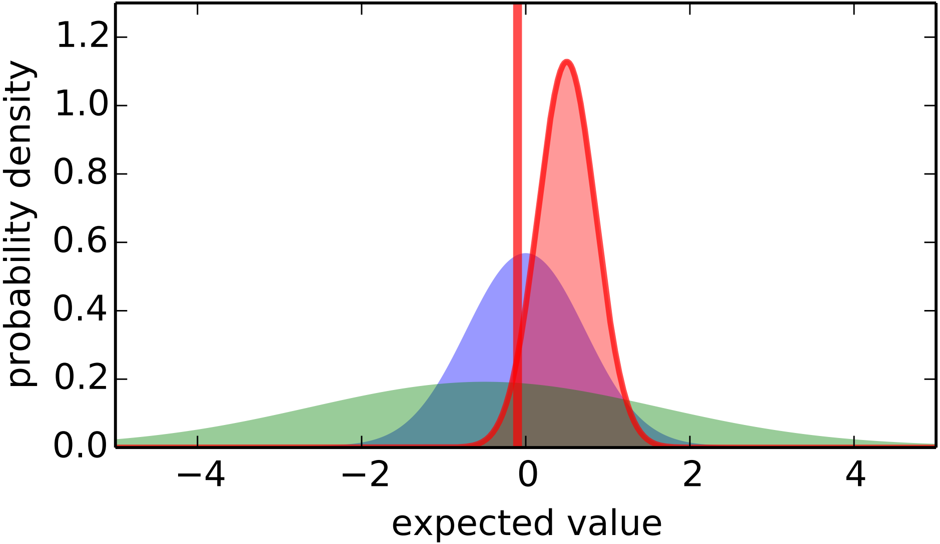

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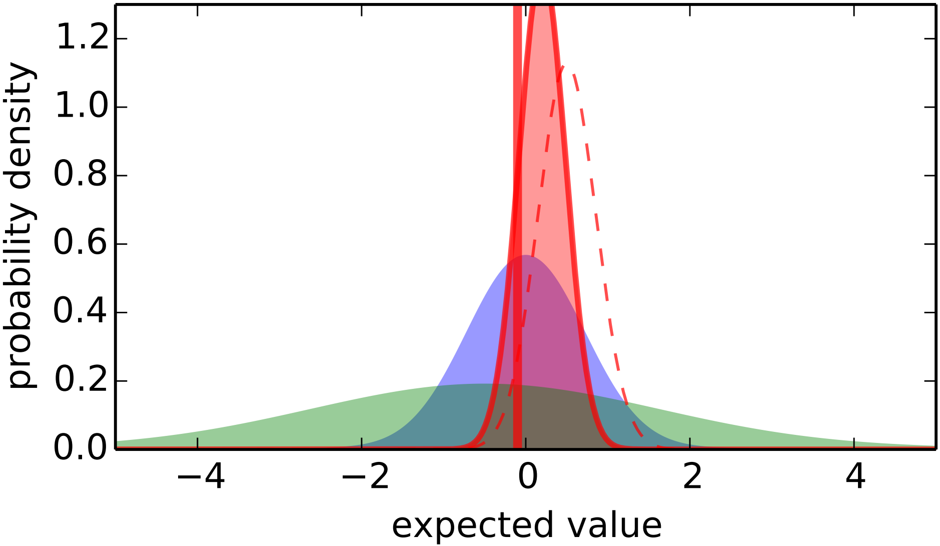

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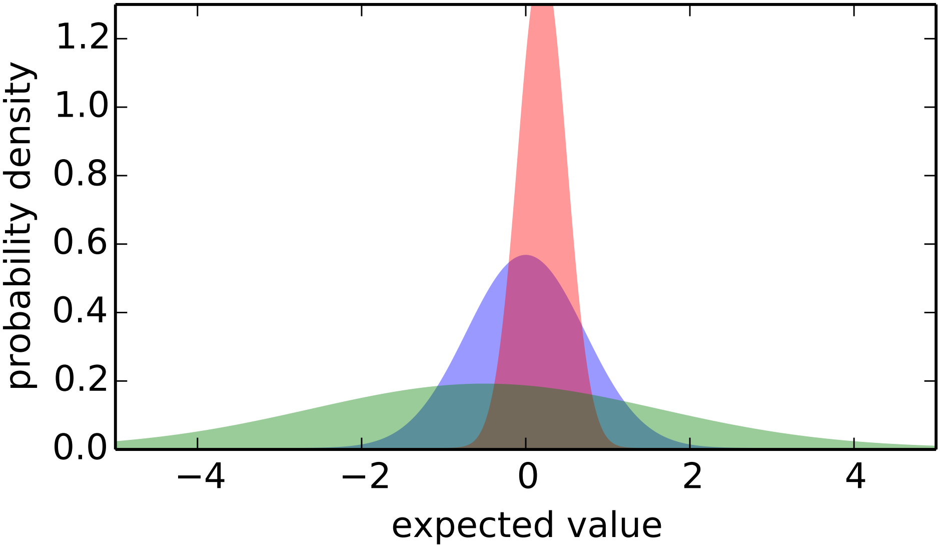
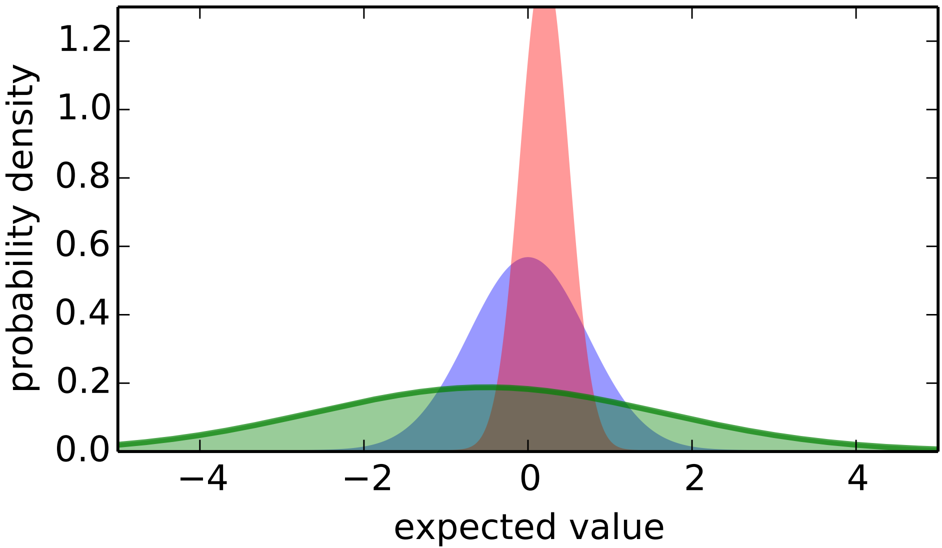
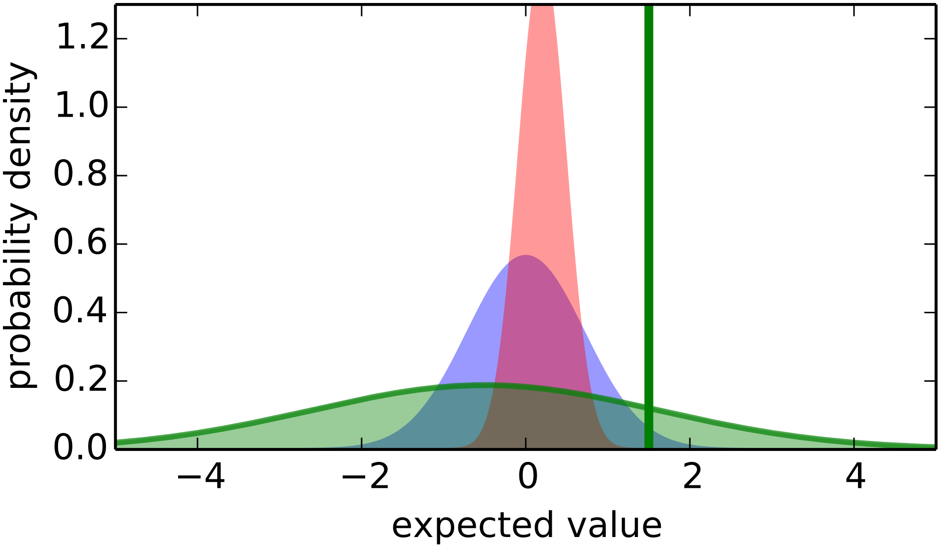


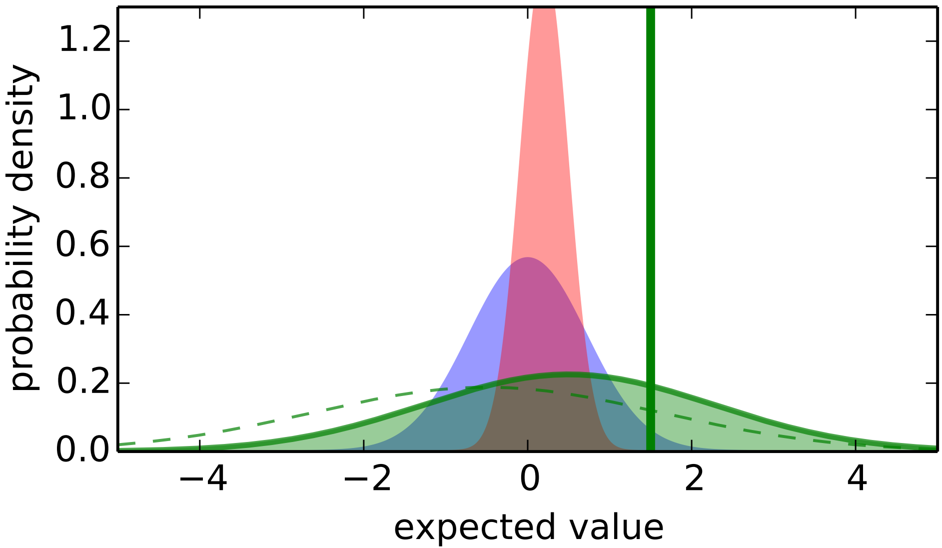
Optimism in the Face of Uncertainty



Optimism in the Face of Uncertainty



Optimism in the Face of Uncertainty



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 depends on the number of times $N(a)$ 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)
- For averages the uncertainty decreases as $\sqrt{N_t(a)}$, by the central limit theorem (If variance of rewards is bounded.)
- Can we derive an optimal algorithm?

Algorithm idea

- Recall, we want to minimize: $\sum_a N_t(a)\Delta_a$
- If Δ_a is big, we want $N_t(a)$ to be small
- If $N_t(a)$ is big, we want Δ_a to be small
- Not all $N_t(a)$ can be small (as their sum has to be t)
- We know $N_t(a)$; can we also know something about Δ_a?

Hoeffding's Inequality

Theorem (Hoeffding's Inequality)

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

$$p\left(\mathbb{E}\left[X\right] \geq \overline{X}_n + u\right) \leq e^{-2nu^2}$$

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

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

Calculating Upper Confidence Bounds

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

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

- 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 we select optimal action much more often as $t \to \infty$

UCB

- This leads to the UCB algorithm

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

where c can be considered a hyper-parameter

Theorem (Auer et al., 2002)

The UCB algorithm (with $c = \sqrt{2}$) achieves logarithmic expected total regret

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

UCB

- UCB:

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

- Intuition:
  - Suppose that Δ_a is large.
  - Then, $N_t(a)$ will be small, because $U_t(a)$ rarely spans the whole gap.
  - So, either Δ_a is low, or $N_t(a)$ is low.
  - In fact, $\Delta_a N_t(a) \leq O(\log t)$, for all a

Values or Models?

- This is a value-based algorithm:

$$Q_t(A_t) = Q_{t-1}(A_t) + \alpha_t(R_t - Q_{t-1}(A_t))\,.$$

- What about a model-based approach?

$$\hat{\mathcal{R}}_t(A_t) = \hat{\mathcal{R}}_{t-1}(A_t) + \alpha_t(R_t - \hat{\mathcal{R}}_{t-1}(A_t))\,.$$

- Indistinguishable?
- We could model more, e.g., the distribution of rewards

Bayesian Bandits

- Bayesian bandits model parameterized distributions over rewards, $p(R_t \mid \theta, a)$
- Compute posterior distribution over θ

$$p_t(\theta \mid a) \quad \propto \quad p(R_t \mid \theta, a) p_{t-1}(\theta \mid a)$$

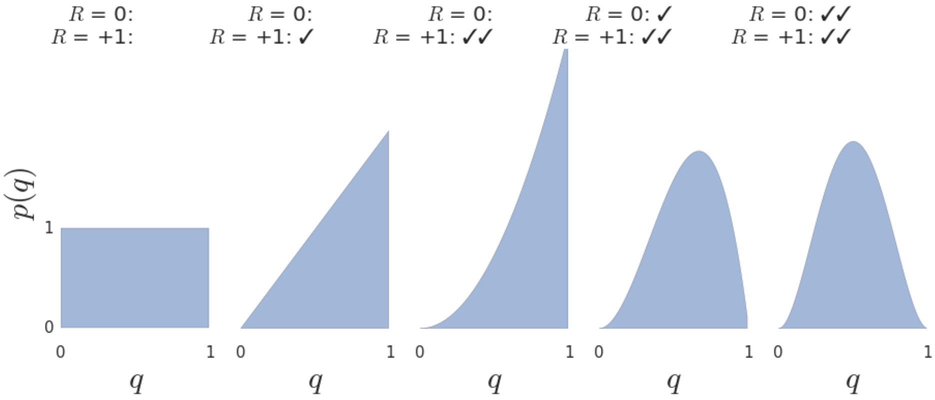
- Allows us to inject rich prior knowledge $p_0(\theta \mid a)$
- Use posterior to guide exploration
  - Upper confidence bounds
  - Probability matching

Bayesian Bandits: Example

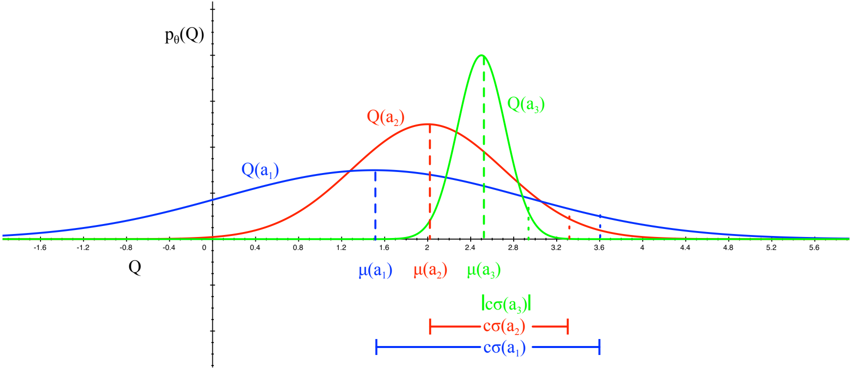
- Consider bandits with Bernoulli reward distribution: rewards are 0 or $+1$
- For each action, the prior could be a uniform distribution on $[0, 1]$
- This means we think each mean reward in $[0, 1]$ is equally likely
- The posterior is a Beta distribution $\text{Beta}(x_a, y_a)$ with initial parameters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



- Compute posterior distribution over action-values
- Estimate upper confidence from posterior
  - e.g., $U_t(a) = c\sigma_t(a)$ where $\sigma(a)$ is std dev of $p_t(q(a))$
- Pick action that maximizes $Q_t(a) + c\sigma(a)$

Probability Matching

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

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

- Probability matching is optimistic in the face of uncertainty:
  Uncertain actions have higher probability of being max
- Can be difficult to compute $\pi(a)$ analytically from posterior

Thompson Sampling

- Thompson sampling:
  - 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

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

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

Value of Information

- Exploration is valuable because information is valuable
- Can we quantify the value of information?
- You gain more information when you are uncertain
- Therefore it makes sense to explore novel situations more
- If we know value of information, we can trade-off exploration and exploitation

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 $\tilde{s}$ summarising all information accumulated so far
- Each action a causes a transition to a new information state $\tilde{s}'$ (by adding information), with probability $p(\tilde{s}' \mid a, \tilde{s})$
- We then have a Markov decision problem
- Here states = observations = internal information state
- Even in bandits, actions affect the future after all, because they affect learning

Example: Bernoulli Bandits

- Consider a Bernoulli bandit, such that

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

- 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 $\tilde{s} = \langle \alpha, \beta \rangle$
  - 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 formulated the bandit as an infinite MDP over information states
- This 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)
- The latter approach is known as Bayes-adaptive RL
- Finds Bayes-optimal exploration/exploitation trade-off with respect to the prior distribution
- Can be unwieldy... unclear how to scale

Policy search

- What about learning policies $\pi(a)$ directly?
- Lets parameterize the policy — can we learn this without learning values?
- For instance, define action preferences $H_t(a)$ and a policy

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

- The preferences do not have to have value semantics
- Instead, view them as learnable parameters
- Can we optimize the preferences

Policy gradients

- Idea: update policy parameters such that the expected value increases
- We can consider gradient ascent on the expected value
- So, in the bandit case, we want to update:

$$\theta = \theta + \alpha \nabla_\theta \mathbb{E}[R_t | \theta] \, ,$$

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

Gradient bandits

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

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

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:

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

- $\Rightarrow$

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

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

Policy gradients with baselines

- Note that $\sum_a \pi_\theta(a) = 1$. Therefore, for any b,

$$\begin{aligned}\sum_a b \nabla_\theta \pi_\theta(a) &= \nabla_\theta \sum_a b \pi_\theta(a) \\ &= \nabla_\theta b \\ &= 0\end{aligned}$$

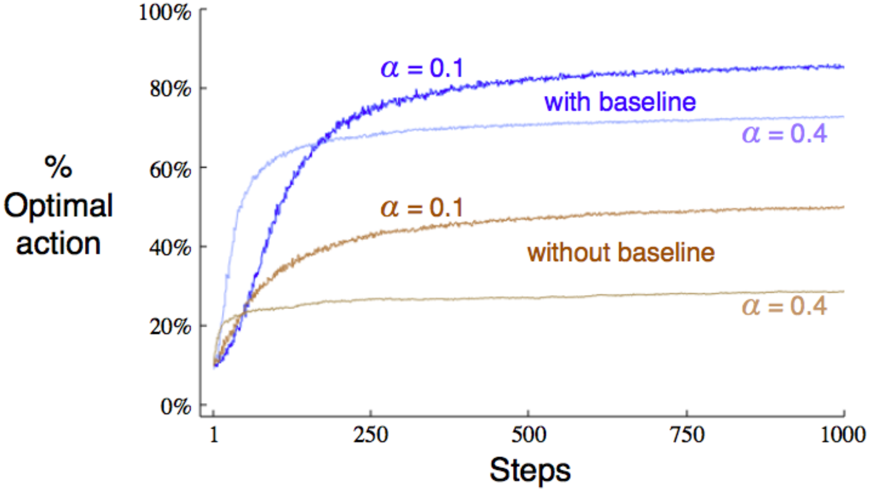
  as long as b does not depend on θ or a.
- This means we can add a baseline, and instead use

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

- Baselines <u>do not</u> change the expected update, but they <u>do</u> change variance

Policy gradients with baselines

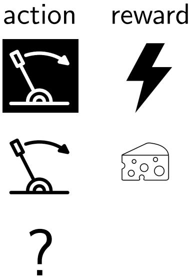
A natural baseline is the average reward $\frac{1}{t}\sum_{i=1}^{t} R_i$



Gradient bandits

- These gradient methods can be extended
  - ...to include context
  - ...to full MDPs
  - ...to partial observability
- We will discuss them again in lecture on policy gradients

Rat Example

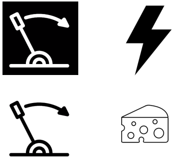


probability of selecting black

- Greedy: ?
- ϵ-greedy: ?
- UCB: ?
- Thompson sampling: ?

Rat Example

action reward



?

probability of selecting black

- Greedy: 0
- ϵ-greedy: $\epsilon/2$
- UCB: 0
- Thompson sampling: 0.25