Lecture 2: Exploration and Exploitation in Multi-Armed Bandits

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Outline

1 Recap

2 Introduction

3 Multi-Armed Bandits

4 Contextual Bandits

5 Policy-Based methods

Previous lecture

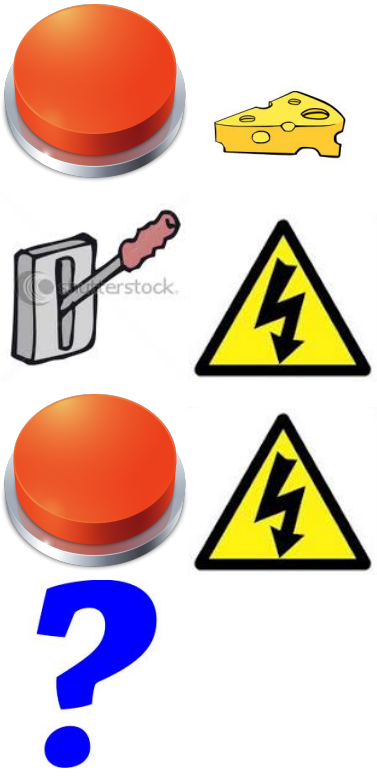
- Reinforcement learning is the science of learning to make decisions
- We can do this by learning one or more of:
  - policy
  - value function
  - model
- The general problem involves taking into account time and consequences
- Our decisions affect the reward, our internal knowledge, and the state of the environment

This Lecture

- Multiple actions, but (mostly) only one state
- Decisions do not affect the state of the environment
- Goal: optimize immediate reward in a repeated 'game against nature'
- History (no observations):

$$H_t = A_1, R_1, A_2, R_2, \ldots, A_t, R_t$$

Rat Example



Exploration vs. Exploitation

- Online decision-making involves a fundamental choice:
  - Exploitation: Maximize return given current knowledge
  - Exploration: Increase knowledge
- The best long-term strategy may involve short-term sacrifices
- Gather enough information to make the best overall decisions

Examples

- Restaurant Selection

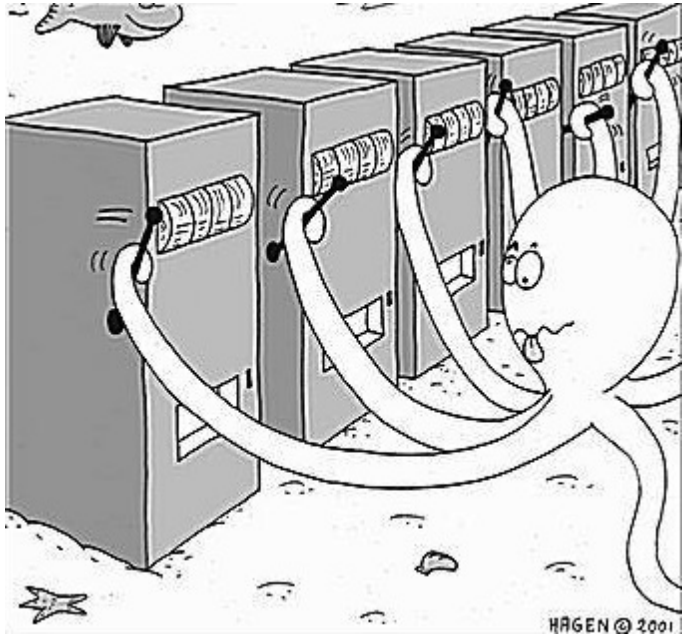
  Exploitation: Go to your favourite restaurant
  Exploration: Try a new restaurant

- Online Banner Advertisements

  Exploitation: Show the most successful advert
  Exploration: Show a different advert

The Multi-Armed Bandit

- A multi-armed bandit is a tuple $\langle \mathcal{A}, \mathcal{R} \rangle$
- $\mathcal{A}$ is a known set of actions (or "arms")
- $\mathcal{R}^a(r) = \mathbb{P}[R_t = r | A_t = a]$ 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 $R_t \sim \mathcal{R}^{A_t}$
- The goal is to maximize cumulative reward $\sum_{i=1}^{t} R_i$
- Repeated 'game against nature'



Action values

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

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

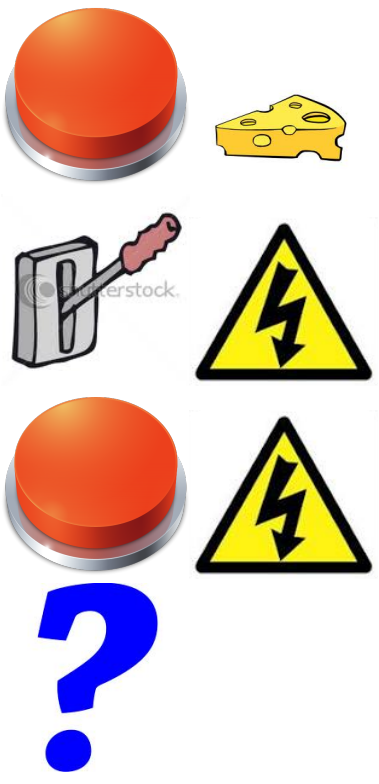
- We consider algorithms that estimate $Q_t(a) \approx q(a)$
- The *count* $N_t(a)$ is number of times we selected action a
- Monte-Carlo estimates:

$$Q_t(a) = \frac{1}{N_t(a)} \sum_{t=1}^{T} R_t \mathcal{I}(A_t = a)$$

- The *greedy* algorithm selects action with highest value

$$a_t^g = \underset{a \in \mathcal{A}}{\operatorname{argmax}}\ Q_t(a)$$

Rat Example

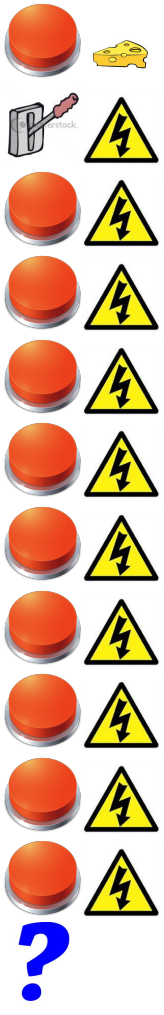


- Cheese: $R = +1$
- Shock: $R = -1$
- We can estimate action values:

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

- When should we stop being greedy?

Rat Example



- Cheese: $R = +1$
- Shock: $R = -1$
- We can estimate action values:

$$Q_3(\text{button}) = -\mathbf{0.8}$$
$$Q_3(\text{lever}) = -1$$

- When should we stop being greedy?

Regret

- The *optimal value* v_* 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 is the opportunity loss for one step

$$v_* - q(A_t)$$

  - I might regret fruit instead of pancakes for breakfast
  - I might regret porridge instead of pancakes even more

Regret

- 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: cumulation here extends over termination of 'episode'
- View extends over 'lifetime of learning', rather than over 'current episode'

Counting Regret

- The *gap* Δ_a is the difference in value between action a and optimal action a_*, $\Delta_a = v_* - q(a)$
- Total regret depends on gaps and counts

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

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

Exploration

- We need to explore to learn about the values of all actions
- What is a good way to explore?
- One common solution: ϵ-greedy
  - Select greedy action (exploit) w.p. $1 - \epsilon$
  - Select random action (explore) w.p. ϵ
- Used in Atari
- 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 $a = \underset{a \in \mathcal{A}}{\text{argmax}}\ Q_t(a)$
  - With probability ϵ select a random action
  - Constant ϵ ensures minimum expected regret

$$\mathbb{E}\left[v_* - q(A_t)\right] \geq \frac{\epsilon}{\mathcal{A}} \sum_{a \in \mathcal{A}} \Delta_a$$

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

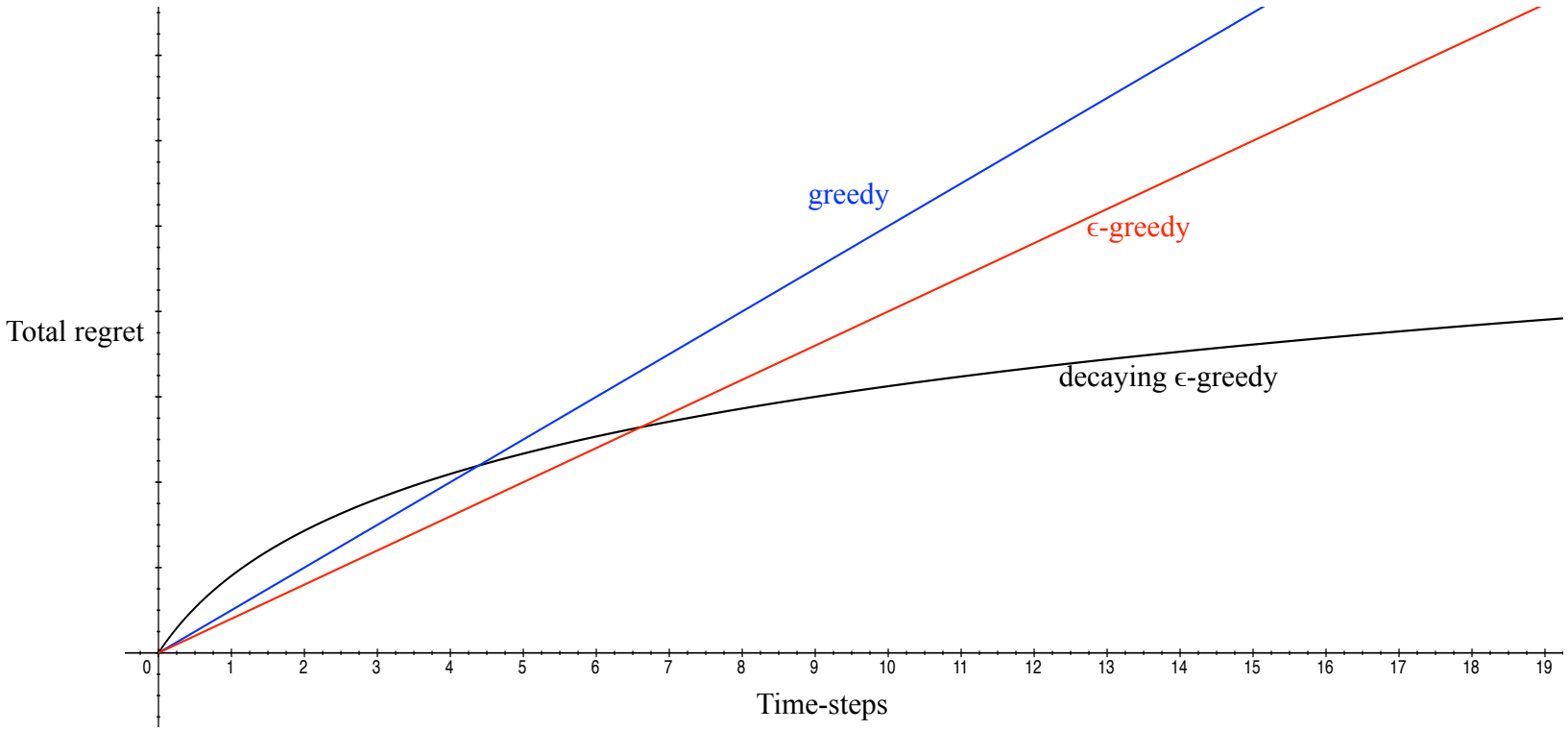
Decaying ϵ_t-Greedy Algorithm

- Pick a decay schedule for $\epsilon_1, \epsilon_2, ...$
- 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, requires advance knowledge of gaps
- Goal: find an algorithm with sublinear regret for any multi-armed bandit (without knowledge of $\mathcal{R}$)

Linear or Sublinear Regret



Lower Bound

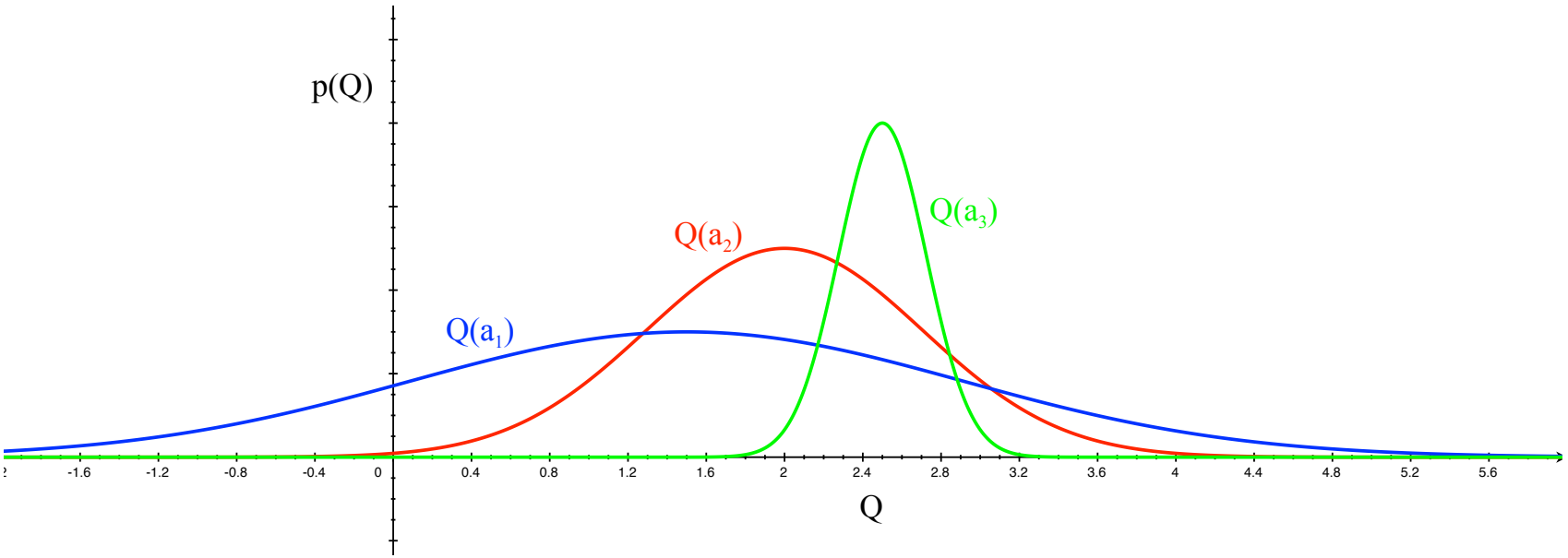
- The performance of any algorithm is determined by similarity between optimal arm and other arms
- Hard problems have arms with similar distributions but different means
- This is described formally by the gap Δ_a and the similarity in distributions $KL(\mathcal{R}^a||\mathcal{R}^a*)$

Theorem (Lai and Robbins)

Asymptotic total regret is at least logarithmic in number of steps

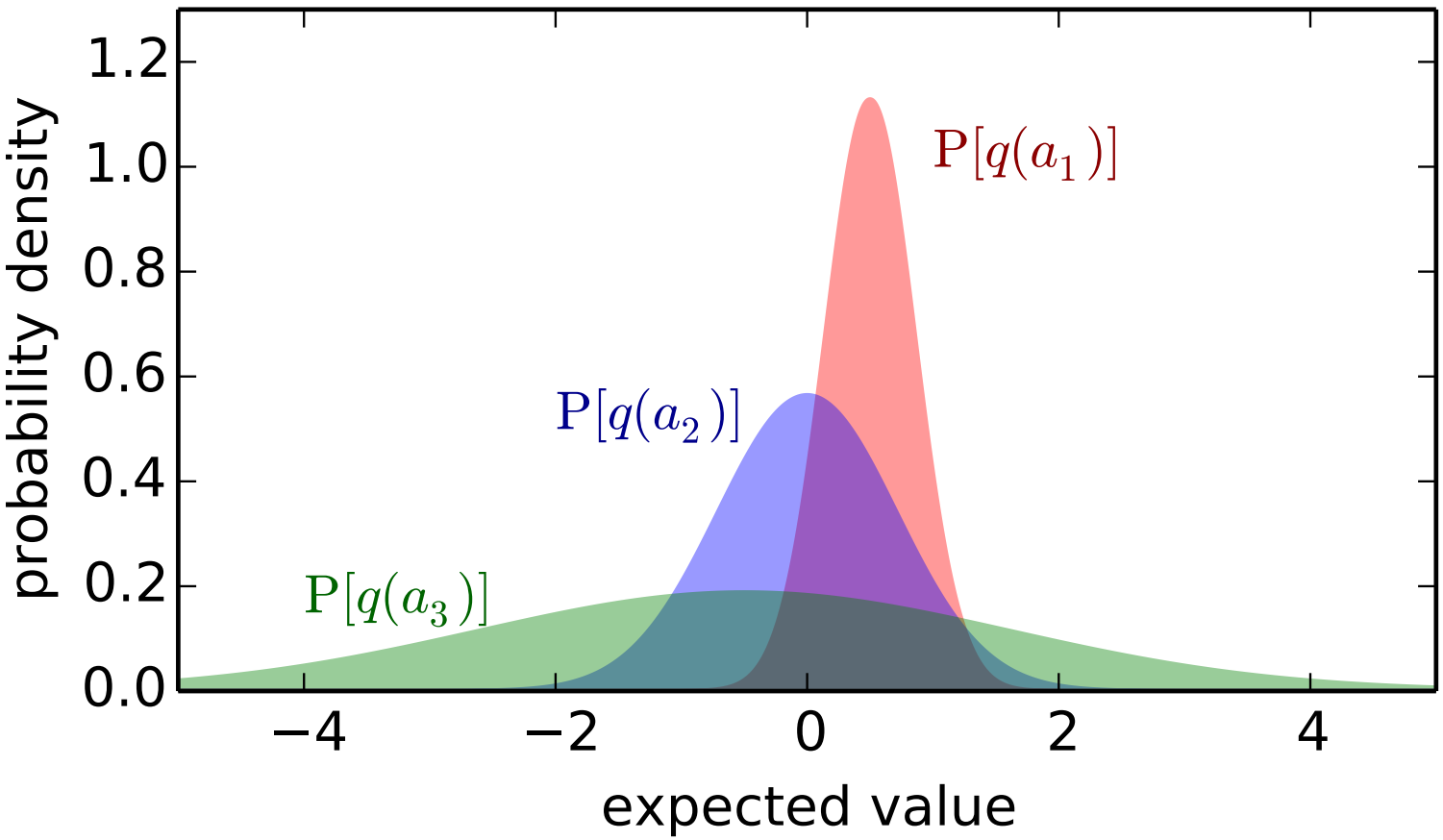
$$\lim_{t\to\infty} L_t \geq \log t \sum_{a|\Delta_a>0} \frac{\Delta_a}{KL(\mathcal{R}^a||\mathcal{R}^{a*})}$$

Optimism in the Face of Uncertainty



- Which action should we pick?
- More uncertainty: more important to explore that action
- It could turn out to be the best action

Optimism in the Face of Uncertainty



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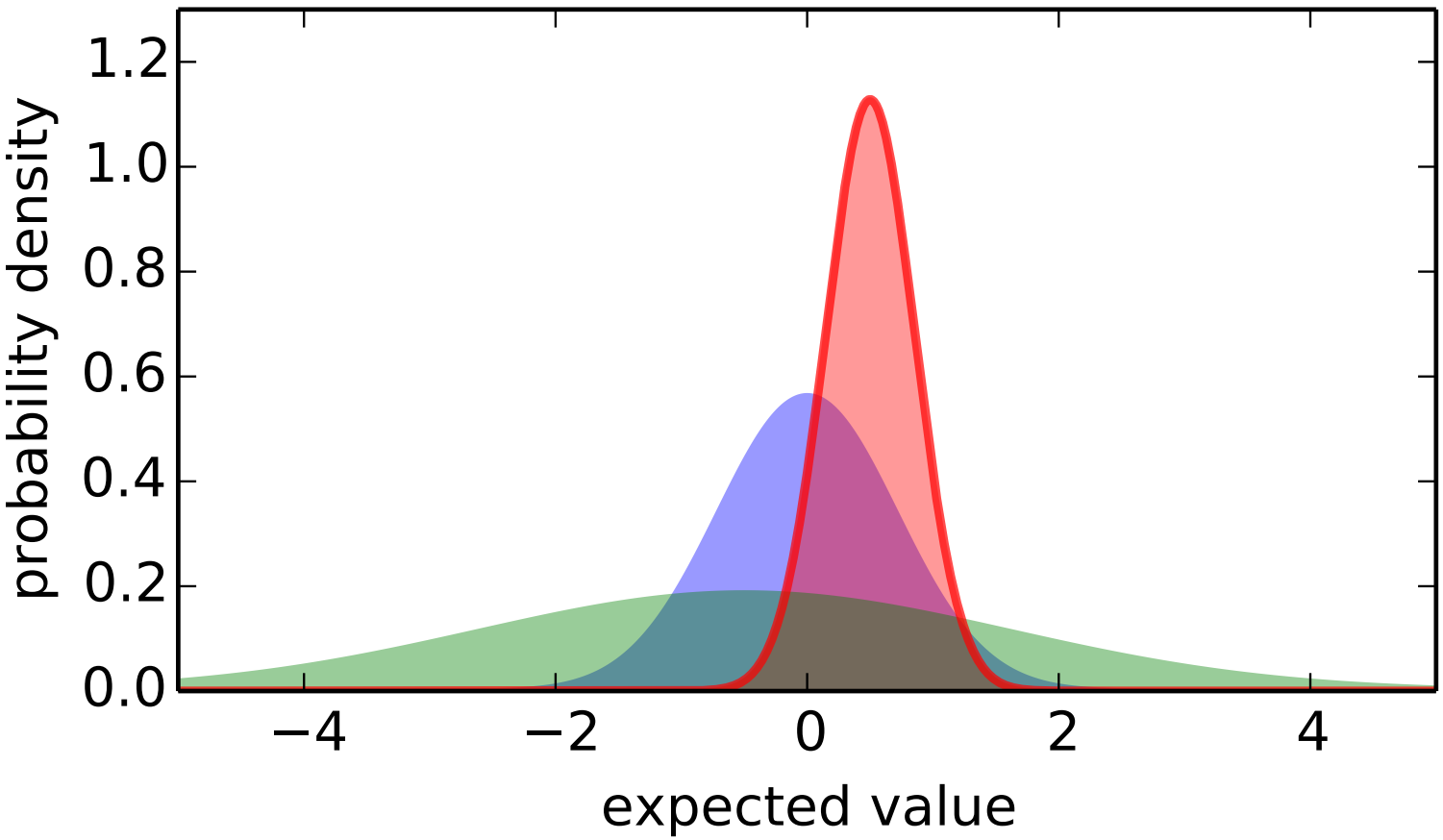

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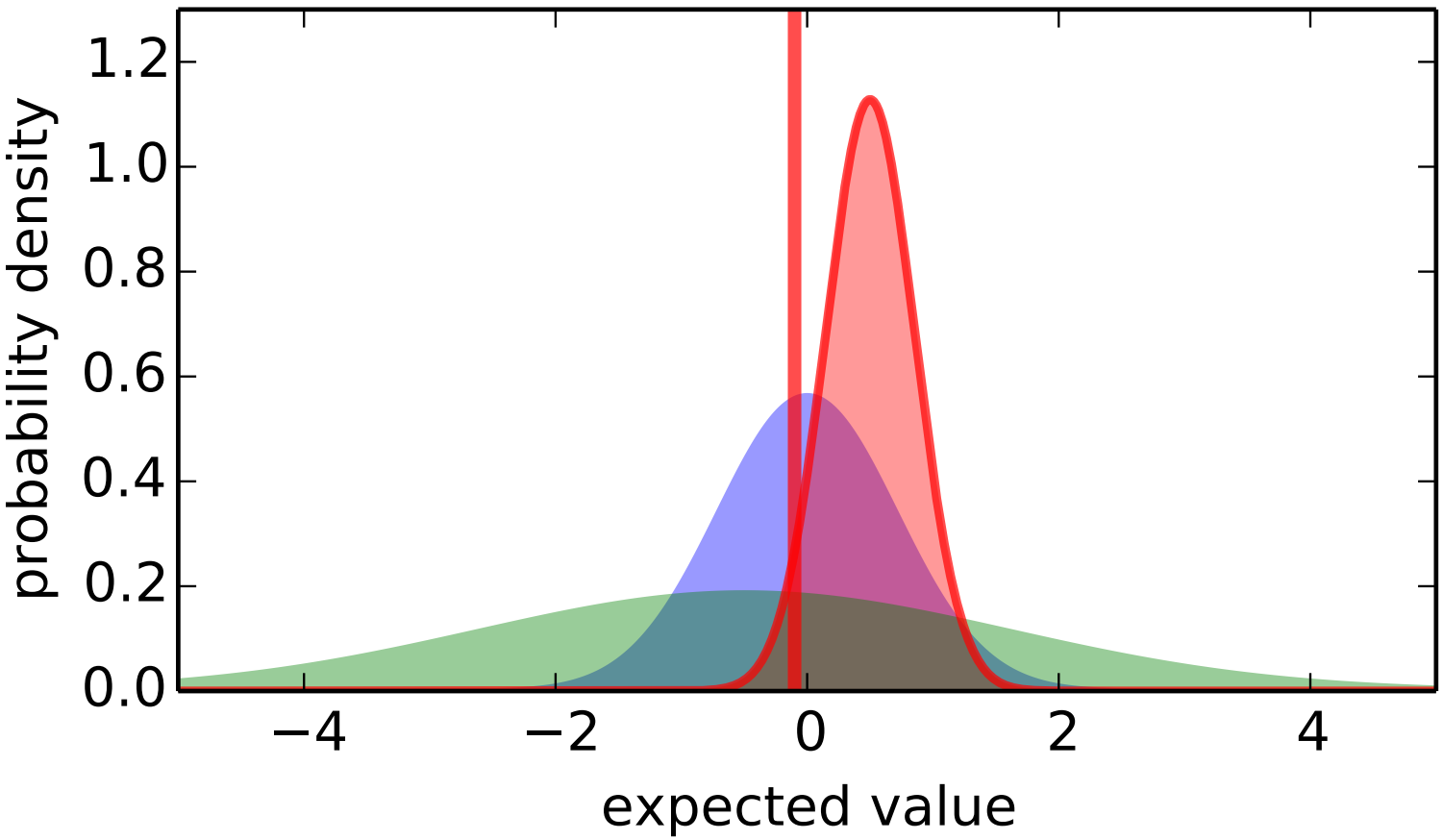

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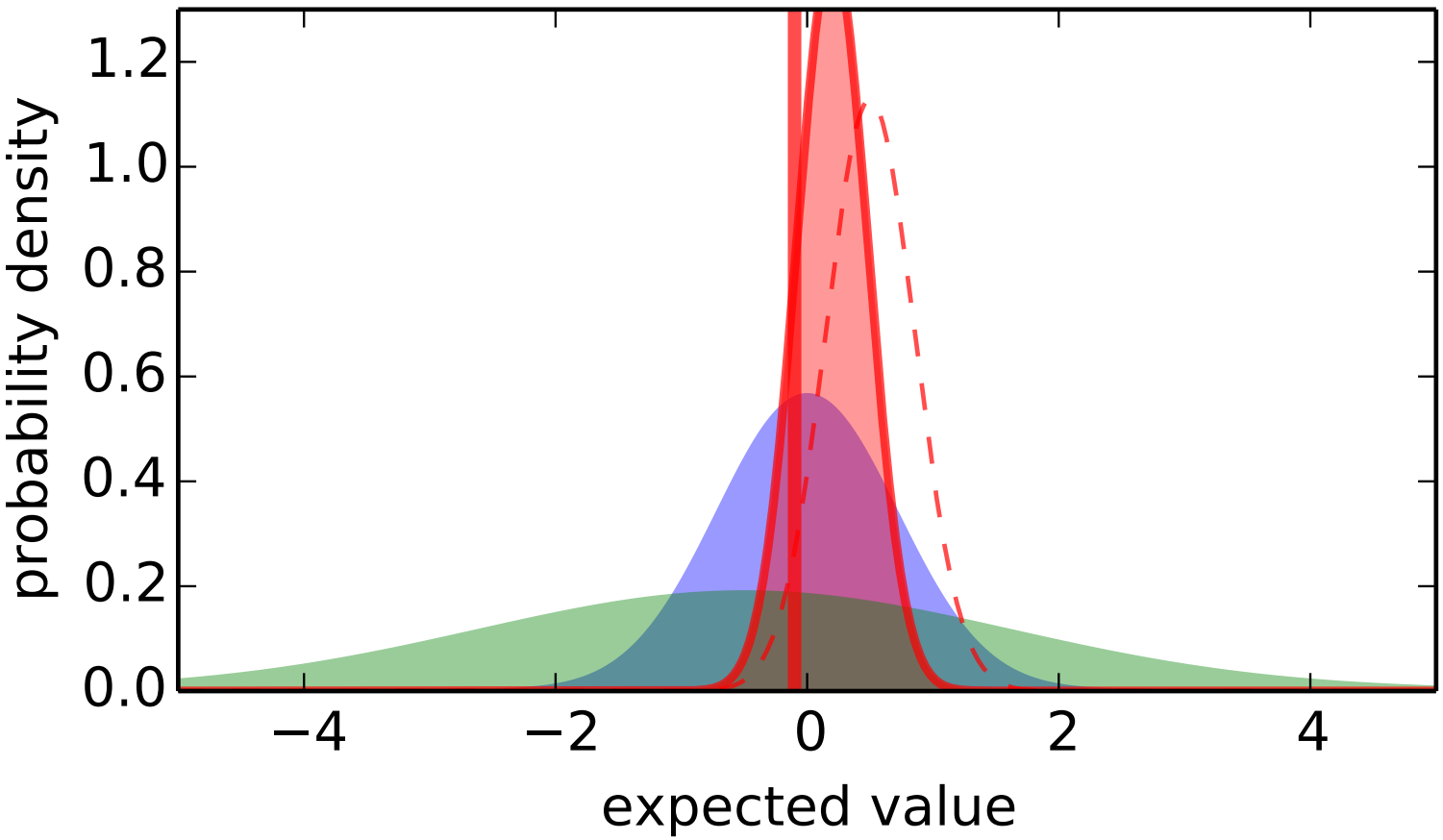

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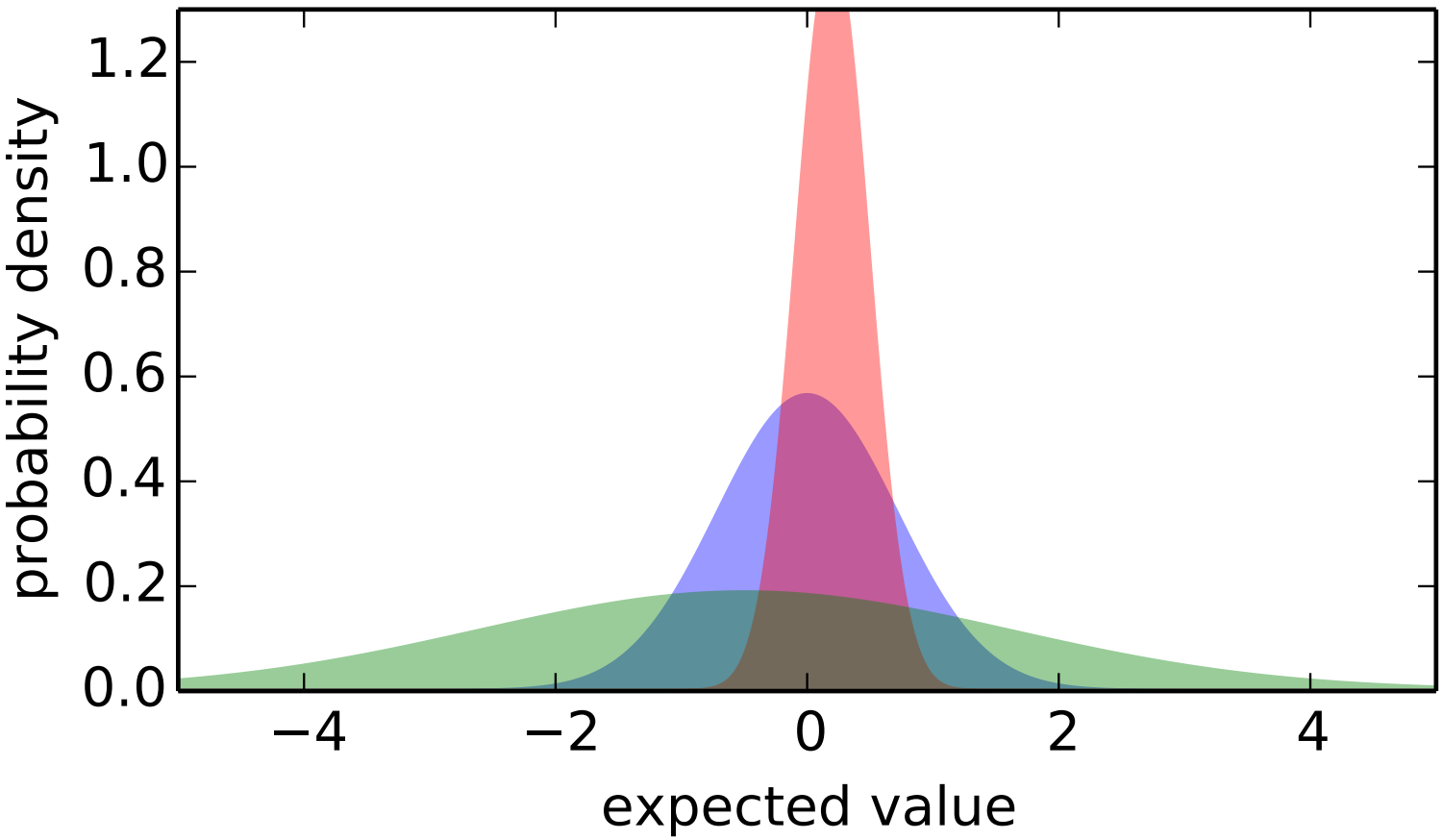

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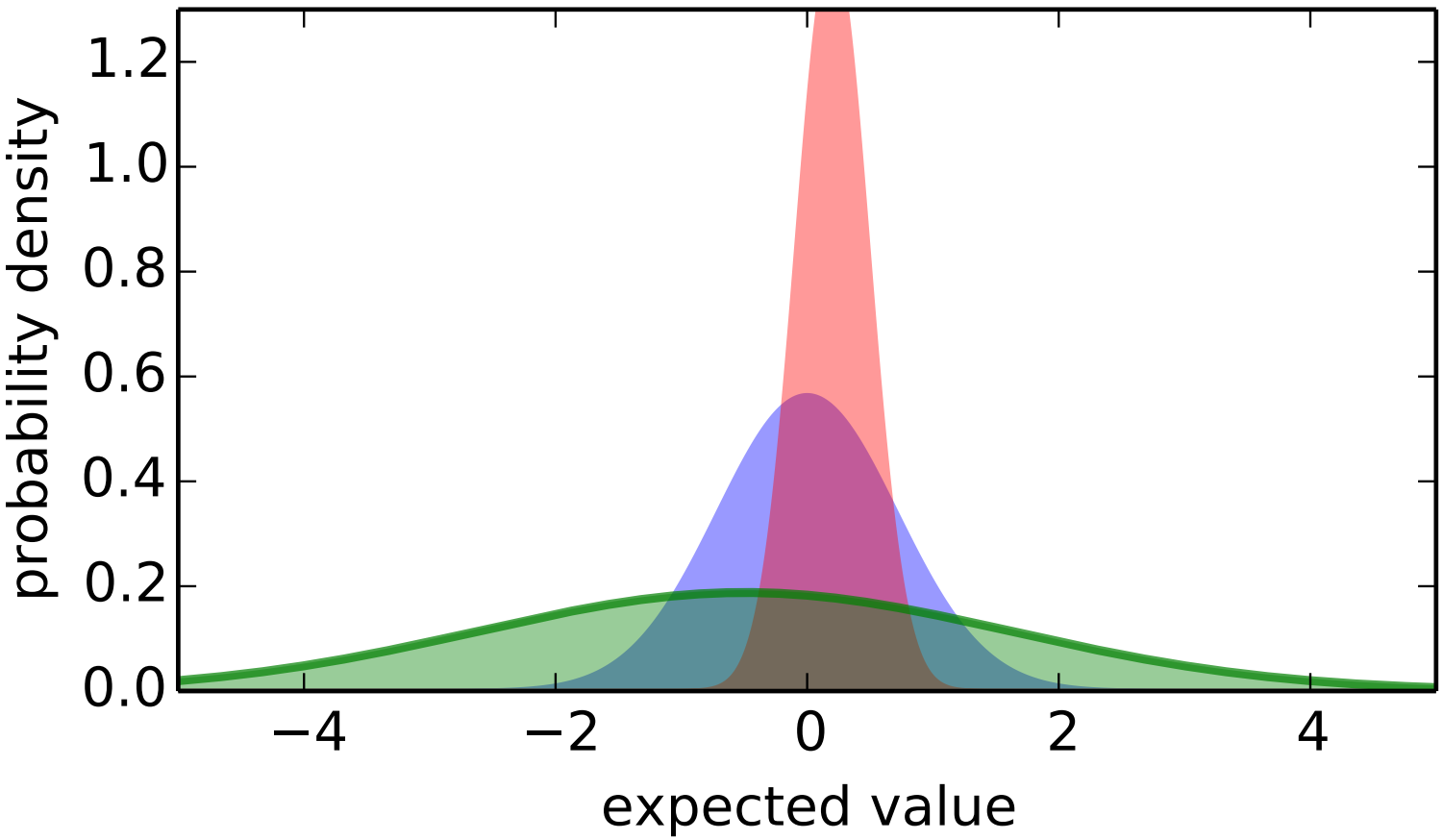
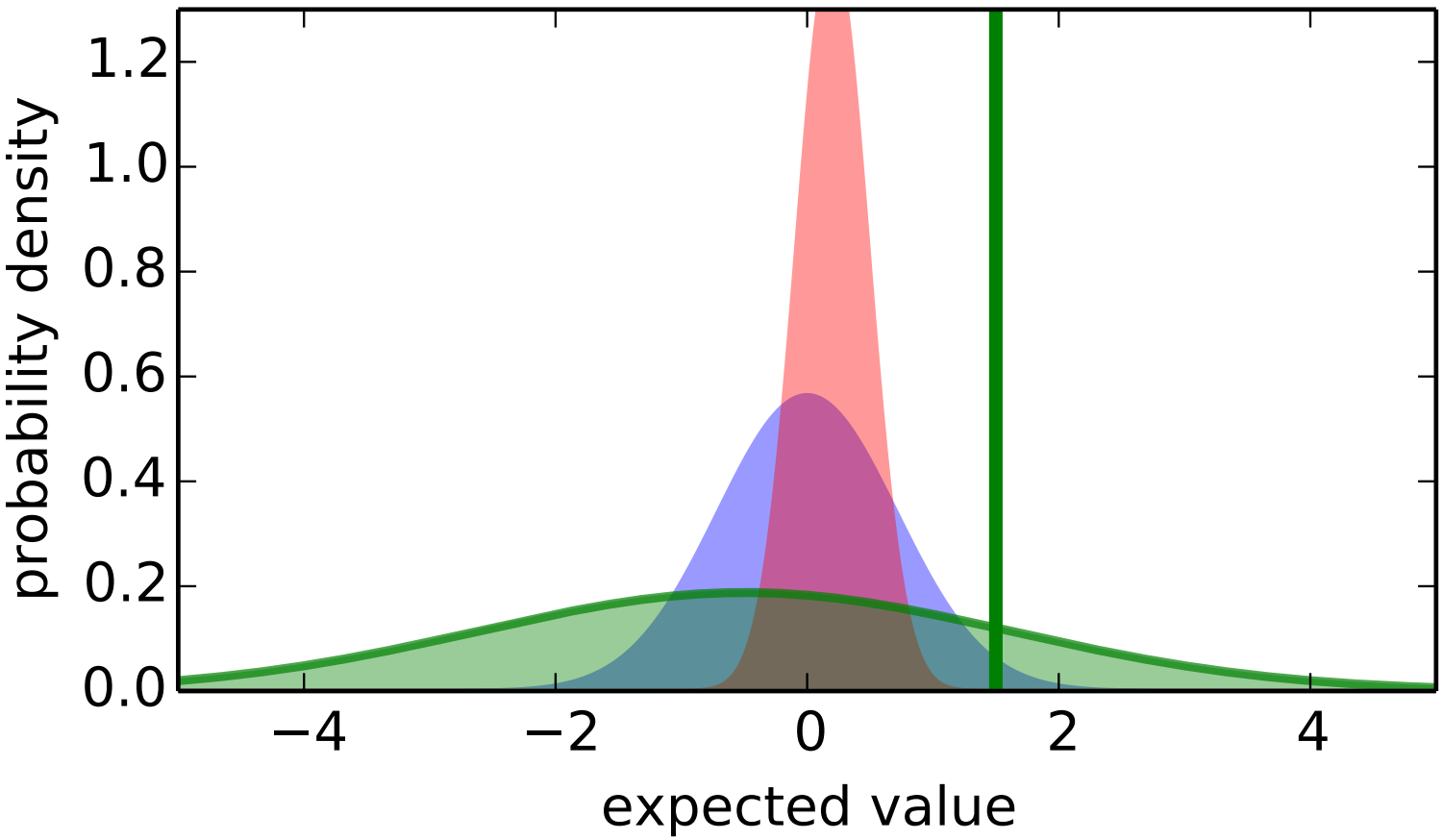


Optimism in the Face of Uncertainty



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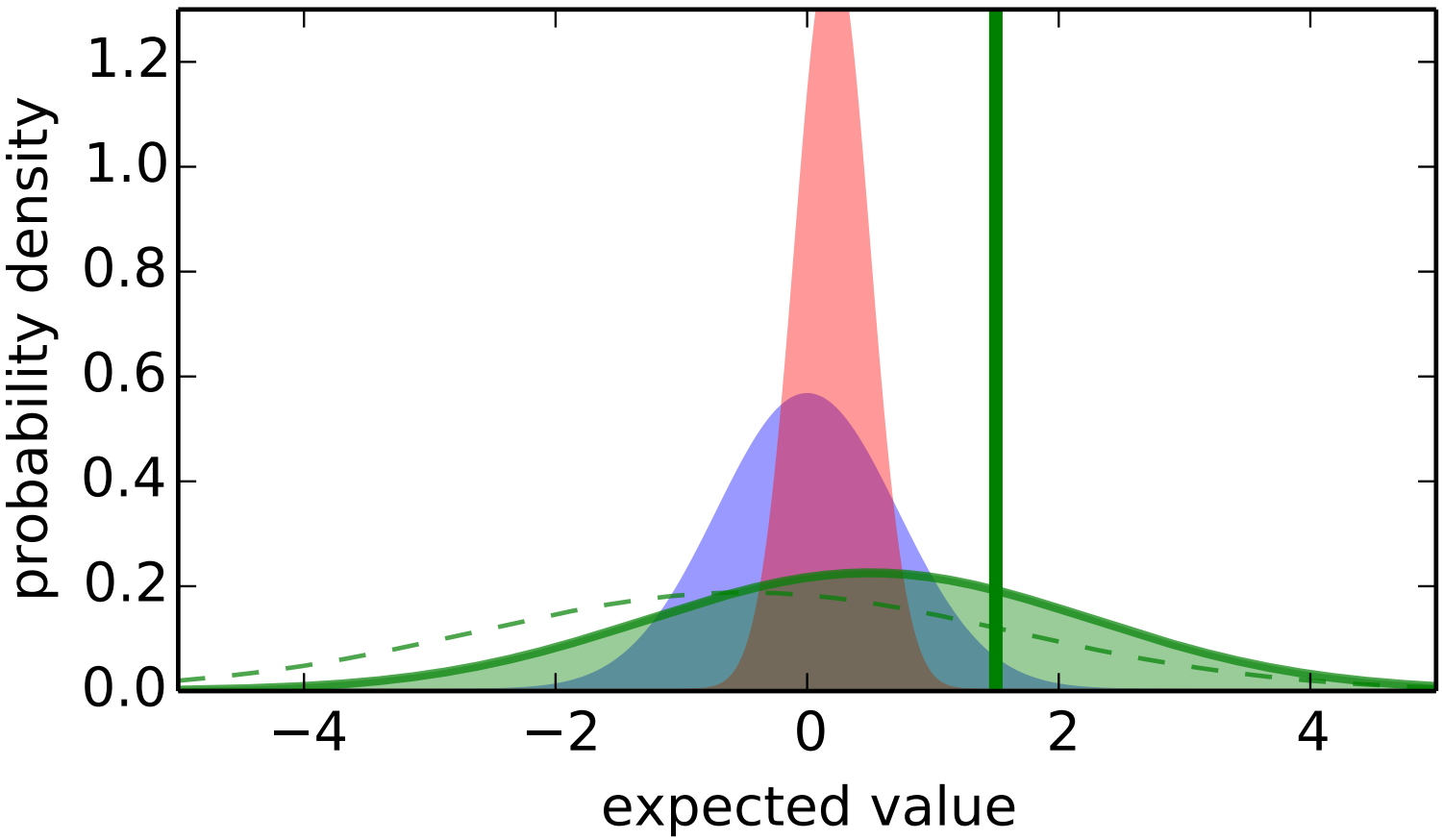


Upper Confidence Bounds

- 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
- 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)
- Select action maximizing Upper Confidence Bound (UCB)

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

Hoeffding's Inequality

Theorem (Hoeffding's Inequality)

Let $\Sigma_1, ..., \Sigma_t$ be i.i.d. random variables in [0,1], and let $\overline{X}_t = \frac{1}{t}\sum_{i=1}^{t}\Sigma_i$ be the sample mean. Then

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

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

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

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

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

Theorem (Auer et al., 2002)

The UCB algorithm achieves logarithmic expected total regret

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

for any t

Values or Models?

- This is a value-based algorithm:

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

- (Same as before, but rewritten as update)
- What about a model-based approach?

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

- Indistinguishable?
- Not if we model *distribution of rewards*

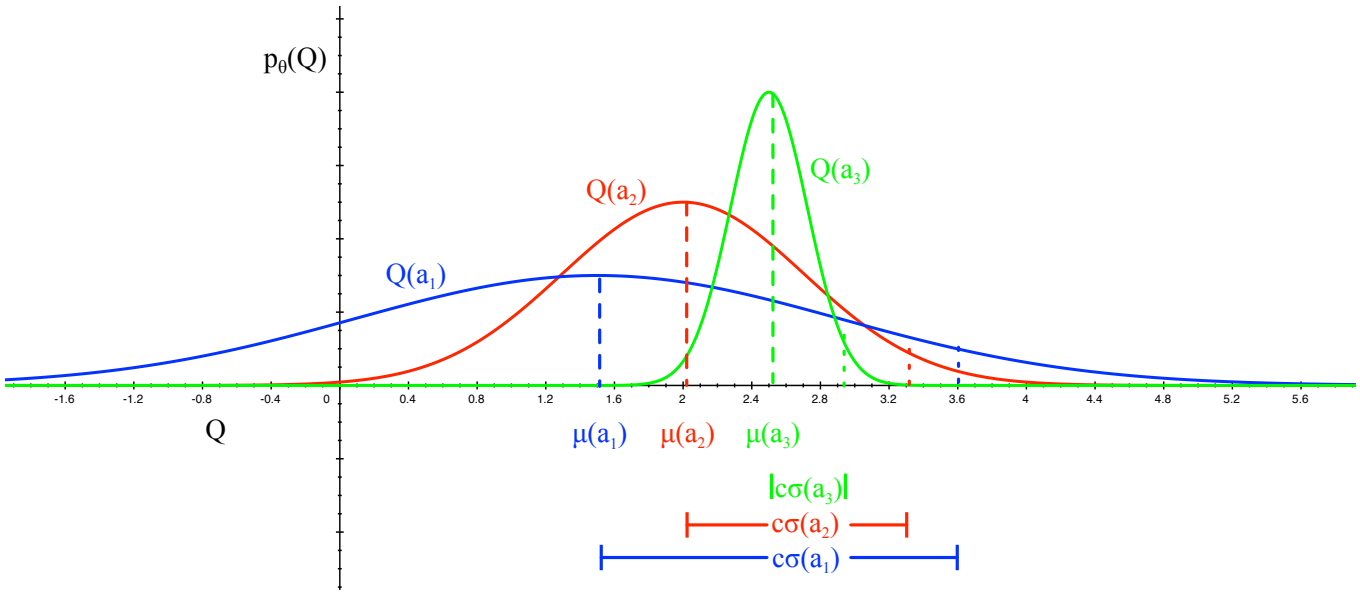
Bayesian Bandits

- *Bayesian bandits* model parameterized distributions over rewards, $p\left[\mathcal{R}^a|\theta\right]$
  - e.g., Gaussians: $\theta = [\mu(a_1), \sigma^2(a_1), ..., \mu(a_{|\mathcal{A}|}), \sigma^2(a_{|\mathcal{A}|})]$
- Compute posterior distribution over θ

$$p\left[\theta|H_t\right] \quad \propto \quad p\left[H_t|\theta\right] p\left[\theta\right]$$

- Allows us to inject rich prior knowledge $p\left[\theta\right]$
- Use posterior to guide exploration
  - Upper confidence bounds
  - Probability matching
- Better performance if prior is accurate

Bayesian Bandits with Upper Confidence Bounds



- Compute posterior distribution over action-values

$$p\left[q(a)|H_{t-1}\right] = \int_\theta p\left[q(a)|\theta\right] p\left[\theta|H_{t-1}\right] \, \mathrm{d}\theta$$

- Estimate upper confidence from posterior, e.g., $U_t(a) = c\sigma_t(a)$
  - where $\sigma(a)$ is std dev of $p(q(a) \mid \theta)$
- 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

$$\pi_t(a) = \mathbb{P}\left[q(a) = \max_{a'} q(a') \mid H_{t-1}\right]$$

- 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 $Q_t(a) \sim p\left[q(a)|H_{t-1}\right], \forall a$
  - Select action maximising sample, $a_t = \underset{a \in \mathcal{A}}{\text{argmax}}\ Q_t(a)$
- Thompson sampling is sample-based probability matching

$$\pi_t(a) = \mathbb{E}\left[\mathcal{I}(Q_t(a) = \max_{a'} Q_t(a')) \mid H_{t-1}\right]$$
$$= \mathbb{P}\left[q(a) = \max_{a'} q(a') \mid H_{t-1}\right]$$

- For Bernoulli bandits, Thompson sampling achieves Lai and Robbins lower bound on regret!

Value of Information

- Exploration is valuable because information is valuable
- Can we quantify the value of information?
- 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* $\tilde{s}$ summarising all information accumulated so far
- Each action a causes a transition to a new information state $\tilde{s}'$ (by adding information), with probability $\mathcal{P}^a_{\tilde{s},\tilde{s}'}$
- We then have a Markov decision problem
- Here states = observations = internal information state

Example: Bernoulli Bandits

- Consider a Bernoulli bandit, such that

$$\mathbb{P}[R_t = 1 \mid A_t = a] = \mu_a$$
$$\mathbb{P}[R_t = 0 \mid A_t = a] = 1 - \mu_a$$

- 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 $\tilde{s} = \langle \alpha, \beta \rangle$
  - 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 have formulated the bandit as an infinite MDP over information states
- 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)
- Latter approach is known as *Bayes-adaptive* RL
- Finds Bayes-optimal exploration/exploitation trade-off with respect to prior distribution

Contextual Bandits

- Lets bring back external observations
- In bandits, this is often called context
- A contextual bandit is a tuple $\langle \mathcal{A}, \mathcal{C}, \mathcal{R} \rangle$
- $\mathcal{A}$ is a known set of actions (or "arms")
- $\mathcal{C} = \mathbb{P}[s]$ is an unknown distribution over states
- At each step t
  - Environment generates state $S_t \sim \mathcal{C}$
  - 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 $\sum_{i=1}^{t} R_i$
- Actions do not affect state!

Linear Regression

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

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

- Suppose we have feature vectors $\phi_t \equiv \phi(S_t)$, where $\phi : \mathcal{S} \to \mathbb{R}^n$
- We can estimate value function with a linear approximation

$$\hat{q}(s, a; \{\theta(a)\}_{a \in \mathcal{A}}) \;=\; \phi(s)^\top \theta(a) \;\approx\; q(s, a)$$

- Estimate parameters by least squares regression

Linear Regression

Estimate parameters by least squares regression...

$$\theta_*(a) = \operatorname*{argmin}_\theta \mathbb{E}\left[\left(q(S_t, a) - \phi_t^\top \theta\right)^2\right]$$

$$\Rightarrow \theta_*(a) = \mathbb{E}\left[\phi_t \phi_t^\top | A_t = a\right]^{-1} \mathbb{E}\left[\phi_t R_t | A_t = a\right]$$

$$\Sigma_t(a) = \sum_{i=1}^{t} \mathcal{I}(A_i = a)\phi_i \phi_i^\top \qquad \text{(feature statistics)}$$

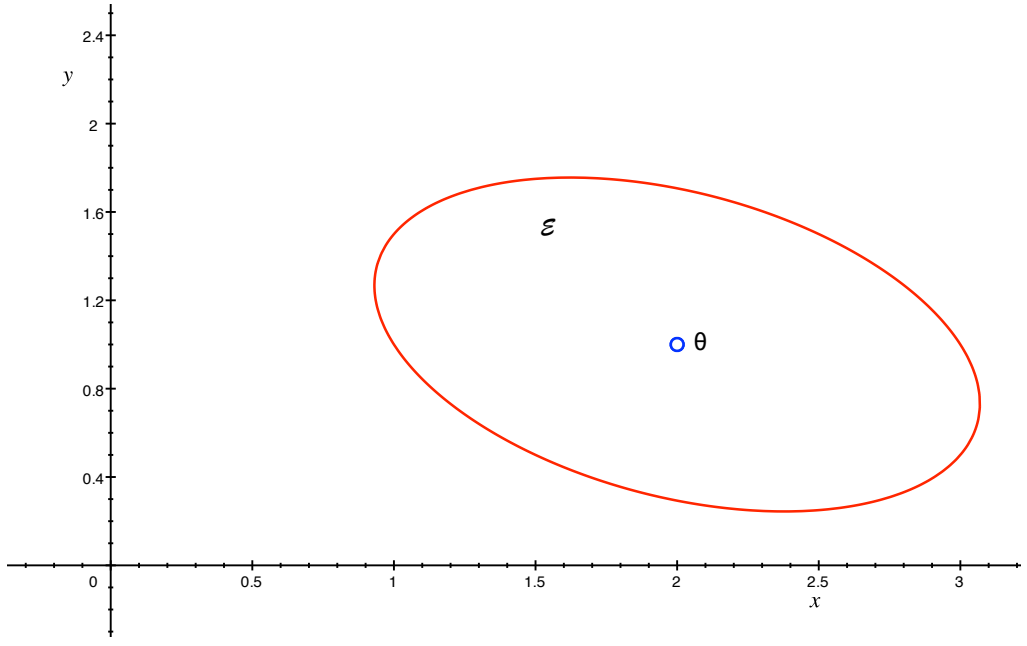
$$b_t(a) = \sum_{i=1}^{t} \mathcal{I}(A_i = a)\phi_i R_i \qquad \text{(reward statistics)}$$

$$\theta_t(a) = \Sigma_t(a)^{-1} b_t(a)$$

Linear Upper Confidence Bounds

- Least squares regression estimates the mean
- Can also estimate the value uncertainty due to parameter estimation error $\sigma^2(s, a; \theta)$
- Can use as uncertainty bonus: $U_\theta(s, a) = c\sigma(s, a; \theta)$
- i.e. define UCB to be c standard deviations above the mean

Geometric Interpretation



- Define confidence ellipsoid $\mathcal{E}_t$ that includes true parameters θ_* with high probability
- Use this to estimate the uncertainty of action values
- Pick parameters within ellipsoid that maximize action value

$$\underset{\theta \in \mathcal{E}}{\text{argmax}}\ \hat{q}(s, a; \theta)$$

Calculating Linear Upper Confidence Bounds

- For least squares regression, parameter covariance is $\Sigma_t(a)^{-1}$
- Action-value is linear in features: $\hat{q}(s, a; \theta) = \phi(s)^\top \theta_a$
- So action-value variance is quadratic,

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

- Upper confidence bound is $\hat{q}(s, a; \theta) + c\sigma(s, a; \theta)$
- Select action maximising upper confidence bound

$$a_t = \underset{a \in \mathcal{A}}{\operatorname{argmax}}\ \hat{q}(S_t, a; \theta) + c\sigma(s, a; \theta)$$

Gradient bandits

- What about learning policies $\pi(a) = \mathbb{P}[A_t = a]$ directly?
- For instance, define action preferences $Y_t(a)$ and the use

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

- The preferences do not have to have semantics of cumulative rewards
- Instead, view them as tunable parameters
- We can then optimize preferences

Gradient bandits

- Gradient ascent on value:

$$
\begin{aligned}
Y_{t+1}(a) &= Y_t(a) + \alpha \frac{\partial \mathbb{E}\left[R_t | \pi_t\right]}{\partial Y_t(a)} \\
&= Y_t(a) + \alpha \frac{\partial}{\partial Y_t(a)} \sum_a \pi_t(a) q(a) \\
&= Y_t(a) + \alpha \sum_a q(a) \frac{\partial \pi_t(a)}{\partial Y_t(a)} \\
&= Y_t(a) + \alpha \sum_a \pi(a) q(a) \frac{\partial \log \pi_t(a)}{\partial Y_t(a)} \\
&= Y_t(a) + \alpha \mathbb{E}\left[R_t \frac{\partial \log \pi_t(a)}{\partial Y_t(a)}\right]
\end{aligned}
$$

Gradient bandits

- For soft max:

$$\begin{aligned} Y_{t+1}(a) &= Y_t(a) + \alpha \mathbb{E}\left[R_t \frac{\partial \log \pi_t(a)}{\partial Y_t(a)}\right] \\ &= Y_t(a) + \alpha \mathbb{E}\left[R_t(\mathcal{I}(a = A_t) - \pi_t(a))\right] \end{aligned}$$

- $\Rightarrow$

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

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

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