Carnegie Mellon

School of Computer Science

Deep Reinforcement Learning and Control

Multi-armed bandits

Spring 2021, CMU 10-403

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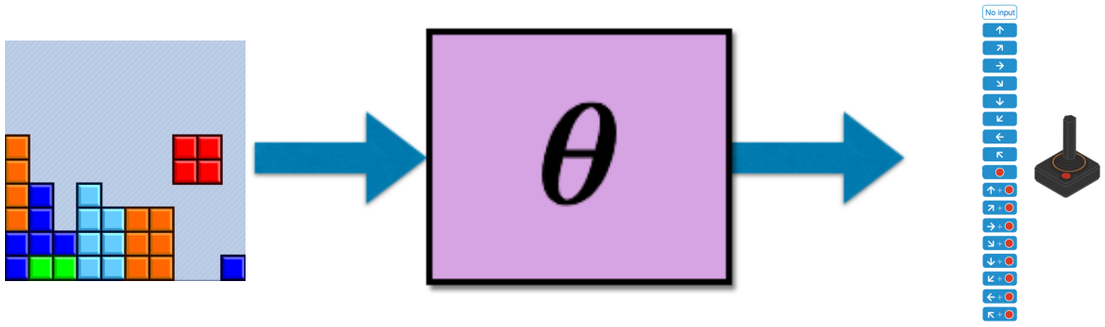
Used Materials

- **Disclaimer:** Some material and slides for this lecture were borrowed from Rich Sutton's lecture on multi-armed bandits.

LL: Reinforcement Learning via Evolution



$$\pi(a \mid s, \theta)$$

Given an initial state distribution $\mu_0(s_0)$, estimate parameters θ of a policy π_θ so that, the trajectories τ sampled from this policy have maximum returns, i.e., sum of rewards $R(\tau)$.

$$\max_{\theta} . \quad U(\theta) = \mathbb{E}_{\tau \sim \pi_\theta} \left[R(\tau) \mid \pi_\theta, \mu_0(s_0) \right]$$

τ : trajectory, a sequence of state, action, rewards, a game fragment or a full game:

$$\tau : s_0, a_0, r_0, s_1, a_1, r_1, s_2, a_2, r_2, \ldots s_T, a_T, r_T$$

$R(\tau)$: reward of a trajectory: (discounted) sum of the rewards of the individual state/actions

$$R(\tau) = \sum_{t=1}^{T} r_t$$

LL: Evolutionary methods for policy search

$$\max_{\theta} . \quad U(\theta) = \mathbb{E}_{\tau \sim \pi_\theta} \left[R(\tau) \,|\, \pi_\theta, \mu_0(s_0) \right]$$

General algorithm:

Initialize a population of parameter vectors (genotypes)

1. *Make random perturbations (mutations) to each parameter vector*
2. *Evaluate the perturbed parameter vector (fitness)*
3. *Keep the perturbed vector if the result improves (selection)*
4. *GOTO 1*

Simple and biologically plausible…

LL: Natural Evolutionary Strategies (NES)

- In CEM and CMA-ES, we have been selecting the best (elite) parameter offsprings.
- NES considers every offspring.

Algorithm 1: Evolutionary Strategies

1. **Input**: Learning rate α, noise standard deviation σ, initial policy parameters θ_0
2. **for** $t = 0,1,2,\cdots$ do
3. Sample $\epsilon_1, \cdots, \epsilon_n \sim \mathcal{N}(0, \mathbf{I}_d)$
4. Compute returns $F_i = F\left(\mu_t + \sigma\epsilon_i\right)$ for $i = 1,2,\cdots,n$
5. Set $\mu_{t+1} \leftarrow \mu_t + \alpha \frac{1}{n\sigma} \sum_{i=1}^{n} F_i \epsilon_i$

6. end for

This lecture - Motivation

Learning to act in a non-sequential (single action) setups:

- Each action results in an immediate reward.
- We want to choose actions that maximize our immediate reward in expectation.
  - Q: Why in expectation?
  - A: Because rewards are not deterministic.
- For example, displaying an advertisement can generate different click rates in different days. Actions: the advertisements to be displayed, Rewards: the user click rate. We want to pick the advertisement that maximizes the click rate on average

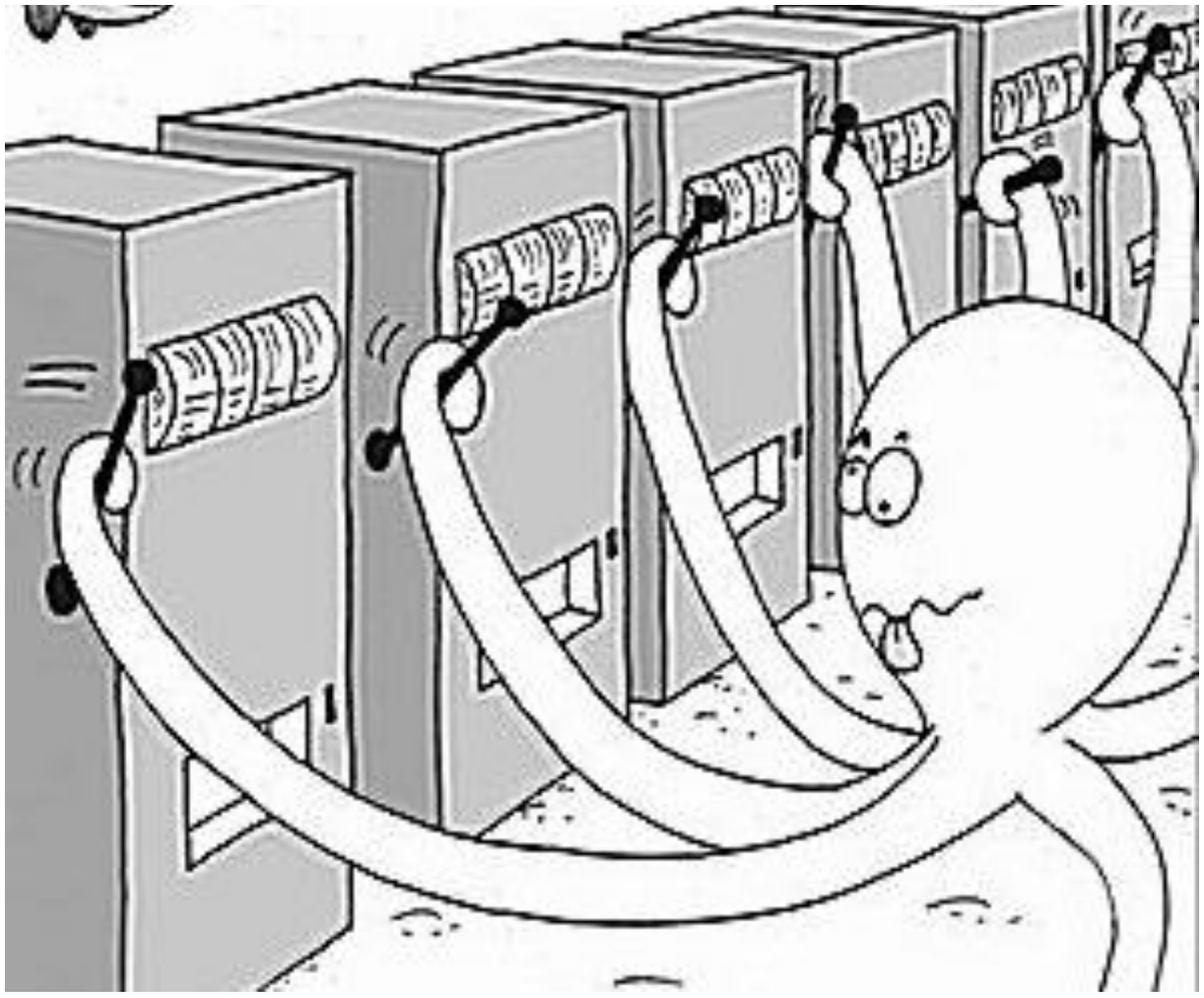
Multi-Armed Bandits

One-armed bandit= Slot machine (English slang)

source: infoslotmachine.com

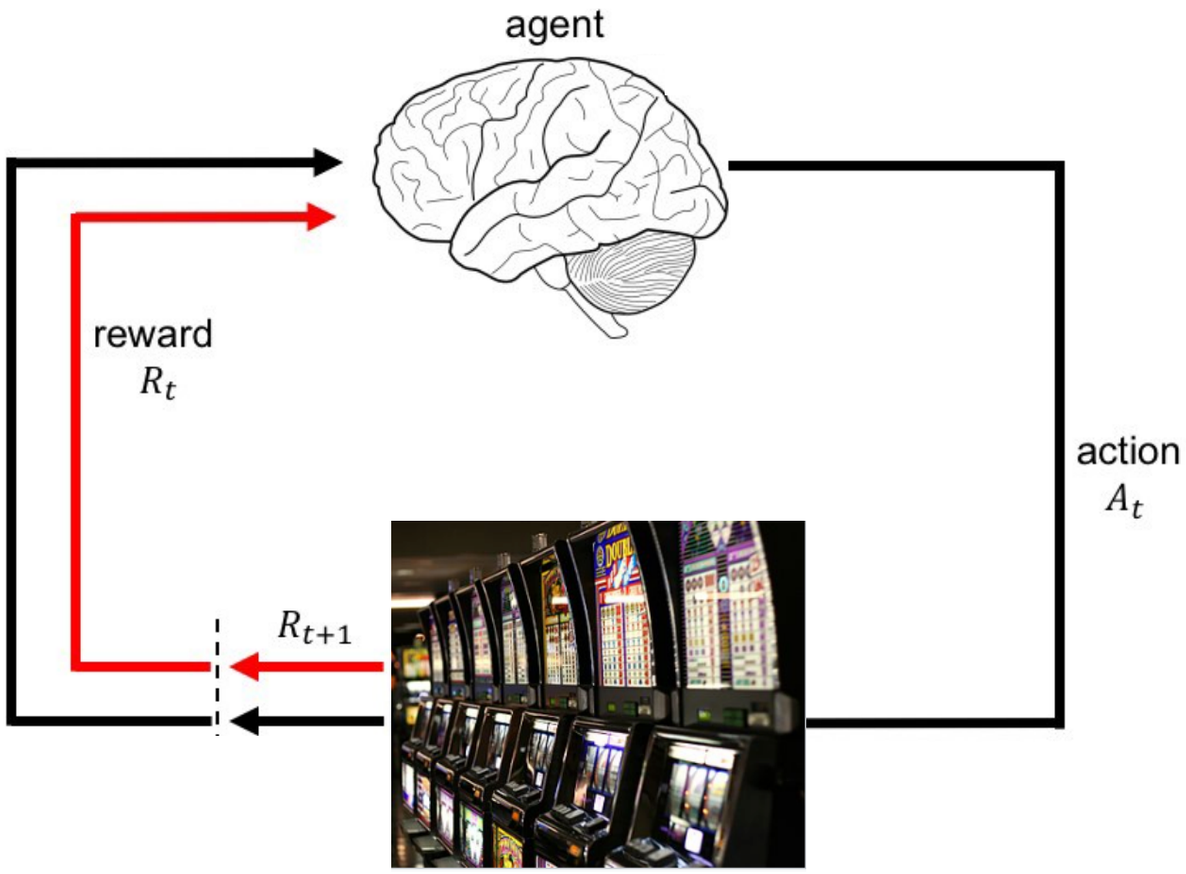
Multi-Armed Bandits

Multi-Armed bandit = Multiple Slot Machine



source: Microsoft Research

Multi-Armed Bandits



$$A_t, R_{t+1}, A_{t+1}, R_{t+2}, A_{t+2}, A_{t+3}, R_{t+3}, \ldots$$

The state does not change! (a.k.a. stateless)

Multi-Armed Bandit Problem

At each timestep t the agent chooses one of the K arms and plays it.

The k th arm produces reward $r_{k,t}$ when played at timestep t .

The rewards $r_{k,t}$ are drawn from a probability distribution $\mathscr{P}_k$ with mean μ_k .

The agent does not know neither the full arm reward distributions neither their means.

source: Pandey et al.'s slide

Agent's Objective: Maximize cumulative rewards (over an infinite horizon).

This is equivalent to finding the arm with the highest **mean** reward. Why?

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source: Pandey et al.'s slide

Definition: The action-value for action α (here arm k) is its mean reward:

$$q_*(a) \doteq \mathbb{E}[R_t | A_t = a]$$

The Exploration/Exploitation Dilemma

- Suppose you form estimates

$$Q_t(a) \approx q_*(a), \quad \forall a$$

action-value estimates

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  If $A_t \neq A_t{}^*$ then you are *exploring*

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- You can't do both, but you need to do both

- You can never stop exploring, but maybe you should explore less with time.

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

Exploration vs Exploitation Dilemma

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  - Exploration: Gather more information
- The best long-term strategy may involve short-term sacrifices
- Gather enough information to make the best overall decisions
- The exploration/exploitation dilemma is not a problem encountered in computational RL or deep RL: It is a fundamental problem in decision making of any intelligent agent.

Exploration vs. Exploitation Dilemma

- Restaurant Selection
  - Exploitation: Go to your favorite restaurant
  - Exploration: Try a new restaurant
- 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

Example: Bernoulli Bandits

Recall: The **Bernoulli distribution** is the discrete probability distribution of a random variable which takes the value 1 with probability p and the value 0 with probability q=1-p, that is, the probability distribution of any single experiment that asks a yes–no question.

- Each action (arm when played) results in success or failure, rewards are binary.
- Mean reward for each arm represents the probability of success.
- Action (arm) $k \in \{1 \ldots K\}$ produces a success with probability $\theta_k \in [0,1]$.

θ_1

win 0.6
of time

θ_2

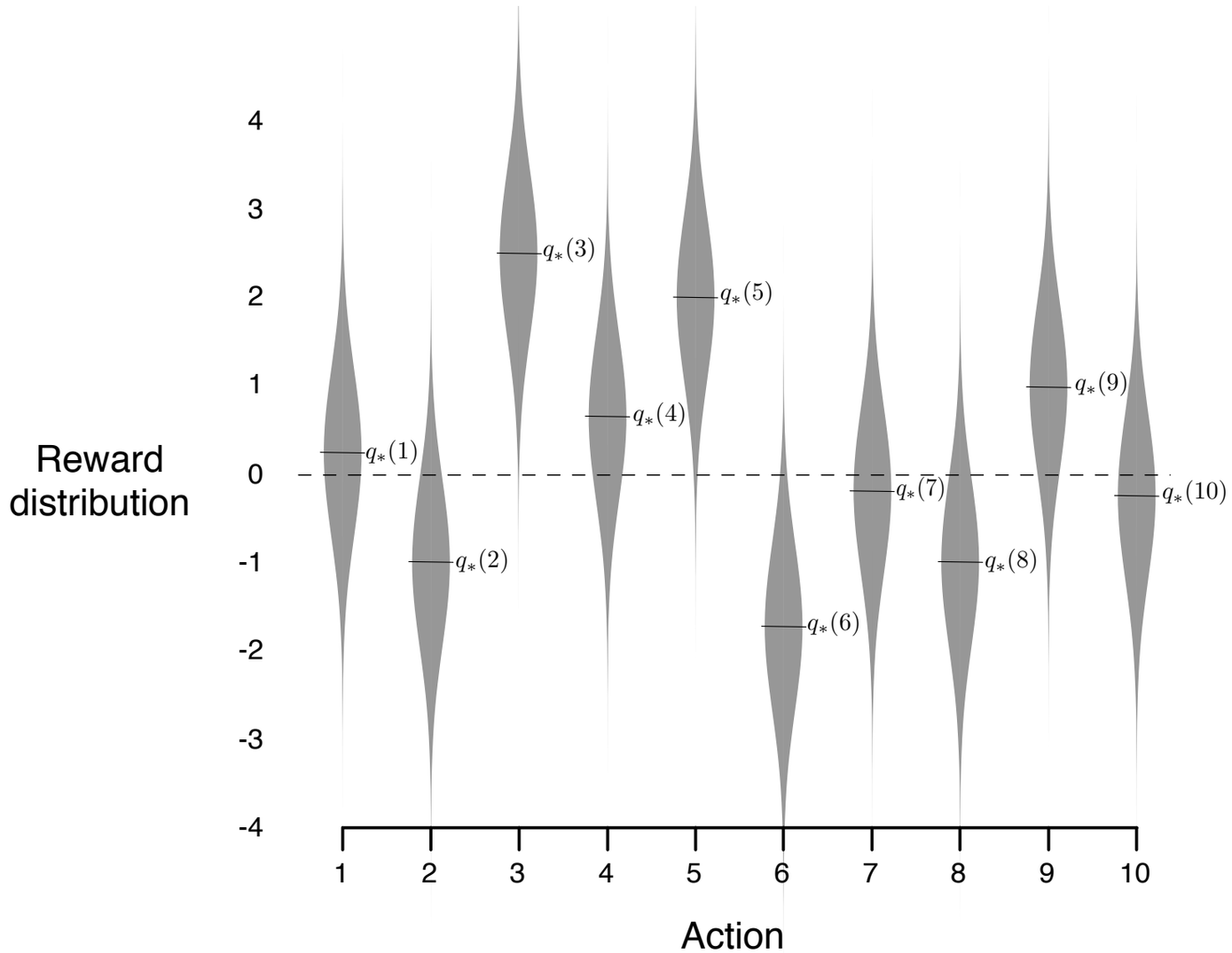
win 0.4
of time

θ_3

win 0.45
of time

Example: Gaussian Bandits

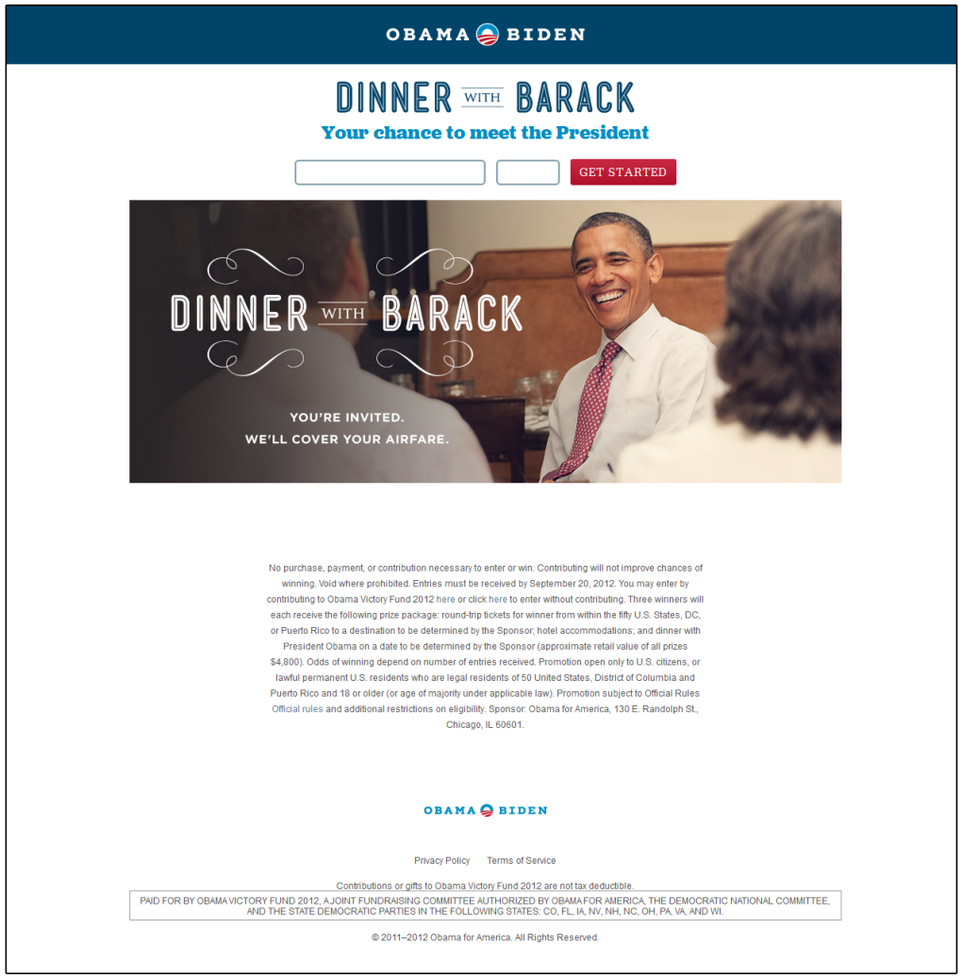
- Each action (arm when played) results in a real number.
- Action (arm) $k \in \{1 \ldots K\}$ produces on average reward equal to the mean of its Gaussian distribution.

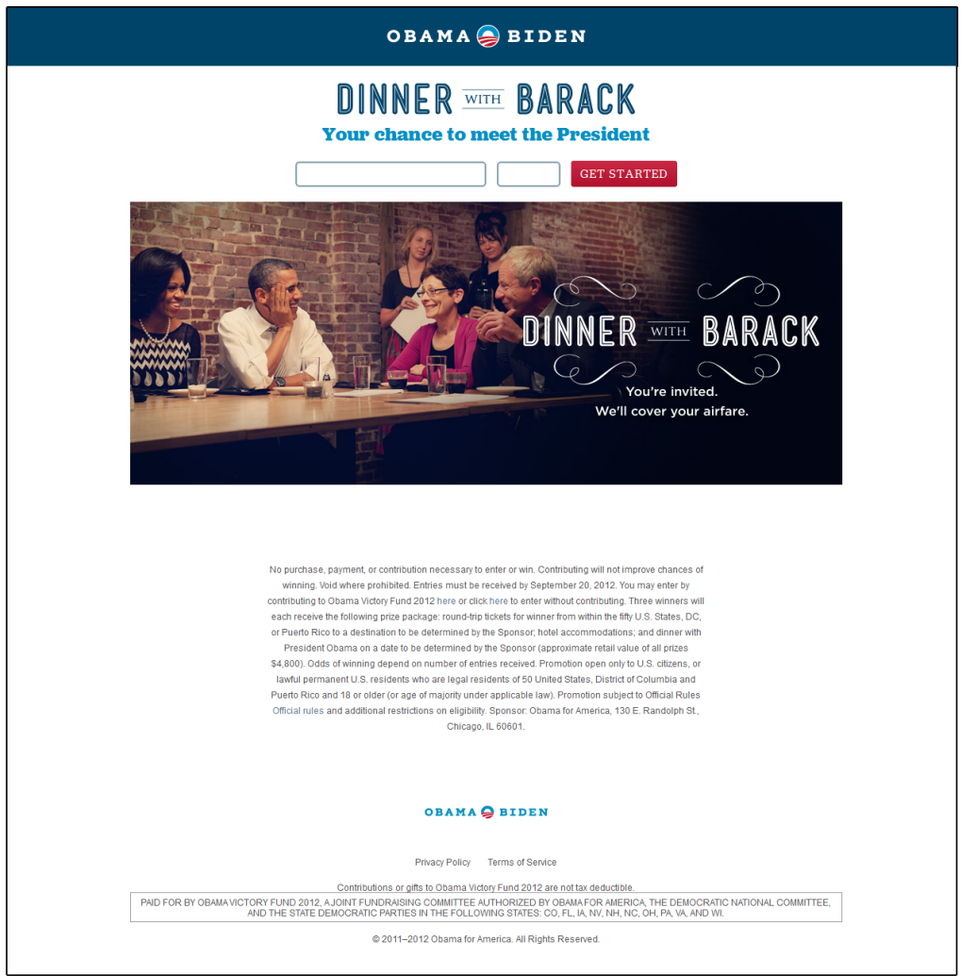


Real world motivation: content presentation

We have two variations of content of a webpage, A and B, and we want to decide which one to display to engage more users.

- Two arm bandits: each arm corresponds to a content variation shown to users (not necessarily the same user).
- Mean rewards: the total percentage of users that would click on each invitation

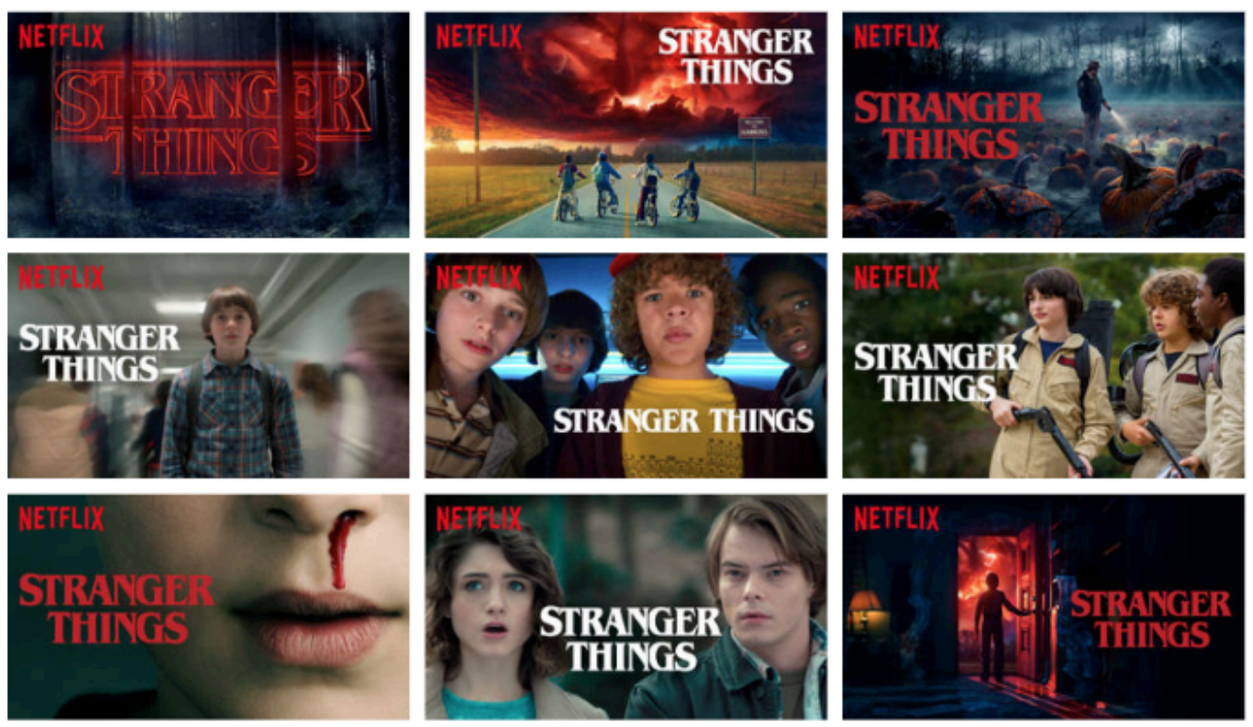




Real world motivation: NETFLIX artwork

For a particular movie, we want to decide what image to show (to all the NEFLIX users)

- Actions: uploading one of the K images to a user's home screen
- Mean rewards: the percentage of users that clicked and watched (quality engagement, not clickbait)



Netflix Artwork

Regret

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

$$q_*(a) \doteq \mathbb{E}[R_t | A_t = a], \quad \forall a \in \{1, \ldots, k\}$$

- The optimal value is

$$v_* = q(a^*) = \max_{a \in \mathcal{A}} q_*(a)$$

- The regret is the opportunity loss for one step

$$I_t = \mathbb{E}[v_* - q_*(a_t)] \qquad \text{reward} = -\text{regret}$$

- The total regret is the total opportunity loss

$$L_T = \mathbb{E}\left[\sum_{t=1}^{T} v_* - q_*(a_t)\right]$$

- Maximize cumulative reward = minimize total regret

Regret

- The count $N_t(a)$: the number of times that action a has been selected prior to time t
- The gap Δa 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

$$L_T = \mathbb{E}\left[\sum_{t=1}^{T} v_* - q_*(a_t)\right]$$

$$= \sum_{a \in \mathcal{A}} \mathbb{E}[N_t(a)](v_* - q_*(a))$$

$$= \sum_{a \in \mathcal{A}} \mathbb{E}[N_t(a)]\Delta_a$$

Forming Action-Value Estimates

- To simplify notation, let us focus on one action
  - We consider only its rewards, and its estimate after n+1 rewards:

$$Q_n \doteq \frac{R_1 + R_2 + \cdots + R_{n-1}}{n-1}$$

- How can we do this incrementally (without storing all the rewards)?
- Could store a running sum and count (and divide), or equivalently:

$$Q_{n+1} = Q_n + \frac{1}{n}\Big[R_n - Q_n\Big]$$

- This is a standard form for learning/update rules:

$$NewEstimate \leftarrow OldEstimate \; + \; StepSize \; \Big[Target - OldEstimate\Big]$$

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- This is a standard form for learning/update rules: error

$$NewEstimate \leftarrow OldEstimate \; + \; StepSize \Big[Target - OldEstimate\Big]$$

Derivation of incremental update

$$Q_n \doteq \frac{R_1 + R_2 + \cdots + R_{n-1}}{n-1}$$

$$\begin{aligned}
Q_{n+1} &= \frac{1}{n}\sum_{i=1}^{n} R_i \\
&= \frac{1}{n}\left(R_n + \sum_{i=1}^{n-1} R_i\right) \\
&= \frac{1}{n}\left(R_n + (n-1)\frac{1}{n-1}\sum_{i=1}^{n-1} R_i\right) \\
&= \frac{1}{n}\Big(R_n + (n-1)Q_n\Big) \\
&= \frac{1}{n}\Big(R_n + nQ_n - Q_n\Big) \\
&= Q_n + \frac{1}{n}\Big[R_n - Q_n\Big],
\end{aligned}$$

Non-stationary bandits

- Suppose the true action values change slowly over time
  - then we say that the problem is *nonstationary*
- In this case, sample averages are not a good idea
  - Why?

Non-stationary bandits

- Suppose the true action values change slowly over time
  - then we say that the problem is *nonstationary*
- In this case, sample averages are not a good idea
- Better is an “exponential, recency-weighted average”:

$$
\begin{aligned}
Q_{n+1} &\doteq Q_n + \alpha\Big[R_n - Q_n\Big] \\
&= (1-\alpha)^n Q_1 + \sum_{i=1}^{n} \alpha(1-\alpha)^{n-i} R_i,
\end{aligned}
$$

where $\alpha \in (0,1]$ and constant

The smaller the i, the smaller the multiplier-> forgetting earlier rewards

Action selection in multi-armed bandits

Fixed exploration period + Greedy

1. Allocate a fixed time period to exploration when you try bandits uniformly at random

2. Estimate mean rewards for all actions: $Q_t(a) = \frac{1}{N_t(a)} \sum_{i=1}^{t-1} r_i \mathbf{1}(A_i = a)$

3. Select the action that is optimal for the estimated mean rewards, breaking ties at random: $a_t = \underset{a \in \mathcal{A}}{\text{argmax}}\, Q_t(a)$

4. GOTO 2

Fixed exploration period + Greedy

- After the fixed exploration period we have formed the following reward estimates

$Q_t(a_1) = 0.3$

$Q_t(a_2) = 0.5$

$Q_t(a_3) = 0.1$

Q1: Will the greedy method always pick the second action?

Q2: Can greedy lock onto a suboptimal action forever?

⇒ Greedy has linear total regret

ε-Greedy Action Selection

- In greedy action selection, you always exploit
- In ε-greedy, you are usually greedy, but with probability ε you instead pick an action at random (possibly the greedy action again)
- This is perhaps the simplest way to balance exploration and exploitation

ε-Greedy Action Selection

A simple bandit algorithm

Initialize, for $a = 1$ to k:
$Q(a) \leftarrow 0$
$N(a) \leftarrow 0$

Repeat forever:

$$A \leftarrow \begin{cases} \arg\max_a Q(a) & \text{with probability } 1-\varepsilon \quad \text{(breaking ties randomly)} \\ \text{a random action} & \text{with probability } \varepsilon \end{cases}$$

$R \leftarrow bandit(A)$
$N(A) \leftarrow N(A) + 1$
$Q(A) \leftarrow Q(A) + \frac{1}{N(A)}\big[R - Q(A)\big]$

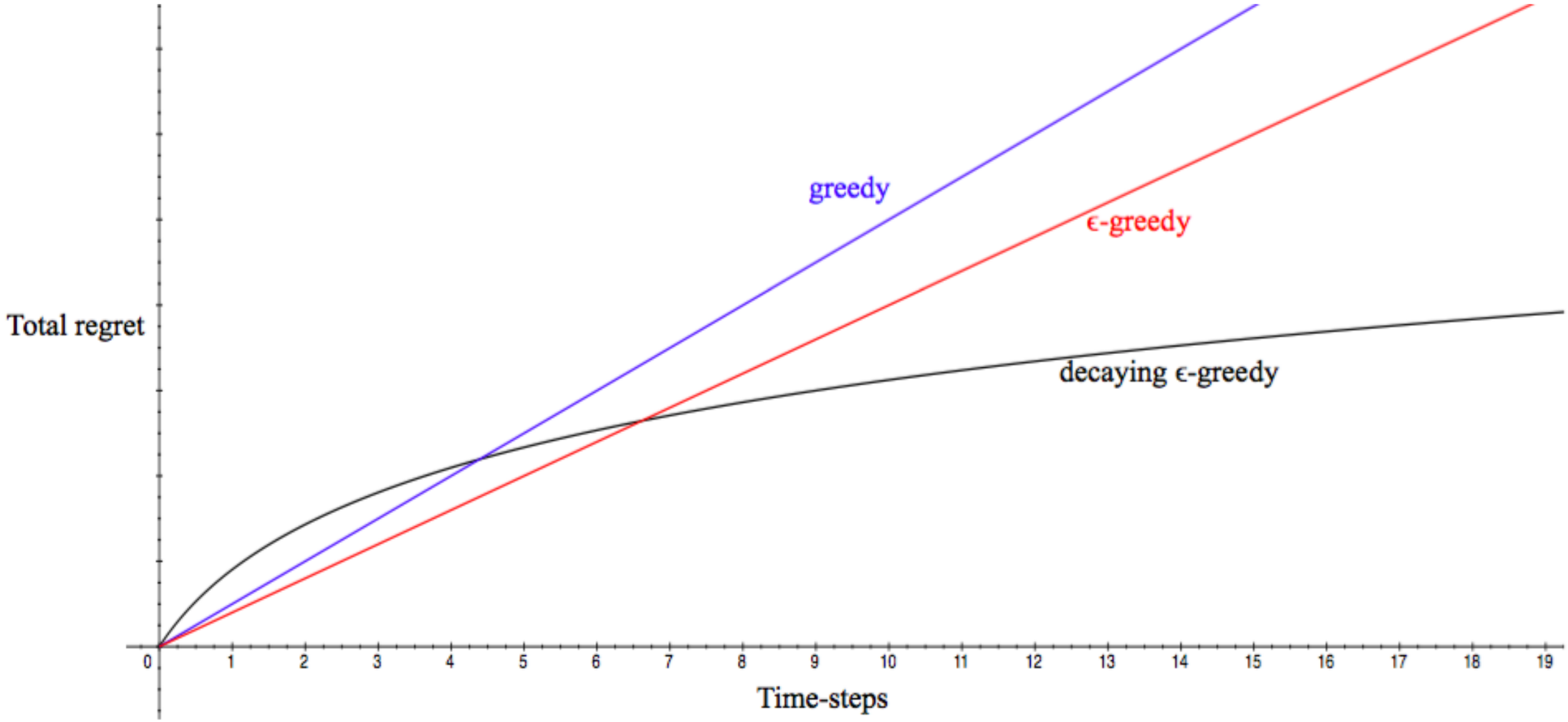
ε-Greedy Algorithm

- The ε-greedy algorithm continues to explore forever
  - With probability 1 − ε select $a_t = \text{argmax}_{a \in \mathcal{A}} Q_t(a)$
  - With probability ε select a random action
- Constant ε ensures minimum regret

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

- ⇒ ε-greedy has linear total regret

Counting Regret

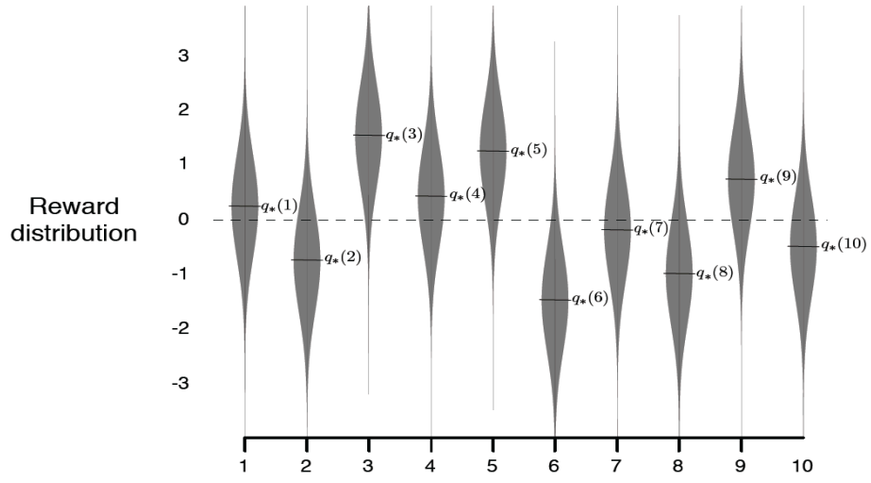


- If an algorithm forever explores it will have linear total regret
- If an algorithm never explores it will have linear total regret

Average reward for three algorithms

We sample 10 arm bandits instantiations:

$$q_*(a) \sim \mathcal{N}(0, 1)$$
$$R_t \sim \mathcal{N}(q_*(a), 1)$$



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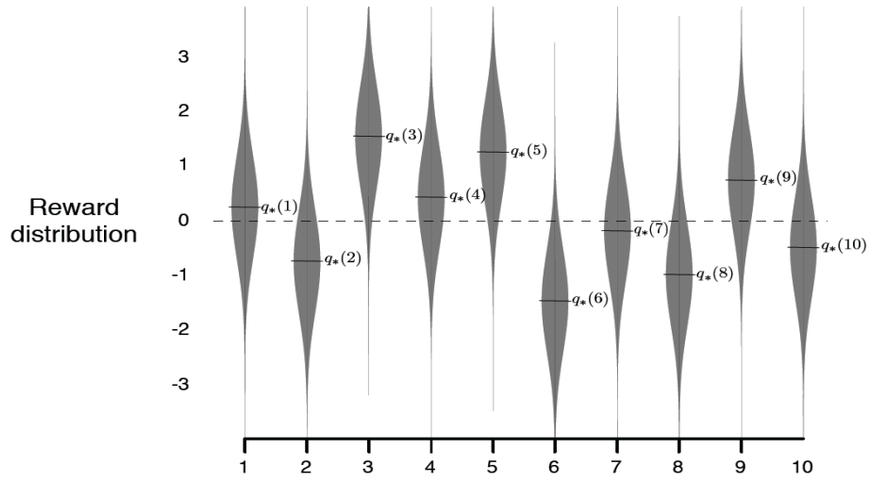

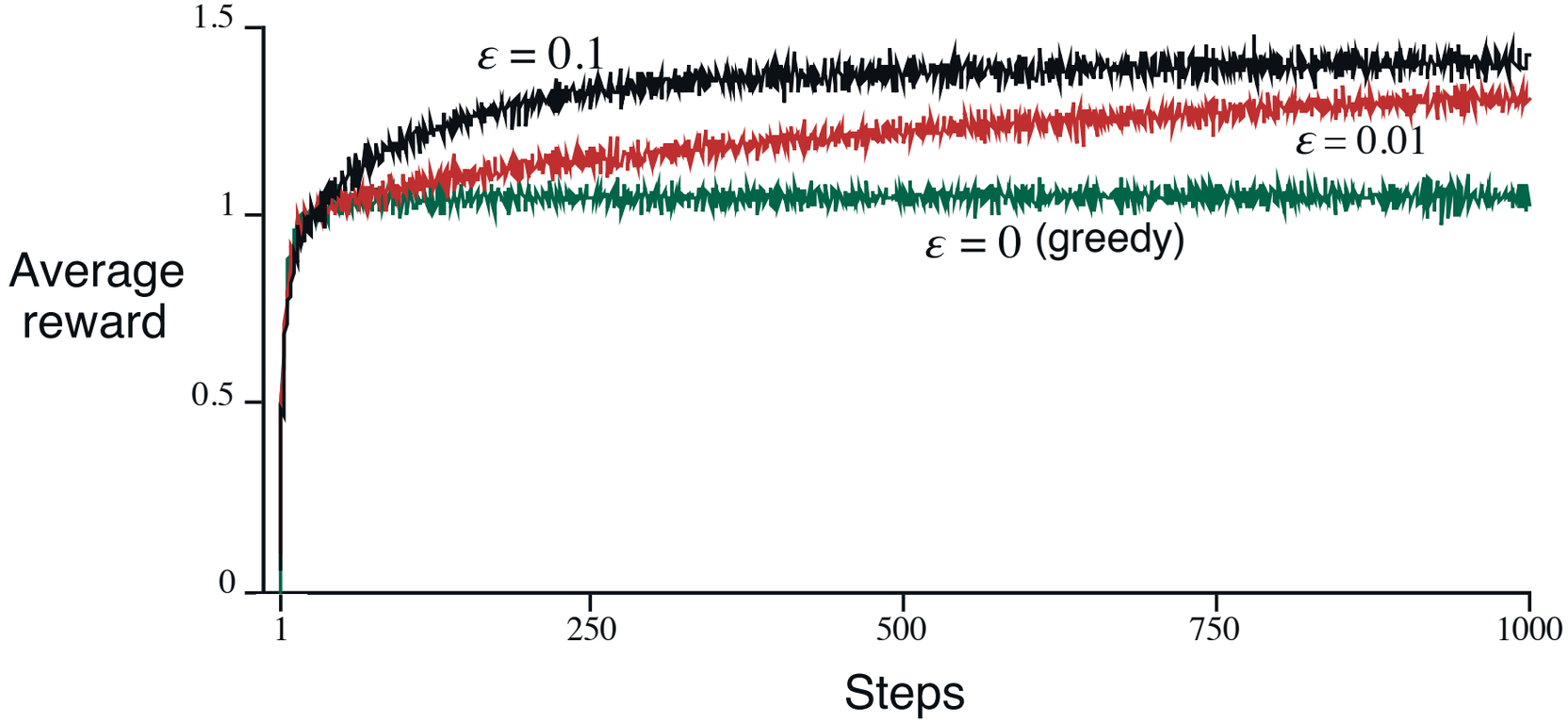

Q: In the limit (after infinite number of steps), which method will result in the largest average reward?

Optimal action for three algorithms

We sample 10 arm bandits instantiations:

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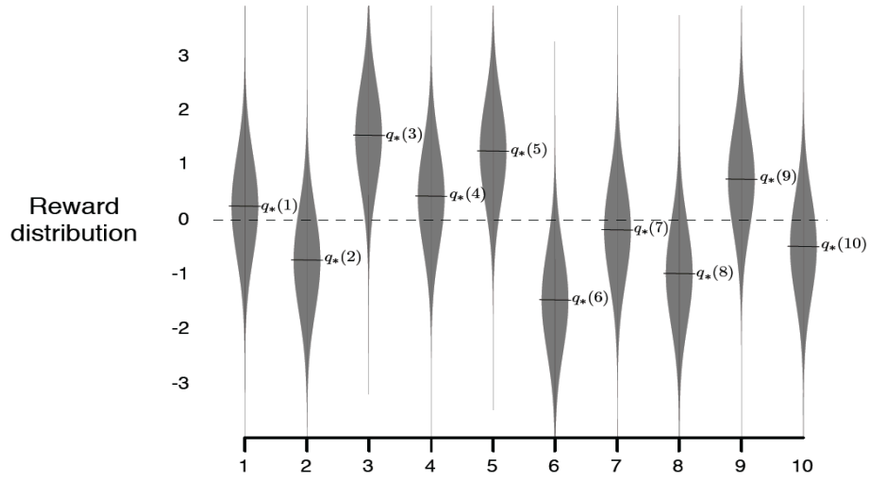

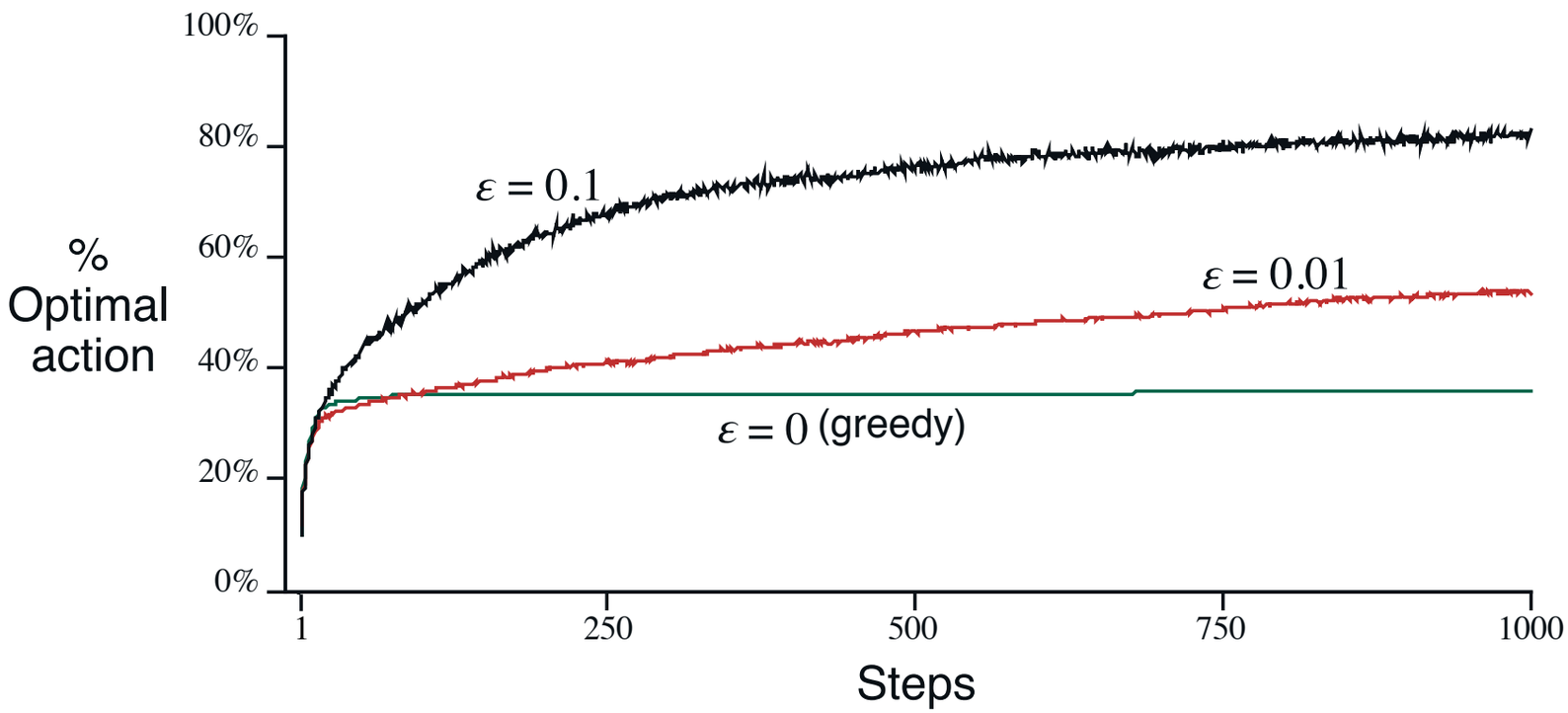

Q: Which method will find the optimal action in the limit?

Optimal action for three algorithms

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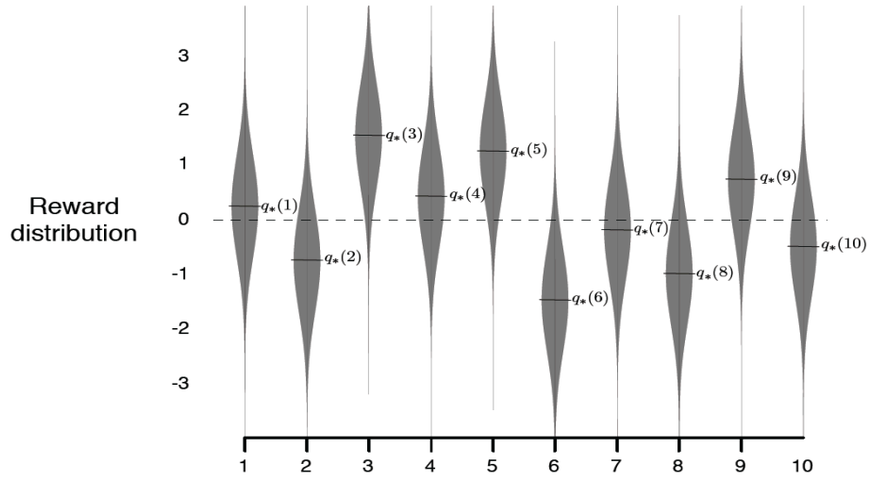
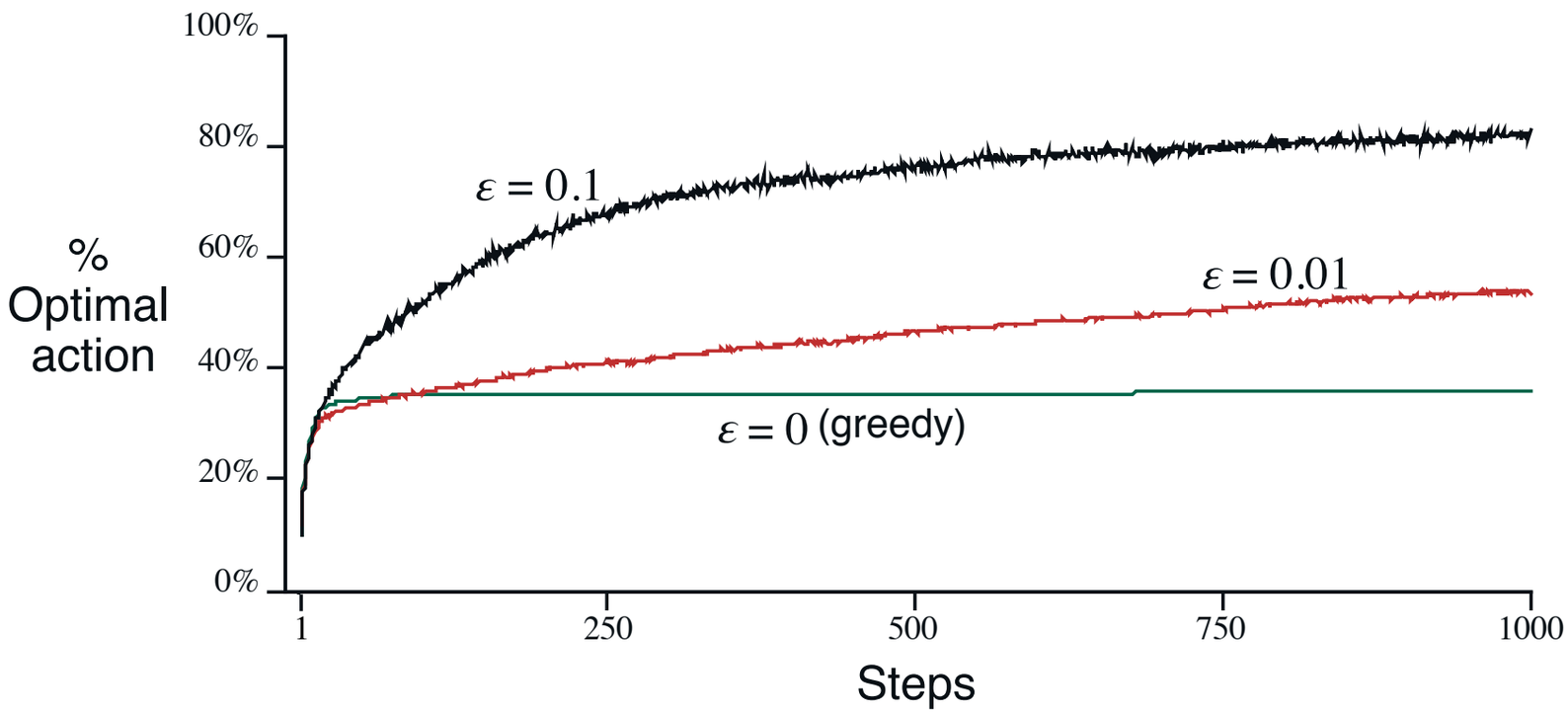




Q: Does the performance of those methods depend on the initialization of the action value estimates?

Optimistic Initialization

- Simple and practical ideas: initialise $Q(a)$ to a high value
- Update action value by incremental Monte-Carlo evaluation
- Starting with $N(a) > 0$,

$$Q_t(a_t) = Q_{t-1}(a_t) + \frac{1}{N_t(a_t)}\left(r_t - Q_{t-1}(a_t)\right)$$

just an incremental estimate of sample mean, including one 'hallucinated' initial optimistic value

- Encourages systematic exploration early on
- But optimistic greedy can still lock onto a suboptimal action if rewards are stochastic.

Optimistic Initial Values

We initialize with the following reward estimates for Bernoulli bandits

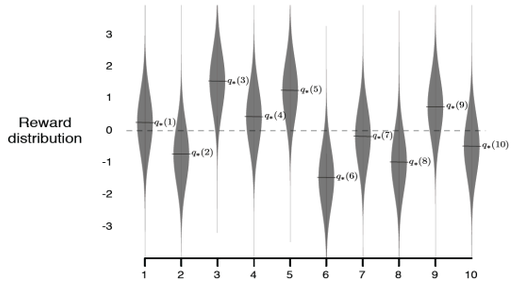
$Q_t(a_1) = 1$ $Q_t(a_2) = 1$ $Q_t(a_3) = 1$

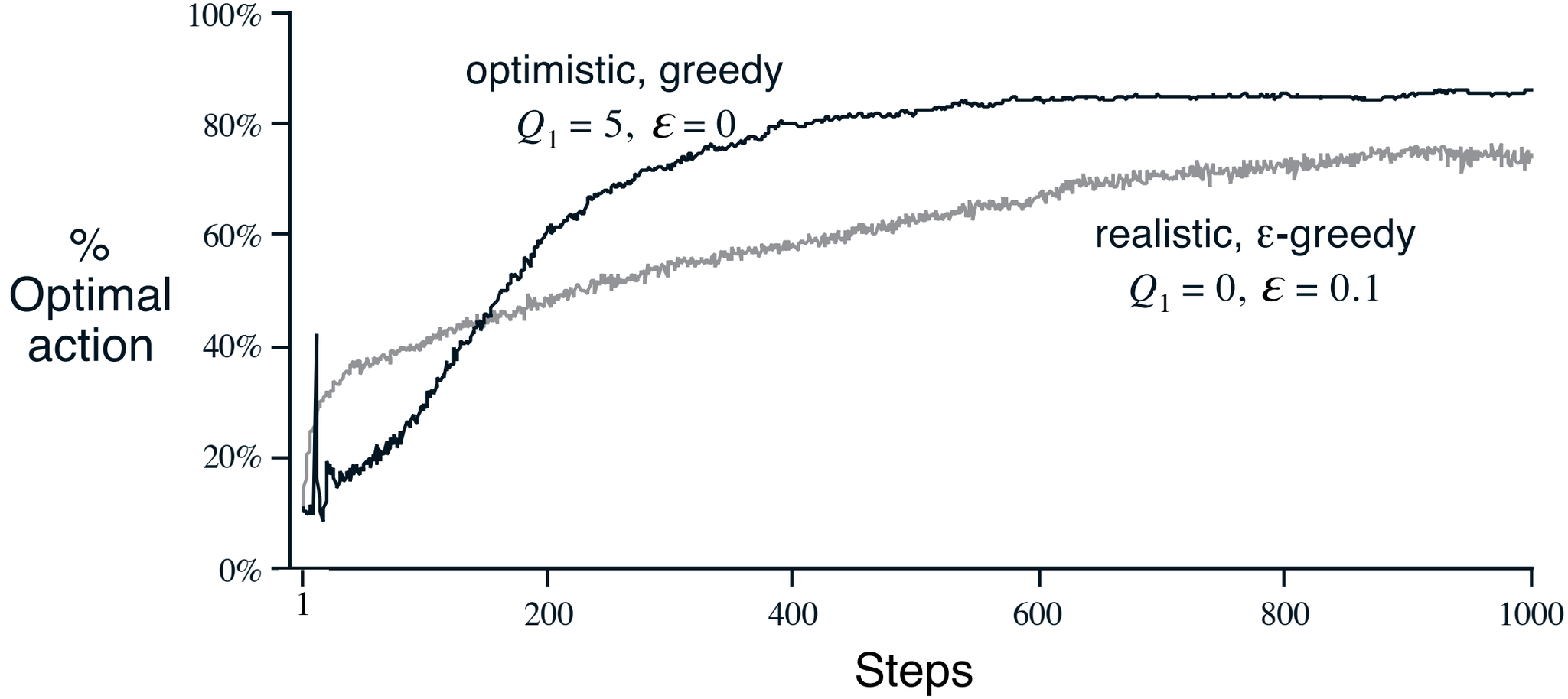
Q: When it is possible that greedy action selection will not try out all the actions?

Optimistic Initial Values

- Suppose we initialize the action values optimistically ($Q_1(a) = 5$), e.g., on the 10-armed testbed

$$q_*(a) \sim \mathcal{N}(0, 1)$$
$$R_t \sim \mathcal{N}(q_*(a), 1)$$





Achieving sub-linear total regret

We need to reason about **uncertainty** of our action value estimates

1000 pulls,
600 wins
Q_t(a_1)=0.6

1000 pulls,
400 wins
Q_t(a_2)=0.4

10 pulls,
4 wins
Q_t(a_1)=0.4

Epsilon-greedy

Repeat forever:

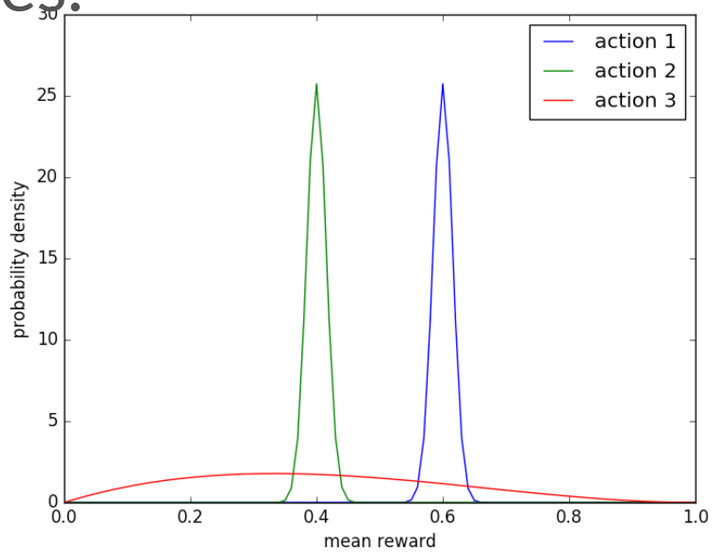
$$A \leftarrow \begin{cases} \arg\max_a Q(a) & \text{with probability } 1-\varepsilon \quad \text{(breaking ties randomly)} \\ \text{a random action} & \text{with probability } \varepsilon \end{cases}$$

$R \leftarrow bandit(A)$

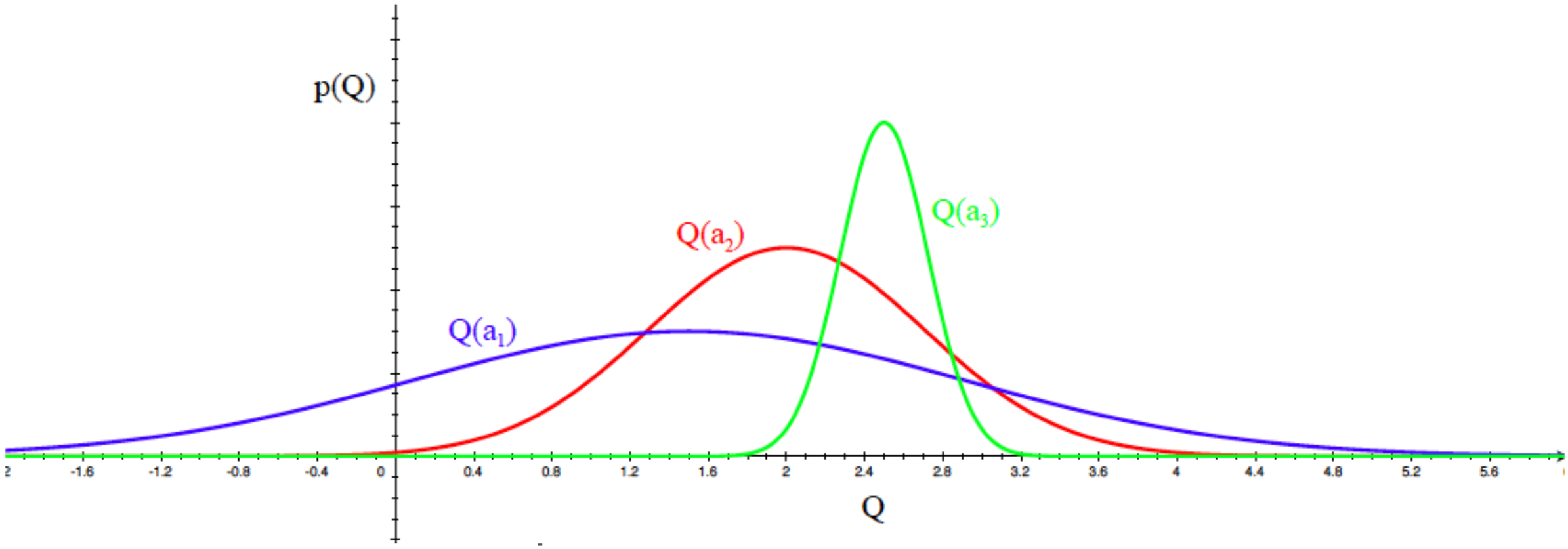
$N(A) \leftarrow N(A) + 1$

$Q(A) \leftarrow Q(A) + \frac{1}{N(A)}\left[R - Q(A)\right]$

The problem with using mean estimates is that we do not reason about uncertainty of those estimates.

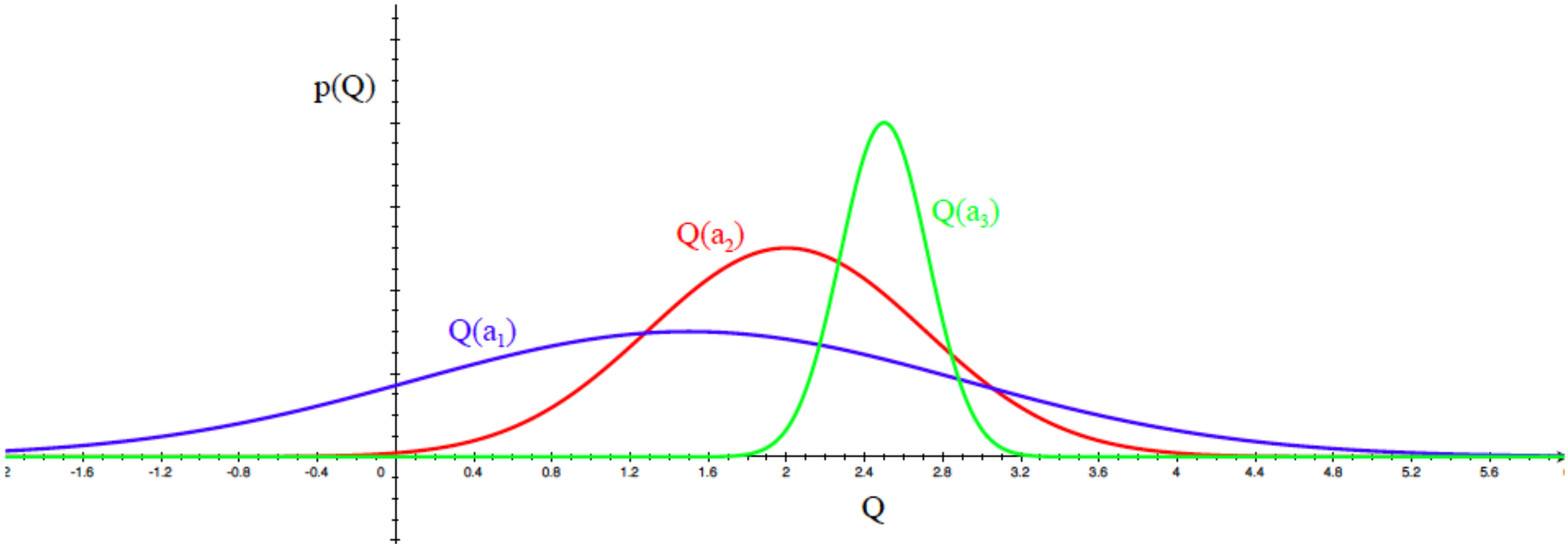


Uncertainty guides Exploration



- 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

Uncertainty guides Exploration



- We are then less uncertain about the value
- And more likely to pick another action
- Until we converge to the best action

Upper Confidence Bounds

- Estimate an upper confidence $U_t(a)$ for each action value
- Such that with high probability

$$q_*(a) \leq Q_t(a) + U_t(a)$$

Estimated mean

Estimated Upper Confidence

- This upper confidence depends on the number of times 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)
- Select action maximizing Upper Confidence Bound (UCB)

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

Upper Confidence Bound (UCB)

- A clever way of reducing exploration over time
- Estimate an upper bound on the true action values
- Select the action with the largest (estimated) upper bound

$$A_t \doteq \arg\max_a \left[Q_t(a) + c\sqrt{\frac{\log t}{N_t(a)}} \right]$$

- c is a hyper-parameter that trades-off explore/exploit
- the confidence bound grows with the total number of actions we have taken t but shrinks with the number of times we have tried this particular action $N_t(a)$. This ensures each action is tried infinitely often but still balances exploration and exploitation.

UCB1: Auer, Cesa-bianchi, and Fischer, Finite-time analysis of the multiarmed bandit problem, 2002

Upper Confidence Bound (UCB)

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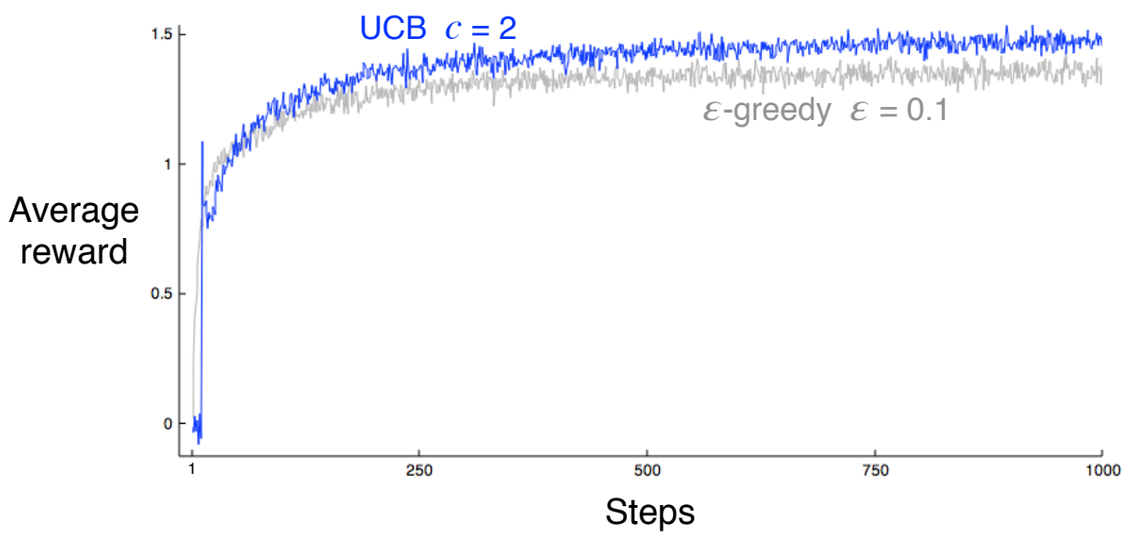


UCB1: Auer, Cesa-bianchi, and Fischer, Finite-time analysis of the multiarmed bandit problem, 2002

UCB1 regret bound

- The regret of UCB1 at a rate of $\ln t$. After t actions it is at most:

$$\sum_{i=1}^{K} \frac{4 \ln t}{\Delta_i} + (1 + \frac{\pi^2}{3})\Delta_i$$

where $\Delta_i = \mu * - \mu_i$

UCB1: Auer, Cesa-bianchi, and Fischer, Finite-time analysis of the multiarmed bandit problem, 2002

Bayesian Bandits

- So far we have made no assumptions about the reward distributions.
  - In UCB we just considered some bounds on rewards
- Bayesian bandits exploit prior knowledge of rewards, $p\left[\mathcal{R}\right]$
- They compute posterior distribution of rewards $p\left[\mathcal{R} \mid h_t\right]$

$$h_t = a_1, r_1, \ldots, a_{t-1}, r_{t-1}$$

- Use posterior to guide exploration: we simply sample from the posterior!

Bayesian learning for model parameters

Step 1: Given n data, $D = x_{1\ldots n} = \{x_1, x_2, \ldots, x_n\}$ write down the expression for likelihood:

$$p(D \mid \theta)$$

Step 2: Specify a prior: $p(\theta)$

Step 3: Compute the posterior:

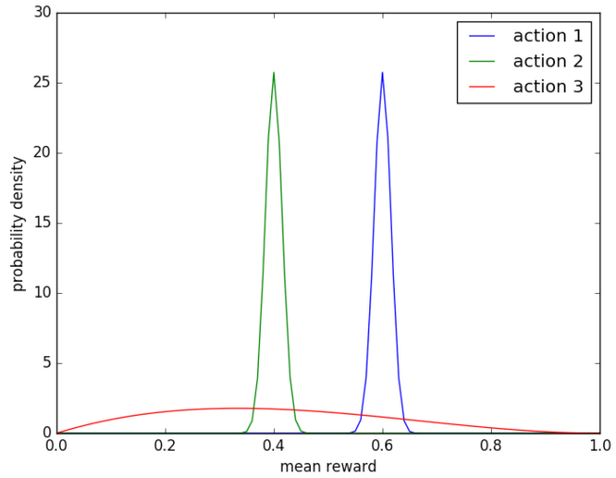
$$p(\theta \mid D) = \frac{p(D \mid \theta)p(\theta)}{p(D)}$$

Thompson Sampling

Represent a distribution for the mean reward of each bandit as opposed to its mean estimate alone. At each timestep:

1. Sample from the reward distribution:
$$\bar{\theta}_1 \sim \hat{p}(\theta_1), \bar{\theta}_2 \sim \hat{p}(\theta_2), \cdots, \bar{\theta}_k \sim \hat{p}(\theta_k)$$

2. Choose action $a = \arg\max_a \mathbb{E}_{\bar{\theta}}[r(a)]$



3. Observe the reward

4. Update the mean reward posterior distributions: $\hat{p}(\theta_1), \hat{p}(\theta_2) \cdots \hat{p}(\theta_k)$

Q: why we use argmax in step 2 and we do not add any noise?

Bernoulli bandits - Prior

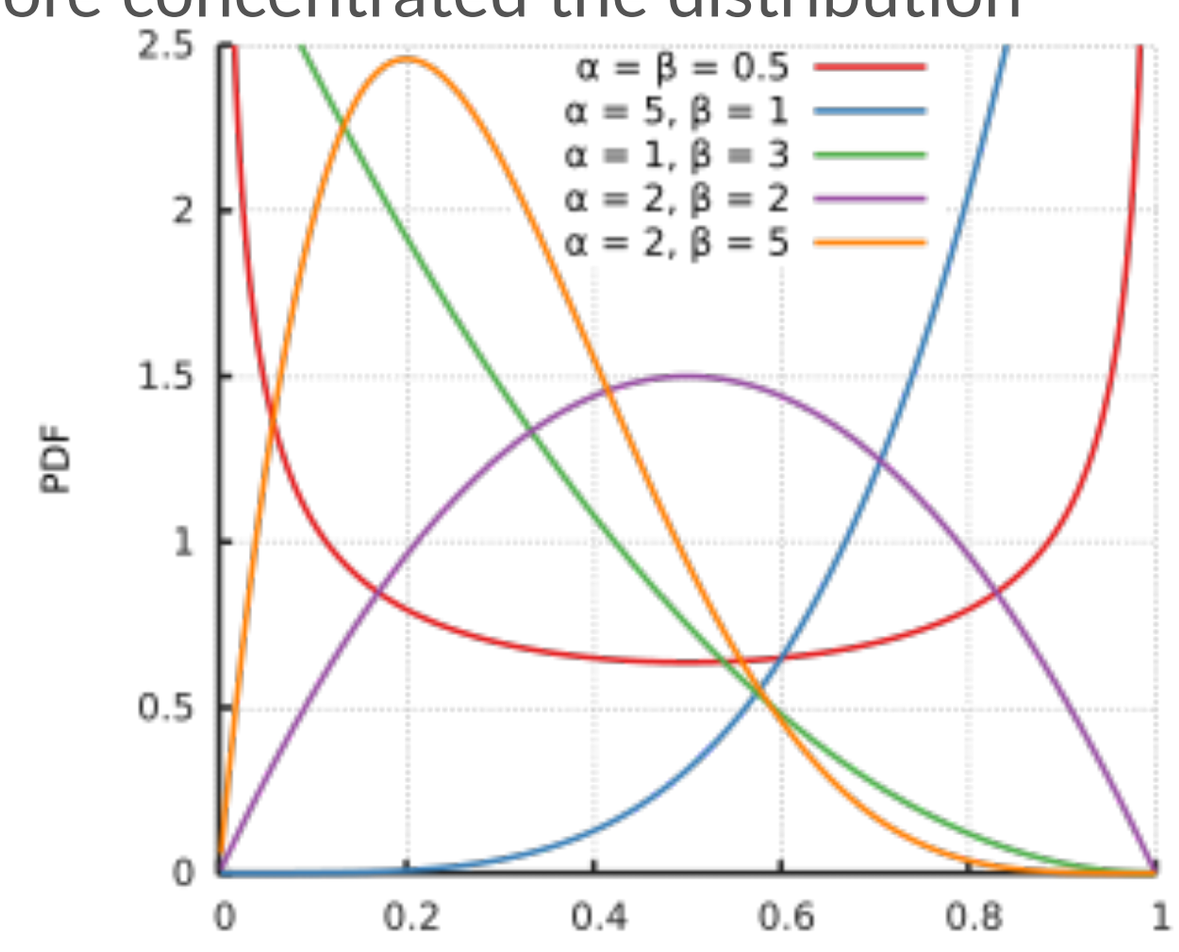
Let's consider a Beta distribution prior over the mean rewards of the Bernoulli bandits:

$$p(\theta_k) = \frac{\Gamma(\alpha_k + \beta_k)}{\Gamma(\alpha_k)\Gamma(\beta_k)} \theta_k^{\alpha_k - 1}(1 - \theta_k)^{\beta_k - 1} \qquad \Gamma(n) = (n-1)!$$

The mean is $\frac{\alpha}{\alpha + \beta}$

The larger the $\alpha + \beta$ the more concentrated the distribution

$\text{Beta}(\alpha, \beta)$



Bernoulli bandits-Posterior

Let's consider a Beta distribution prior over the mean rewards of the Bernoulli bandits:

$$p(\theta_k) = \frac{\Gamma(\alpha_k + \beta_k)}{\Gamma(\alpha_k)\Gamma(\beta_k)} \theta_k^{\alpha_k - 1}(1 - \theta_k)^{\beta_k - 1} \qquad \Gamma(n) = (n-1)!$$

The posterior is also a Beta! Because beta is conjugate distribution for the Bernoulli distribution.

A closed form solution for the bayesian update, possible only for conjugate distributions!

$$(\alpha_k, \beta_k) \leftarrow \begin{cases} (\alpha_k, \beta_k) & \text{if } x_t \neq k \\ (\alpha_k, \beta_k) + (r_t, 1 - r_t) & \text{if } x_t = k. \end{cases}$$

Greedy VS Thompson for Bernoulli bandits

a: success
b: failure

Algorithm 1 BernGreedy(K, α, β)

for $t = 1, 2, \ldots$ **do**
  #estimate model:
  for $k = 1, \ldots, K$ **do**
    $\hat{\theta}_k \leftarrow \alpha_k/(\alpha_k + \beta_k)$
  end for

  #select and apply action:
  $x_t \leftarrow \text{argmax}_k \hat{\theta}_k$
  Apply x_t and observe r_t

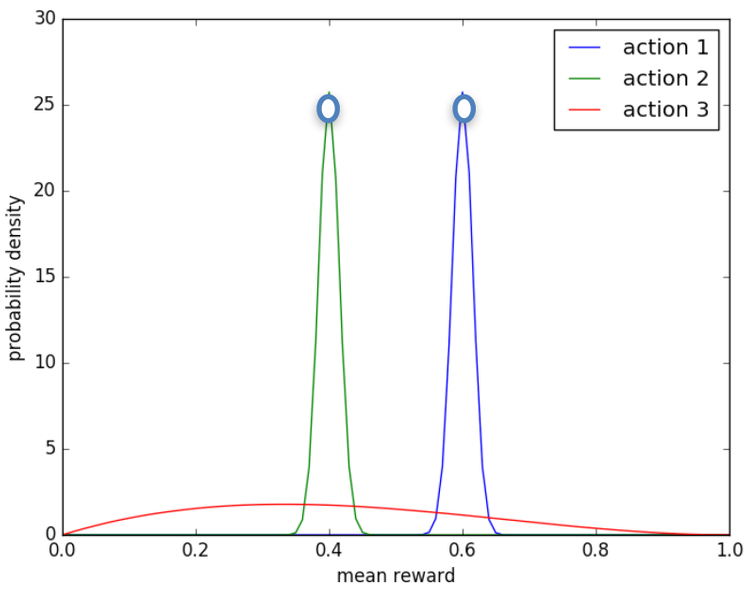
  #update distribution:
  $(\alpha_{x_t}, \beta_{x_t}) \leftarrow (\alpha_{x_t}, \beta_{x_t}) + (r_t, 1 - r_t)$
end for

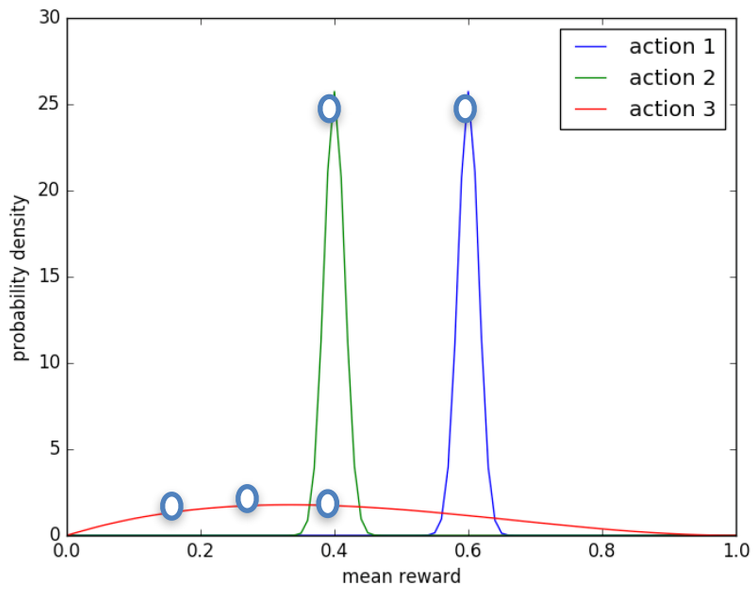
Algorithm 2 BernThompson(K, α, β)

for $t = 1, 2, \ldots$ **do**
  #sample model:
  for $k = 1, \ldots, K$ **do**
    Sample $\hat{\theta}_k \sim \text{beta}(\alpha_k, \beta_k)$
  end for

  #select and apply action:
  $x_t \leftarrow \text{argmax}_k \hat{\theta}_k$
  Apply x_t and observe r_t

  #update distribution:
  $(\alpha_{x_t}, \beta_{x_t}) \leftarrow (\alpha_{x_t}, \beta_{x_t}) + (r_t, 1 - r_t)$
end for





Contextive Bandits (a.k.a Associative Search)

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

Bayesian Bandits VS A/B Hypothesis testing

- Given two actions, A,B, traditional hypothesis testing would require to gather enough samples to decide whether a preference of A versus B is statistically significant.

- Bayesian bandits adapt the actions over time based on the rewards seen thus far: they accomplish smaller cumulative regret

https://analytics.googleblog.com/2013/01/multi-armed-bandit-experiments.html

Real world motivation: Personalized NETFLIX artwork

For a particular title and a particular user, we will use the contextual multi-armed bandit formulation to decide what image to show per title per user

- Actions: uploading an image (available for this movie title) to a user's home screen
- Mean rewards (unknown): the % of NETFLIX users that will click on the title and watch the movie
- Estimated mean rewards: the average click rate (+quality engagement, not clickbait)
- Context (s) : user attributes, e.g., language preferences, gender of films she has watched, time and day of the week, etc.

Netflix Artwork:https://medium.com/netflix-techblog/artwork-personalization-c589f074ad76

Question: was there a train and test phase on our multi-armed bandit algorithms?

No, the setup we explored was: given a set of K arms, how do we select actions to minimize our cumulative regret.

Q: what would be the learning based equivalent of the multi-armed bandit problem?

A:

- We have a training set of N multi-armed bandit instantiations.
- Each K-armed bandit is one training example.
- The agent gets n number of interactions, and obtains a final reward (-regret).
- The agent learns a policy —mapping from its set of actions taken thus far and their outcomes, to a probability over what actions to try next

We will visit this setup in the meta-learning lecture.