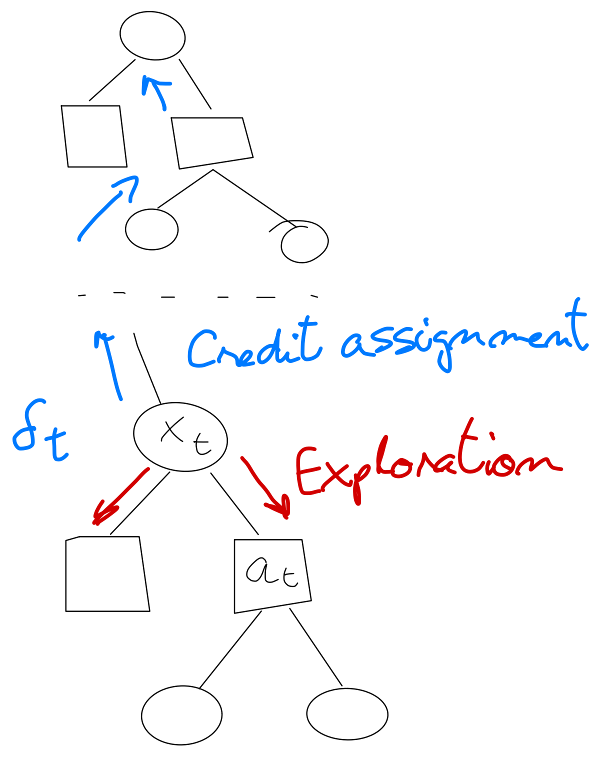
Multi-arm Bandits

Sutton and Barto, Chapter 2

The simplest
reinforcement learning
problem

Recall: Sequential Decision Making

- At time t, agent receives an observation from set $\mathcal{X}$ and can choose an action from set $\mathcal{A}$ (think finite for now)
- Goal of the agent is to maximize long-term return



Simple case: One step!

- No x, take an action, observe a reward immediately
- So, a degenerate tree (not truly sequential)
- This is what we call a simple bandit problem
- No credit assignment, only exploration / exploitation
- Later: contextual bandits (there's x, feedback still immediate)
- Lots of applications in ad placement, more recently in large language models

What is a bandit?

- The simplest kind of structure: every node is a copy of every other node, and they are not connected!
- Which means there are no delayed action effects, simplifying credit assignment!
- Therefore, the main problem in bandits is exploration
- Vanilla multi-arm bandits: nodes do not have any observation
- Contextual bandits have observations (more on that later)

Let's play a bandit!

- Imagine you have two actions
- You play action 1 and get a reward of 0
- You play action 2 and get a reward of 1
- Which action should you prefer?
- Which action should you try next?

Let's play a bandit!

- Imagine you have two actions
- You played action 1 three times and got rewards of 0, 1, -1
- You played action 2 three times and got a rewards of 1, 10, -10
- Which action should you prefer?
- Which action should you try next?

Let's play a bandit!

- Imagine you have two actions
- You played action 1 for 300 times and got rewards of 0 (200 times), 1 (50 times), -1 (50 times)
- You played action 2 for 300 times and got a rewards of 1 (200 times), 10 (50 times), -10 (50 times)
- Which action should you prefer?
- Which action should you try next?

Let's play a bandit!

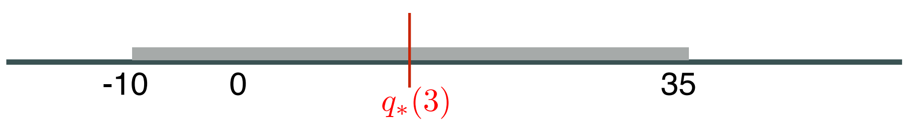
- Imagine you have two actions
- You played action 1 for 3000 times and got rewards of 0 (300 times), 1 (2000 times), -1 (600 times), +10 (100 times)
- You played action 2 for 3000 times and got a rewards of 1 (2000 times), 10 (1000 times), -10 (1000 times)
- Which action should you prefer?
- Which action should you try next?

Main Principles

- Optimize Expected Value
- Other criteria are possible, eg conditional value at risk (CVaR)
- Need to balance exploration (trying all actions) vs exploitation
- Reduce uncertainty in the mean of each action

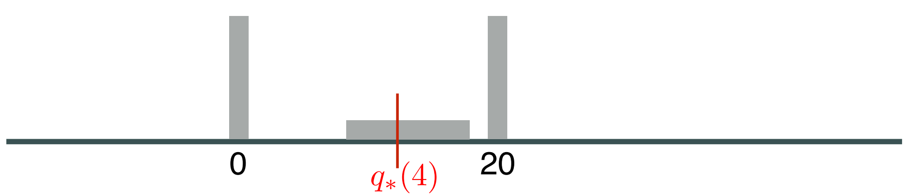
You are the algorithm! (bandit1)

- Action 1 — Reward is always 8
  - value of action 1 is $q_*(1) =$
- Action 2 — 88% chance of 0, 12% chance of 100!
  - value of action 2 is $q_*(2) = .88 \times 0 + .12 \times 100 =$
- Action 3 — Randomly between -10 and 35, equiprobable



$q_*(3) =$

- Action 4 — a third 0, a third 20, and a third from {8,9,…, 18}



$q_*(4) =$

The *k*-armed Bandit Problem

- On each of an infinite sequence of *time steps*, t=1, 2, 3, …, you choose an action A_t from k possibilities, and receive a real-valued *reward* R_t

- The reward depends only on the action taken; it is identically, independently distributed (i.i.d.):

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

- These true values are *unknown*. The distribution is unknown

- Nevertheless, you must maximize your total reward

- You must both try actions to learn their values (explore), and prefer those that appear best (exploit)

The Exploration/Exploitation Dilemma

- Suppose you form estimates

$$Q_t(a) \approx q_*(a), \quad \forall a$$ *action-value estimates*

- Define the *greedy action* at time *t* as

$$A_t^* \doteq \arg\max_a Q_t(a)$$

- If $A_t = A_t^*$ then you are *exploiting*
  If $A_t \neq A_t^*$ then you are *exploring*

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

- You can never stop exploring, but maybe you should explore less with time. Or maybe not.

Action-Value Methods

- Methods that learn action-value estimates and nothing else
- For example, estimate action values as *sample averages*:

$$Q_t(a) \doteq \frac{\text{sum of rewards when } a \text{ taken prior to } t}{\text{number of times } a \text{ taken prior to } t} = \frac{\sum_{i=1}^{t-1} R_i \cdot \mathbf{1}_{A_i=a}}{\sum_{i=1}^{t-1} \mathbf{1}_{A_i=a}}$$

- The sample-average estimates converge to the true values *If* the action is taken an infinite number of times

$$\lim_{N_t(a)\to\infty} Q_t(a) = q_*(a)$$

The number of times action a has been taken by time t

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

A simple bandit algorithm

Initialize, for $a = 1$ to k:

$Q(a) \leftarrow 0$

$N(a) \leftarrow 0$

Repeat forever:

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

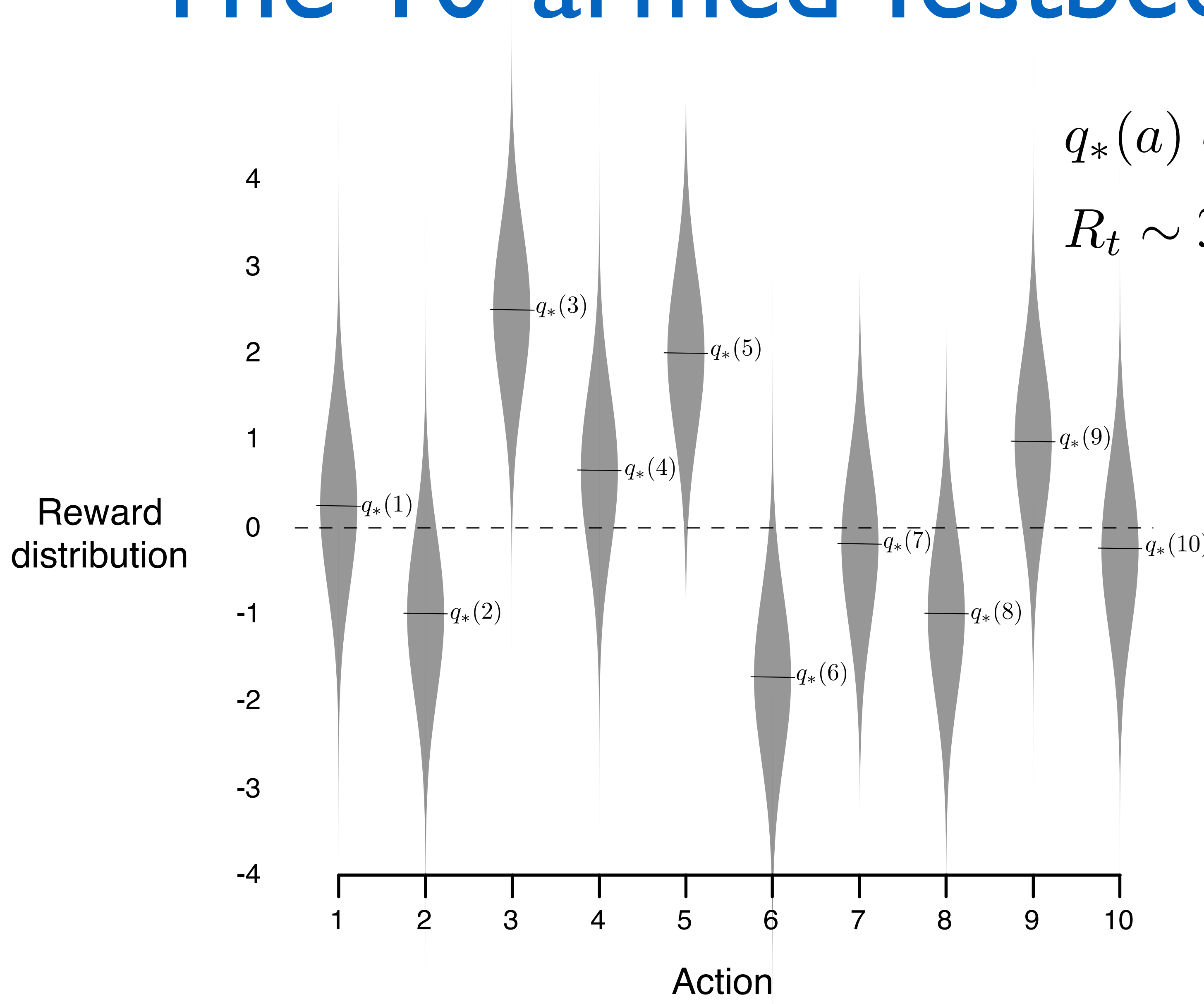
$R \leftarrow bandit(A)$

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

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

One Bandit Task from

The 10-armed Testbed



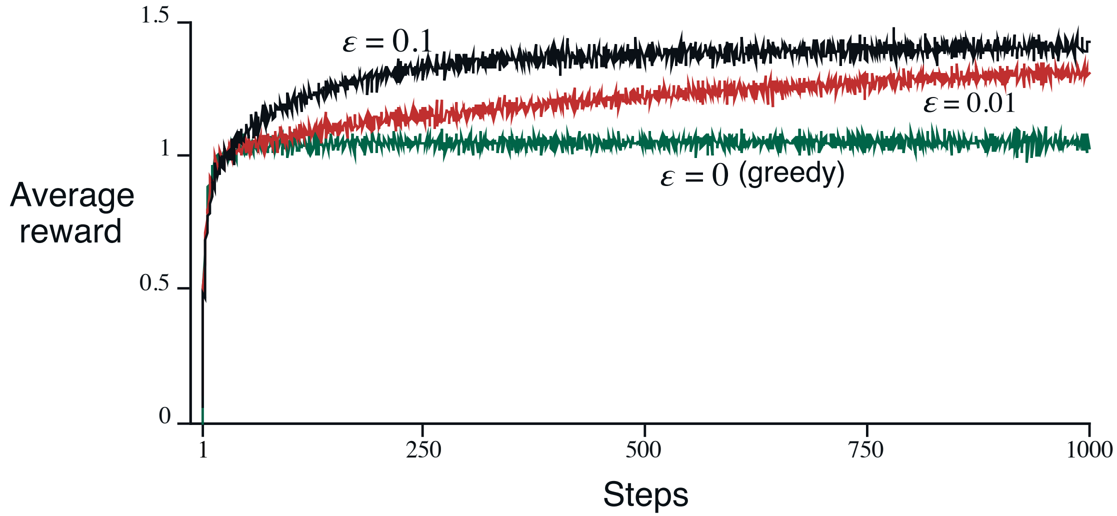
$$q_*(a) \sim \mathcal{N}(0, 1)$$

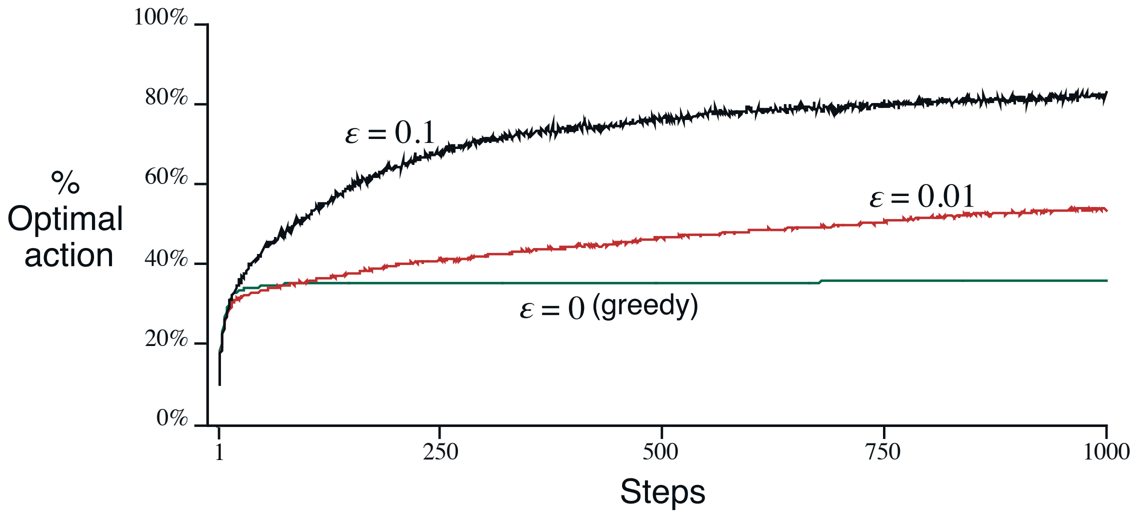
$$R_t \sim \mathcal{N}(q_*(a), 1)$$

Run for 1000 steps

Repeat the whole thing 2000 times with different bandit tasks

ε-Greedy Methods on the 10-Armed Testbed





Averaging $\longrightarrow$ learning rule

- 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:

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

Derivation of incremental update

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

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

Averaging $\longrightarrow$ learning rule

- 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:

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

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

Tracking a Non-stationary Problem

- Suppose the true action values change slowly over time
  - then we say that the problem is *non-stationary*
- In this case, sample averages are not a good idea (Why?)
- Better is an "exponential, recency-weighted average":

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

where α is a constant *step-size parameter*, $\alpha \in (0, 1]$

- There is bias due to Q_1 that becomes smaller over time

Standard stochastic approximation convergence conditions

- To assure convergence with probability 1:

$$\sum_{n=1}^{\infty} \alpha_n(a) = \infty \qquad \text{and} \qquad \sum_{n=1}^{\infty} \alpha_n^2(a) < \infty$$

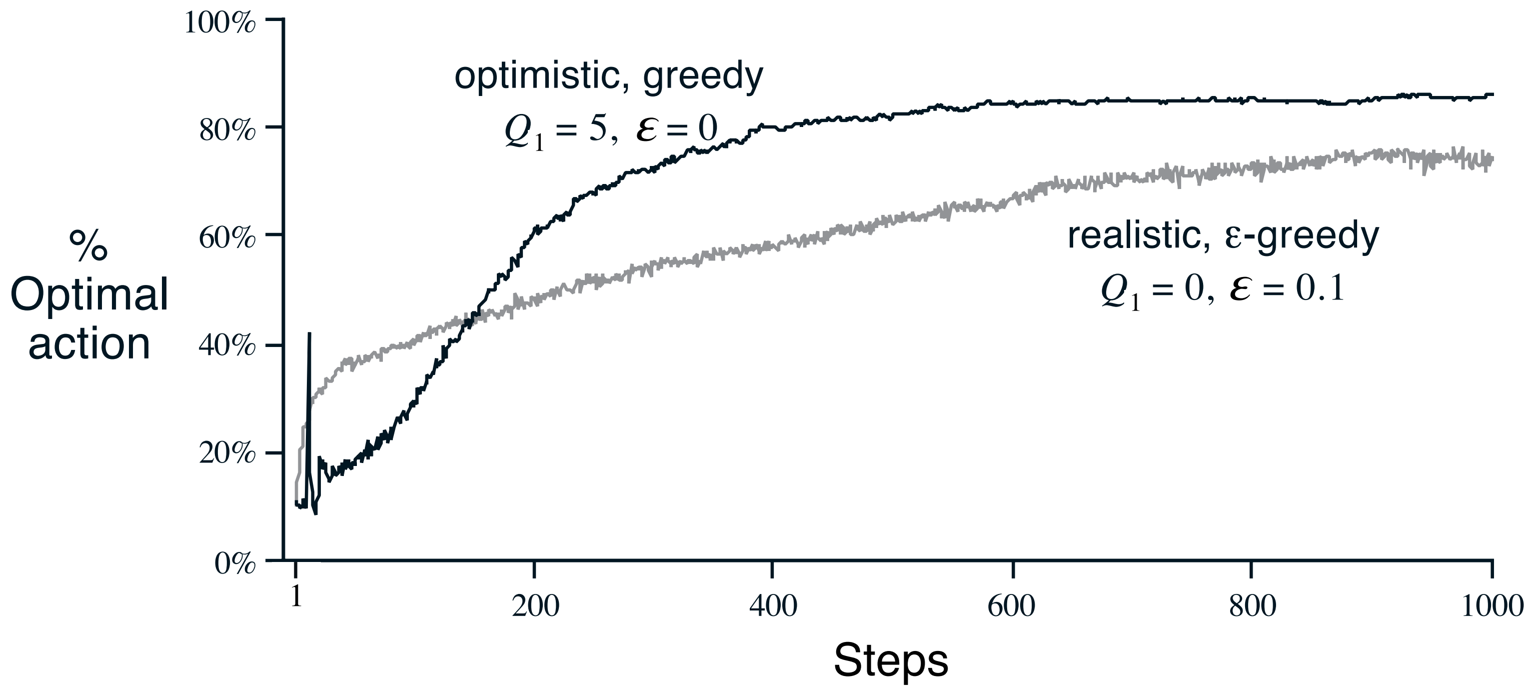
- e.g., $\alpha_n \doteq \frac{1}{n}$
- not $\alpha_n \doteq \frac{1}{n^2}$

if $\alpha_n \doteq n^{-p}, \quad p \in (0,1)$
then convergence is
at the optimal rate:
$O(1/\sqrt{n})$

Optimistic Initial Values

- All methods so far depend on $Q_1(a)$, i.e., they are biased. So far we have used $Q_1(a) = 0$

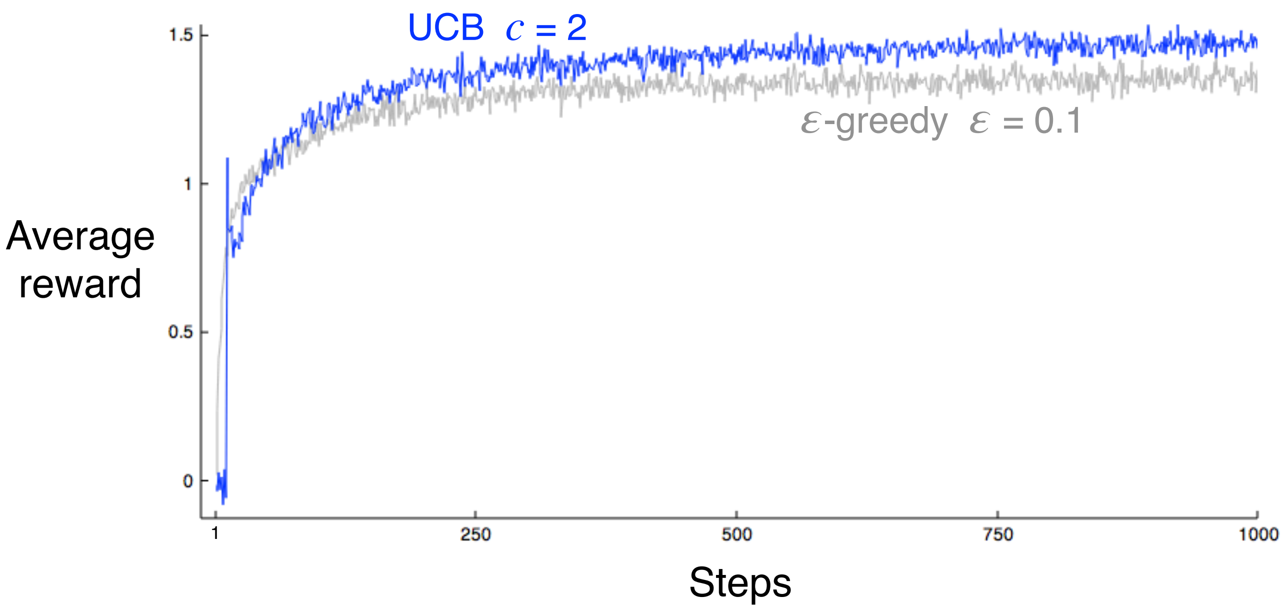
- Suppose we initialize the action values *optimistically* ($Q_1(a) = 5$), e.g., on the 10-armed testbed (with $\alpha = 0.1$)



Upper Confidence Bound (UCB) action selection

- 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

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



Gradient-Bandit Algorithms

- Let $H_t(a)$ be a learned *preference* for taking action a

$$\Pr\{A_t = a\} \doteq \frac{e^{H_t(a)}}{\sum_{b=1}^{k} e^{H_t(b)}} \doteq \pi_t(a)$$

Note that this allows us to work with unnormalized preferences and turn them into probabilities!

Same idea as using potentials in graphical models

Gradient-Bandit Algorithms

- Let $H_t(a)$ be a learned *preference* for taking action a

$$\Pr\{A_t = a\} \doteq \frac{e^{H_t(a)}}{\sum_{b=1}^{k} e^{H_t(b)}} \doteq \pi_t(a)$$

$$H_{t+1}(A_t) \doteq H_t(A_t) + \alpha\big(R_t - \bar{R}_t\big)\big(1 - \pi_t(A_t)\big)$$

$$\bar{R}_t \doteq \frac{1}{t}\sum_{i=1}^{t} R_i$$

Gradient-Bandit Algorithms

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$$H_{t+1}(a) \doteq H_t(a) + \alpha\big(R_t - \bar{R}_t\big)\big(\mathbf{1}_{a=A_t} - \pi_t(a)\big), \qquad \forall a,$$

$$\bar{R}_t \doteq \frac{1}{t}\sum_{i=1}^{t} R_i$$

Gradient-Bandit Algorithms

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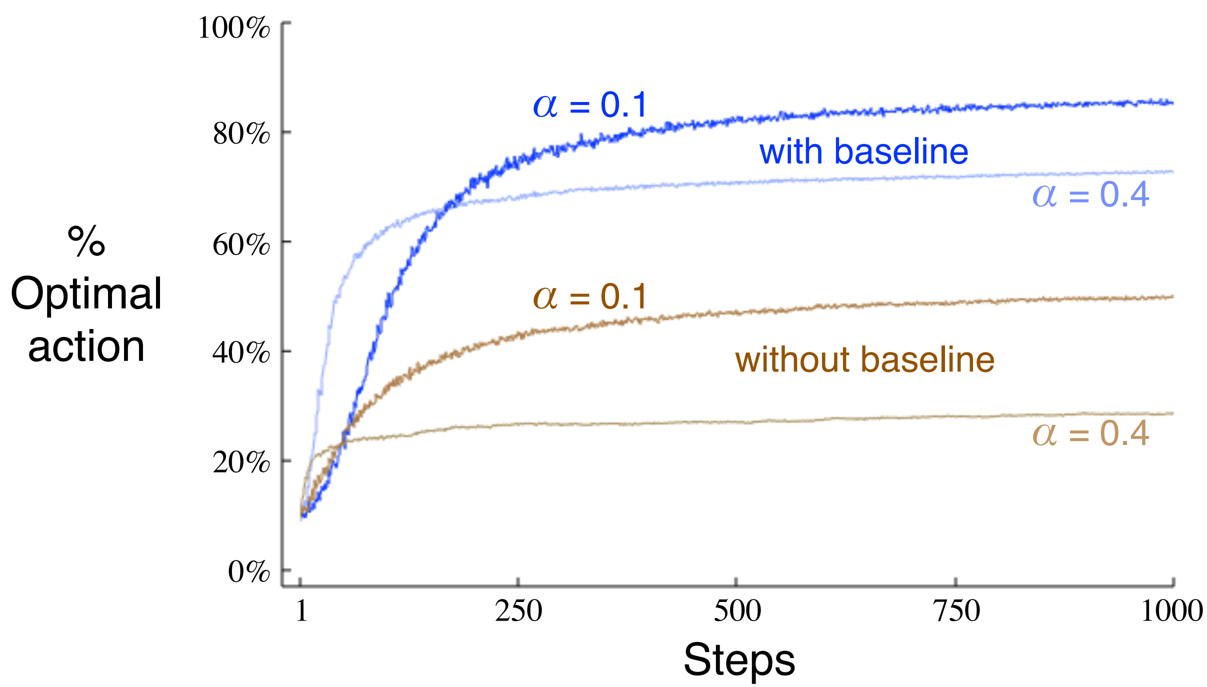

Derivation of gradient-bandit algorithm

In exact *gradient ascent*:

$$H_{t+1}(a) \doteq H_t(a) + \alpha \frac{\partial \mathbb{E}\left[R_t\right]}{\partial H_t(a)}, \tag{1}$$

where:

$$\mathbb{E}[R_t] \doteq \sum_b \pi_t(b) q_*(b),$$

$$\begin{aligned}
\frac{\partial \mathbb{E}[R_t]}{\partial H_t(a)} &= \frac{\partial}{\partial H_t(a)} \left[\sum_b \pi_t(b) q_*(b) \right] \\
&= \sum_b q_*(b) \frac{\partial \pi_t(b)}{\partial H_t(a)} \\
&= \sum_b \left(q_*(b) - X_t \right) \frac{\partial \pi_t(b)}{\partial H_t(a)},
\end{aligned}$$

where X_t does not depend on b, because $\sum_b \frac{\partial \pi_t(b)}{\partial H_t(a)} = 0$.

$$
\begin{aligned}
\frac{\partial\, \mathbb{E}[R_t]}{\partial H_t(a)} &= \sum_b \big(q_*(b) - X_t\big) \frac{\partial\, \pi_t(b)}{\partial H_t(a)} \\
&= \sum_b \pi_t(b) \big(q_*(b) - X_t\big) \frac{\partial\, \pi_t(b)}{\partial H_t(a)} / \pi_t(b) \\
&= \mathbb{E}\left[\big(q_*(A_t) - X_t\big) \frac{\partial\, \pi_t(A_t)}{\partial H_t(a)} / \pi_t(A_t) \right] \\
&= \mathbb{E}\left[\big(R_t - \bar{R}_t\big) \frac{\partial\, \pi_t(A_t)}{\partial H_t(a)} / \pi_t(A_t) \right],
\end{aligned}
$$

where here we have chosen $X_t = \bar{R}_t$ and substituted R_t for $q_*(A_t)$, which is permitted because $\mathbb{E}[R_t|A_t] = q_*(A_t)$.
For now assume: $\frac{\partial\, \pi_t(b)}{\partial H_t(a)} = \pi_t(b)\big(\mathbf{1}_{a=b} - \pi_t(a)\big)$. Then:

$$
\begin{aligned}
&= \mathbb{E}\big[\big(R_t - \bar{R}_t\big)\pi_t(A_t)\big(\mathbf{1}_{a=A_t} - \pi_t(a)\big)/\pi_t(A_t)\big] \\
&= \mathbb{E}\big[\big(R_t - \bar{R}_t\big)\big(\mathbf{1}_{a=A_t} - \pi_t(a)\big)\big].
\end{aligned}
$$

$$
H_{t+1}(a) = H_t(a) + \alpha\big(R_t - \bar{R}_t\big)\big(\mathbf{1}_{a=A_t} - \pi_t(a)\big), \text{ (from (1), QED)}
$$

Thus it remains only to show that

$$\frac{\partial \pi_t(b)}{\partial H_t(a)} = \pi_t(b)\big(\mathbf{1}_{a=b} - \pi_t(a)\big).$$

Recall the standard quotient rule for derivatives:

$$\frac{\partial}{\partial x}\left[\frac{f(x)}{g(x)}\right] = \frac{\frac{\partial f(x)}{\partial x} g(x) - f(x)\frac{\partial g(x)}{\partial x}}{g(x)^2}.$$

Using this, we can write...

Quotient Rule: $$\frac{\partial}{\partial x}\left[\frac{f(x)}{g(x)}\right] = \frac{\frac{\partial f(x)}{\partial x} g(x) - f(x)\frac{\partial g(x)}{\partial x}}{g(x)^2}$$

$$
\begin{aligned}
\frac{\partial \pi_t(b)}{\partial H_t(a)} &= \frac{\partial}{\partial H_t(a)} \pi_t(b) \\
&= \frac{\partial}{\partial H_t(a)} \left[\frac{e^{H_t(b)}}{\sum_{c=1}^{k} e^{H_t(c)}} \right] \\
&= \frac{\frac{\partial e^{H_t(b)}}{\partial H_t(a)} \sum_{c=1}^{k} e^{H_t(c)} - e^{H_t(b)} \frac{\partial \sum_{c=1}^{k} e^{H_t(c)}}{\partial H_t(a)}}{\left(\sum_{c=1}^{k} e^{H_t(c)}\right)^2} && \text{(Q.R.)} \\
&= \frac{\mathbf{1}_{a=b} e^{H_t(a)} \sum_{c=1}^{k} e^{H_t(c)} - e^{H_t(b)} e^{H_t(a)}}{\left(\sum_{c=1}^{k} e^{H_t(c)}\right)^2} && \left(\frac{\partial e^x}{\partial x} = e^x\right) \\
&= \frac{\mathbf{1}_{a=b} e^{H_t(b)}}{\sum_{c=1}^{k} e^{H_t(c)}} - \frac{e^{H_t(b)} e^{H_t(a)}}{\left(\sum_{c=1}^{k} e^{H_t(c)}\right)^2} \\
&= \mathbf{1}_{a=b} \pi_t(b) - \pi_t(b)\pi_t(a) \\
&= \pi_t(b)\big(\mathbf{1}_{a=b} - \pi_t(a)\big). && \text{(Q.E.D.)}
\end{aligned}
$$

Softmax (Boltzmann) Exploration

- Let $H_t(a)$ be a learned *preference* for taking action a

$$\Pr\{A_t = a\} \doteq \frac{e^{H_t(a)}}{\sum_{b=1}^{k} e^{H_t(b)}} \doteq \pi_t(a)$$

Consider $H_t(a) = Q_t(a)/T$

This is Boltzmann or softmax exploration!

If the temperature T is very large (towards infinity) - same as uniform

If temperature T goes to 0, same as greedy

Summary Comparison of Bandit Algorithms