Monte-Carlo Planning: Introduction and Bandit Basics

Alan Fern

Large Worlds

- We have considered basic model-based planning algorithms
- **Model-based planning**: assumes MDP model is available
  - Methods we learned so far are at least poly-time in the number of states and actions
  - Difficult to apply to large state and action spaces (though this is a rich research area)
- We will consider various methods for overcoming this issue

Approaches for Large Worlds

- **Planning with compact MDP representations**
  1. Define a language for compactly describing an MDP
     - MDP is exponentially larger than description
     - E.g. via Dynamic Bayesian Networks
  2. Design a planning algorithm that directly works with that language
- Scalability is still an issue
- Can be difficult to encode the problem you care about in a given language
- May study in last part of course

Approaches for Large Worlds

- **Reinforcement learning w/ function approx.**
  1. Have a learning agent directly interact with environment
  2. Learn a compact description of policy or value function

- Often works quite well for large problems

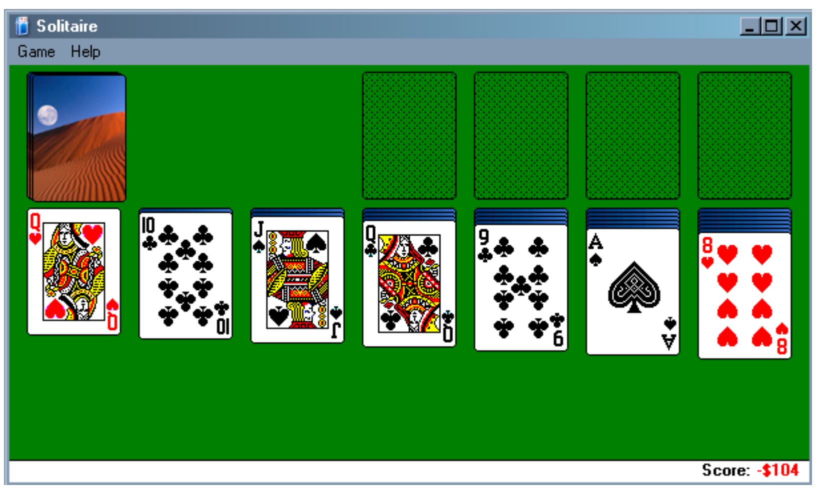
- Doesn't fully exploit a simulator of the environment when available

- We will study reinforcement learning later in the course

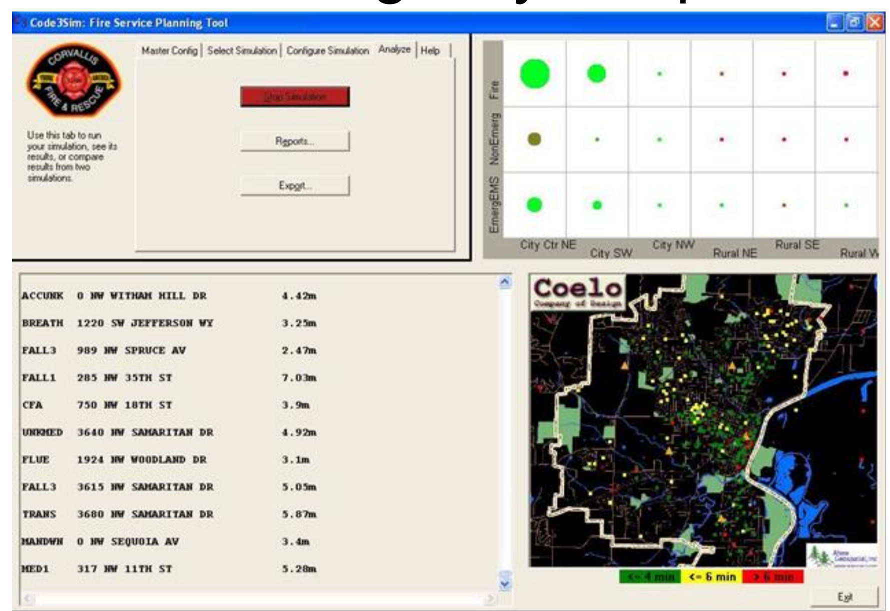
Approaches for Large Worlds: Monte-Carlo Planning

- Often a simulator of a planning domain is available or can be learned/estimated from data

Klondike Solitaire



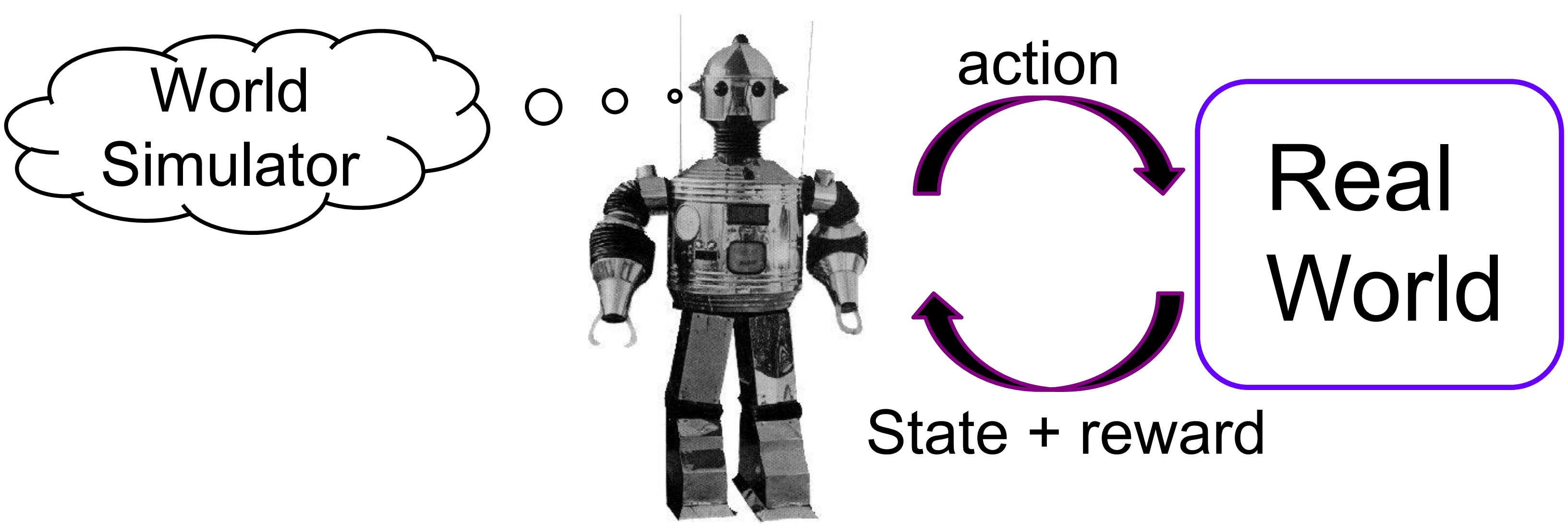
Fire & Emergency Response



Large Worlds: Monte-Carlo Approach

- Often a simulator of a planning domain is available or can be learned from data

- **<u>Monte-Carlo Planning</u>:** compute a good policy for an MDP by interacting with an MDP simulator



Example Domains with Simulators

- Traffic simulators
- Robotics simulators
- Military campaign simulators
- Computer network simulators
- Emergency planning simulators
  - large-scale disaster and municipal
- Forest Fire Simulator
- Board games / Video games
  - Go / RTS

In many cases Monte-Carlo techniques yield state-of-the-art performance. Even in domains where exact MDP models are available.

MDP: Simulation-Based Representation

- A simulation-based representation gives: S, A, R, T, I:
  - finite state set S (|S|=n and is generally very large)
  - finite action set A (|A|=m and will assume is of reasonable size)
- |S| is too large to provide a matrix representation of R, T, and I (see next slide for I)
- A simulation based representation provides us with callable functions for R, T, and I.
  - Think of these as any other library function that you might call
- Our planning algorithms will operate by repeatedly calling those functions in an intelligent way

MDP: Simulation-Based Representation

- A simulation-based representation gives: S, A, R, T, I:
  - finite state set S (|S|=n and is generally very large)
  - finite action set A (|A|=m and will assume is of reasonable size)
  - Stochastic, real-valued, bounded reward function R(s,a) = r
    - Stochastically returns a reward **r** given input s and a
      (note: here rewards can depend on actions and can be stochastic)
  - Stochastic transition function T(s,a) = s' (i.e. a simulator)
    - Stochastically returns a state **s'** given input s and a
    - Probability of returning **s'** is dictated by Pr(s' | s,a) of MDP
  - Stochastic initial state function I.
    - Stochastically returns a state according to an initial state distribution

These stochastic functions can be implemented in any language!

Pure Reinforcement Learning vs. Monte-Carlo Planning

- In pure reinforcement learning:
  - the agent begins with no knowledge
  - wanders around the world observing outcomes
- In Monte-Carlo planning
  - the agent begins with no declarative knowledge of the world
  - has an interface to a world simulator that allows observing the outcome of taking any action in any state
- The simulator gives the agent the ability to "teleport" to any state, at any time, and then apply any action
- A pure RL agent does not have the ability to teleport
  - Can only observe the outcomes that it happens to reach

Pure Reinforcement Learning vs. Monte-Carlo Planning

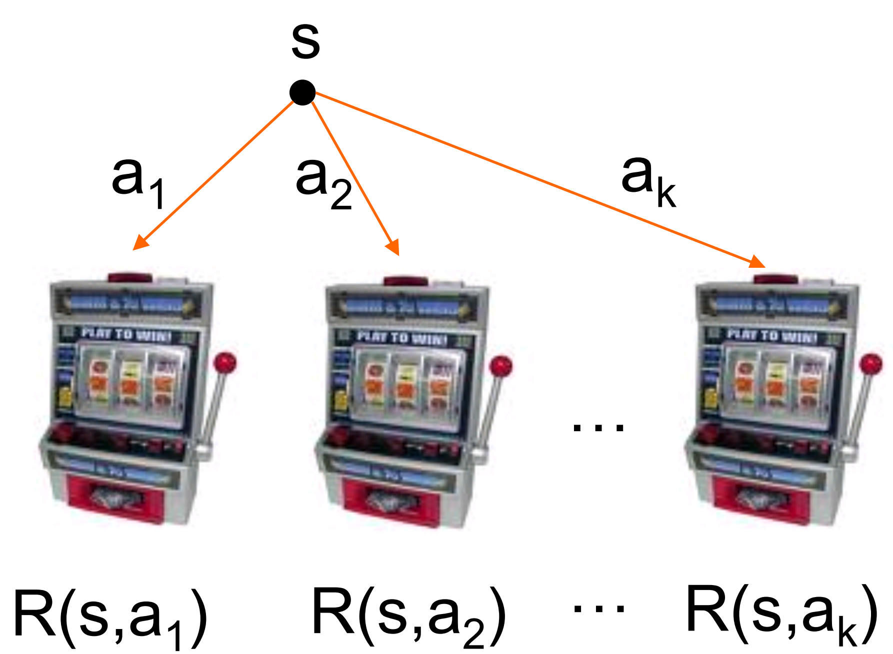
- MC planning is sometimes called RL with a "strong simulator"
  - I.e. a simulator where we can set the current state to any state at any moment
  - Often here we focus on computing action for a start state
- Pure RL is sometimes called RL with a "weak simulator"
  - I.e. a simulator where we cannot set the state
- A strong simulator can emulate a weak simulator
  - So pure RL can be used in the MC planning framework
  - But not vice versa

Monte-Carlo Planning Outline

- Single State Case (multi-armed bandits)
  - A basic tool for other algorithms
- Monte-Carlo Policy Improvement
  - Policy rollout
  - Policy Switching
  - Approximate Policy Iteration
- Monte-Carlo Tree Search
  - Sparse Sampling
  - UCT and variants

Single State Monte-Carlo Planning

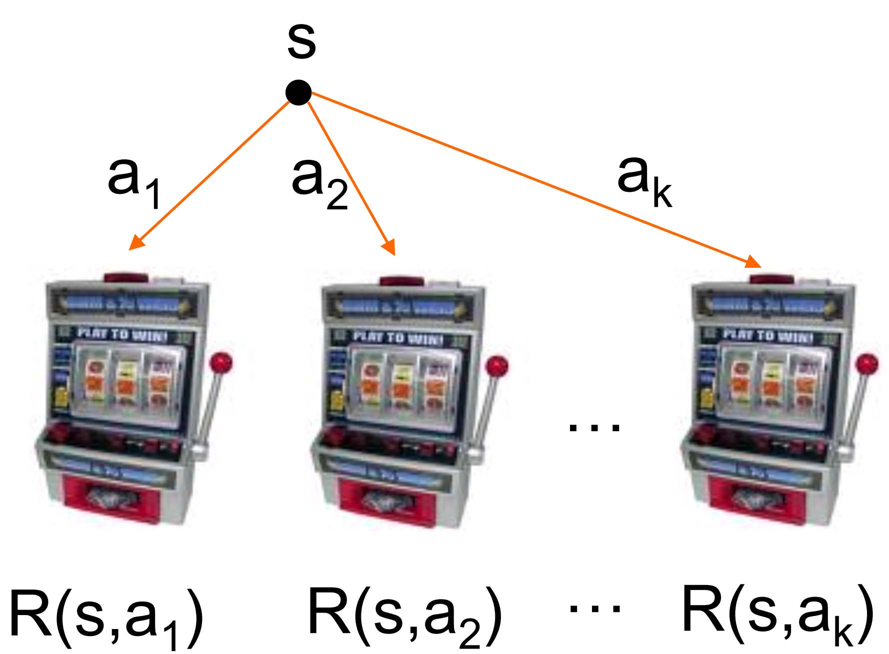
- Suppose MDP has a single state and k actions
  - Can sample rewards of actions using calls to simulator
  - Sampling action *a* is like pulling a slot machine arm with random payoff function *R*(*s*,*a*)



Multi-Armed Bandit Problem

Single State Monte-Carlo Planning

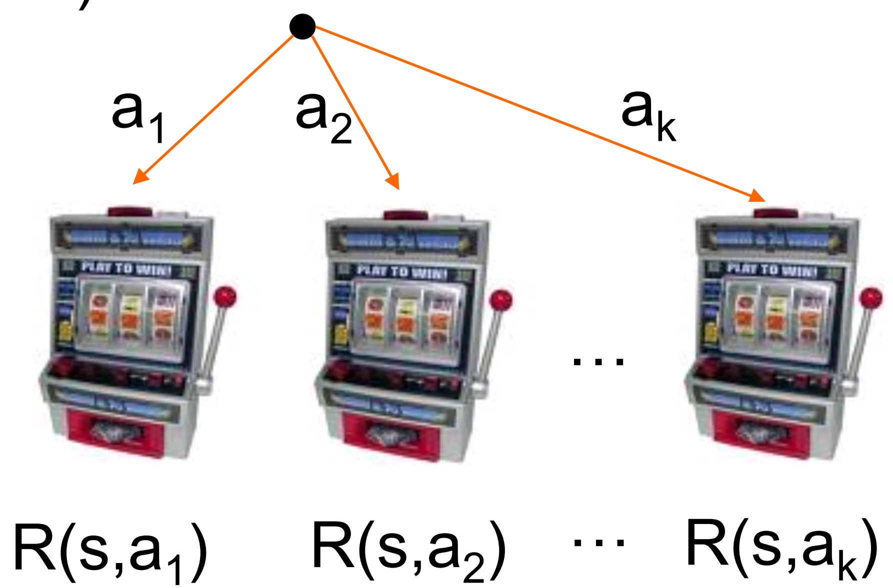
- Bandit problems arise in many situations
  - Clinical trials (arms correspond to treatments)
  - Ad placement (arms correspond to ad selections)



Multi-Armed Bandit Problem

Single State Monte-Carlo Planning

- We will consider three possible bandit objectives
  - **PAC Objective:** find a near optimal arm w/ high probability
  - **Cumulative Regret:** achieve near optimal cumulative reward over lifetime of pulling (in expectation)
  - **Simple Regret:** quickly identify arm with high reward (in expectation)



Multi-Armed Bandit Problem

Multi-Armed Bandits

- Bandit algorithms are not just useful as components for multi-state Monte-Carlo planning
- Pure bandit problems arise in many applications
- Applicable whenever:
  - We have a set of independent options with unknown utilities
  - There is a cost for sampling options or a limit on total samples
  - Want to find the best option or maximize utility of our samples

Multi-Armed Bandits: Examples

- **Clinical Trials**
  - Arms = possible treatments
  - Arm Pulls = application of treatment to inidividual
  - Rewards = outcome of treatment
  - Objective = maximize cumulative reward = maximize benefit to trial population (or find best treatment quickly)
- **Online Advertising**
  - Arms = different ads/ad-types for a web page
  - Arm Pulls = displaying an ad upon a page access
  - Rewards = click through
  - Objective = maximize cumulative reward = maximize clicks (or find best add quickly)

Bounded Reward Assumption

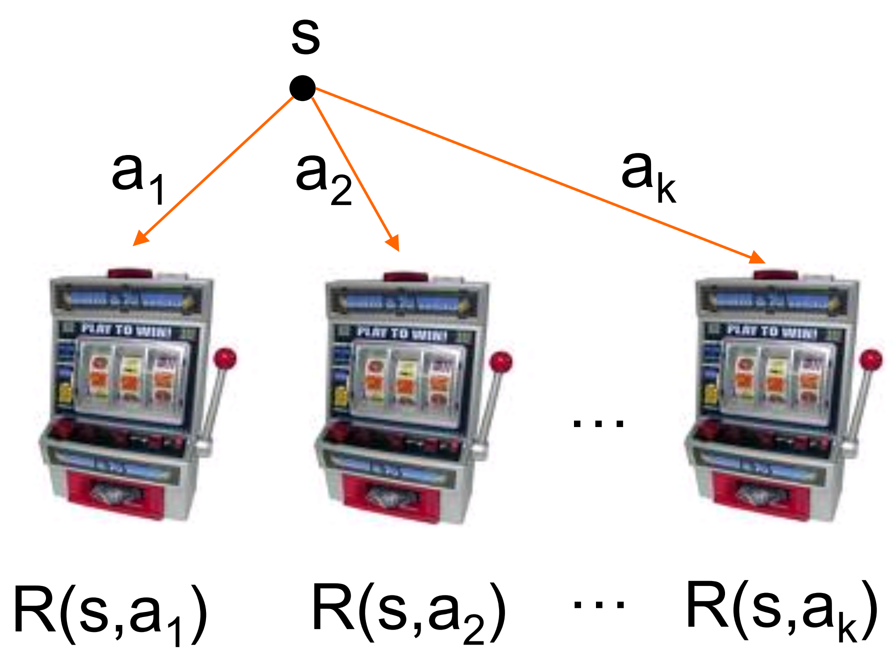
- A common assumption we will make is that rewards are in a bounded interval [-R_{max}, R_{max}].

- I.e., for each i, $\Pr(R(s, a_i) \in [-R_{max}, R_{max}]) = 1$.

- Results are available for other types of assumptions, e.g. Gaussian distributions
  - Require different type of analysis

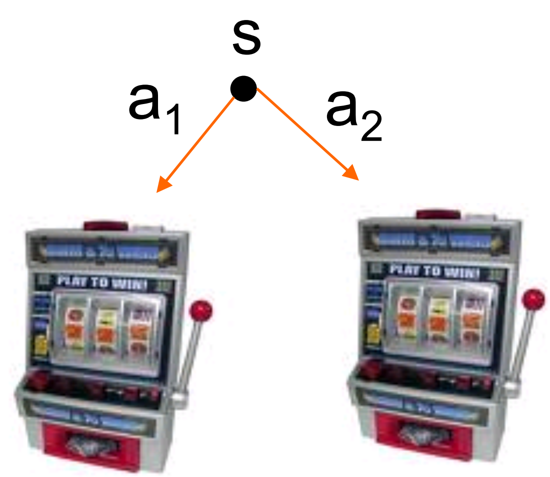
PAC Bandit Objective: Informal

- **Probably Approximately Correct (PAC)**
  - Select an arm that probably (w/ high probability) has approximately the best expected reward
  - Design an algorithm that uses as few simulator calls (or pulls) as possible to guarantee this



Multi-Armed Bandit Problem

Why have "probably" in PAC?



Pr(R(s,a_1)=1) = 0.001

Pr(R(s,a_1)=0) = 0.999

Pr(R(s,a_2)=1) = 0.999

Pr(R(s,a_2)=0) = 0.001

Suppose we are trying to determine the best arm by pulling each arm 1 million times.

Will this procedure <u>ALWAYS</u> identify the best arm?

No! There is a tiny, but non-zero, probability that we observe more rewards = 1 for a_1 than for a_2. (a run of extreme bad luck)

So a bandit algorithm can only be guaranteed to "probably" identify the best arm.

Why have "approximately" in PAC?

s

a_1 a_2

$\Pr(R(s,a_1)=1) = 0.5$

$\Pr(R(s,a_1)=0) = 0.5$

$\Pr(R(s,a_2)=1) = 0.499999$

$\Pr(R(s,a_2)=0) = 0.500001$

Suppose we are trying to determine the best arm.

How many times will we need to pull the arms to determine the absolute best arm?

The arms are nearly identical. Need a huge number of pulls to reliably determine which are is better.

To limit the theoretical number of pulls we only require an algorithm to find an approximately optimal arm.

PAC Bandit Algorithms

- k = # of arms
- $R^* = \max_i E[R(s, a_i)]$ is the optimal expected reward
- Rewards are in $[-R_{max}, R_{max}]$

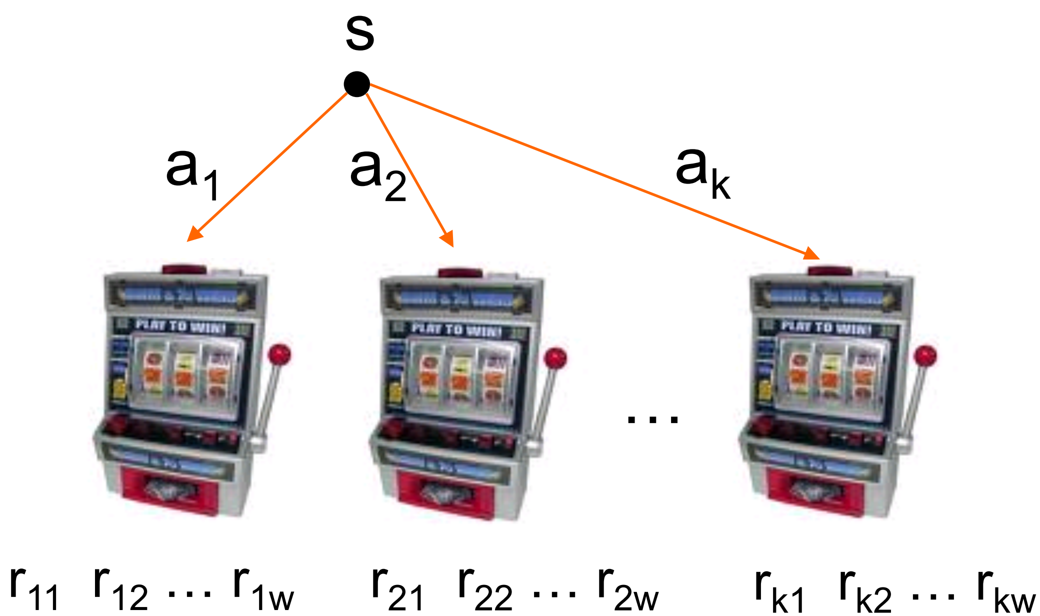
Definition (Efficient PAC Bandit Algorithm): An algorithm ALG is an efficient PAC bandit algorithm iff for any multi-armed bandit problem, for any $0 < \delta < 1$ and any $0 < \epsilon$ (these are inputs to ALG), ALG pulls a number of arms that is **polynomial in $\boldsymbol{1/\epsilon}$, $\boldsymbol{1/\delta}$, $\boldsymbol{R_{max}}$, and $\boldsymbol{k}$** and returns an arm index j such that with probability at least $1 - \delta$ we have $R^* - E\left[R\left(s, a_j\right)\right] \leq \epsilon$

- Such an algorithm is efficient in terms of # of arm pulls, and is probably (with probability $1 - \delta$) approximately correct (picks an arm with expected reward within ϵ of optimal).

UniformBandit Algorithm

Even-Dar, E., Mannor, S., & Mansour, Y. (2002). PAC bounds for multi-armed bandit and Markov decision processes. In *Computational Learning Theory*

1. Pull each arm **w** times (uniform pulling).
2. Return arm with best average reward.



Can we make this an efficient PAC bandit algorithm?

Aside: Additive Chernoff Bound

- Let R be a random variable with maximum absolute value Z. An let r_i i=1,…,w be i.i.d. samples of R
- The **Chernoff bound** gives a bound on the probability that the average of the r_i are far from E[R]

Chernoff Bound

$$\Pr\left(\left|E[R]-\tfrac{1}{w}\sum_{i=1}^{w} r_i\right| \geq \varepsilon\right) \leq \exp\left(-\left(\frac{\varepsilon}{Z}\right)^2 w\right)$$

Equivalent Statement:

With probability at least $1-\delta$ we have that,

$$\left|E[R]-\tfrac{1}{w}\sum_{i=1}^{w} r_i\right| \leq Z\sqrt{\tfrac{1}{w}\ln\tfrac{1}{\delta}}$$

Aside: Coin Flip Example

- Suppose we have a coin with probability of heads equal to *p*.
- Let *X* be a random variable where *X*=1 if the coin flip gives heads and zero otherwise. (so *Z* from bound is 1)

$$E[X] = 1 \cdot p + 0 \cdot (1 - p) = p$$

- After flipping a coin *w* times we can estimate the heads prob. by average of x_i.
- The Chernoff bound tells us that this estimate converges exponentially fast to the true mean (coin bias) *p*.

$$\Pr\left(\left| p - \tfrac{1}{w} \sum_{i=1}^{w} x_i \right| \geq \varepsilon \right) \leq \exp\left(-\varepsilon^2 w \right)$$

UniformBandit Algorithm

Even-Dar, E., Mannor, S., & Mansour, Y. (2002). PAC bounds for multi-armed bandit and Markov decision processes. In *Computational Learning Theory*

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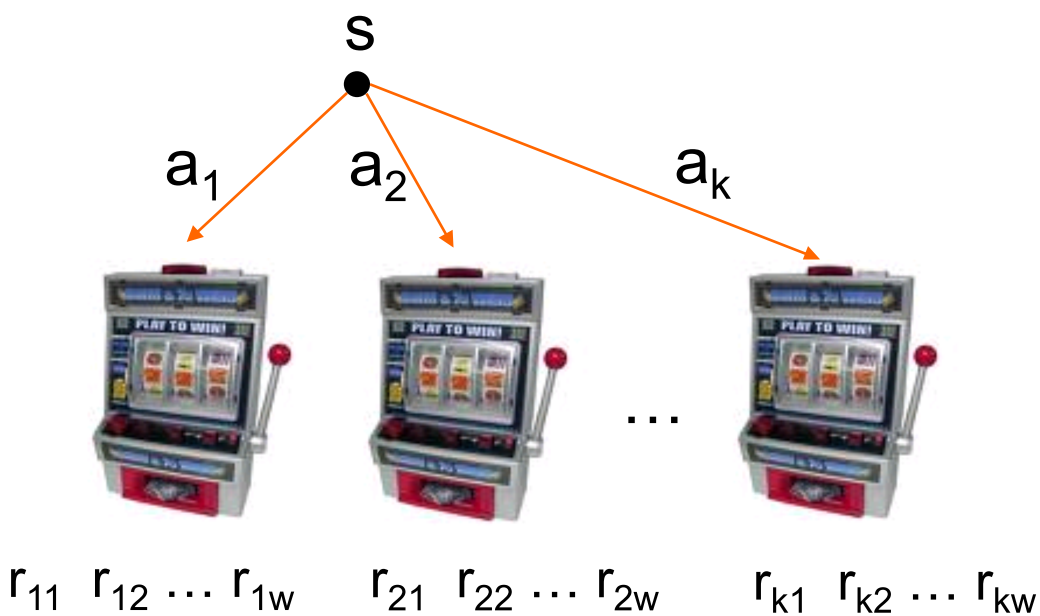


Can we make this an efficient PAC bandit algorithm?

UniformBandit PAC Bound

- For a single bandit arm the Chernoff bound says ($Z = R_{max}$):

  With probability at least $1-\delta'$ we have that,

$$\left| E[R(s,a_i)] - \frac{1}{w}\sum_{j=1}^{w} r_{ij} \right| \le \mathrm{R}_{\max}\sqrt{\frac{1}{w}\ln\frac{1}{\delta'}}$$

- Bounding the error by ε gives:

$$R_{\max}\sqrt{\frac{1}{w}\ln\frac{1}{\delta'}} \le \varepsilon \quad \text{or equivalently} \quad w \ge \left(\frac{R_{\max}}{\varepsilon}\right)^2 \ln\frac{1}{\delta'}$$

- Thus, using this many samples for a single arm will guarantee an ε-accurate estimate with probability at least $1-\delta'$ for a single arm.

UniformBandit PAC Bound

- So we see that with $w \geq \left(\frac{R_{\max}}{\varepsilon}\right)^2 \ln\frac{1}{\delta'}$ samples per arm, there is no more than a δ' probability that an individual arm's estimate will **not** be ε-accurate
  - But we want to bound the probability of any arm being inaccurate

The **union bound** says that for *k* events, the probability that at least one event occurs is bounded by the sum of individual probabilities

$$\Pr(A_1\ or\ A_2\ or \cdots or\ A_k) \leq \sum_{i=1}^{k} \Pr(A_i)$$

- Using the above # samples per arm and the union bound (with events being "arm *i* is not ε-accurate") there is no more than $k\delta'$ probability of any arm not being ε-accurate

- Setting $\delta' = \frac{\delta}{k}$ **all** arms are ε-accurate with prob. at least $1-\delta$

UniformBandit PAC Bound

Putting everything together we get:

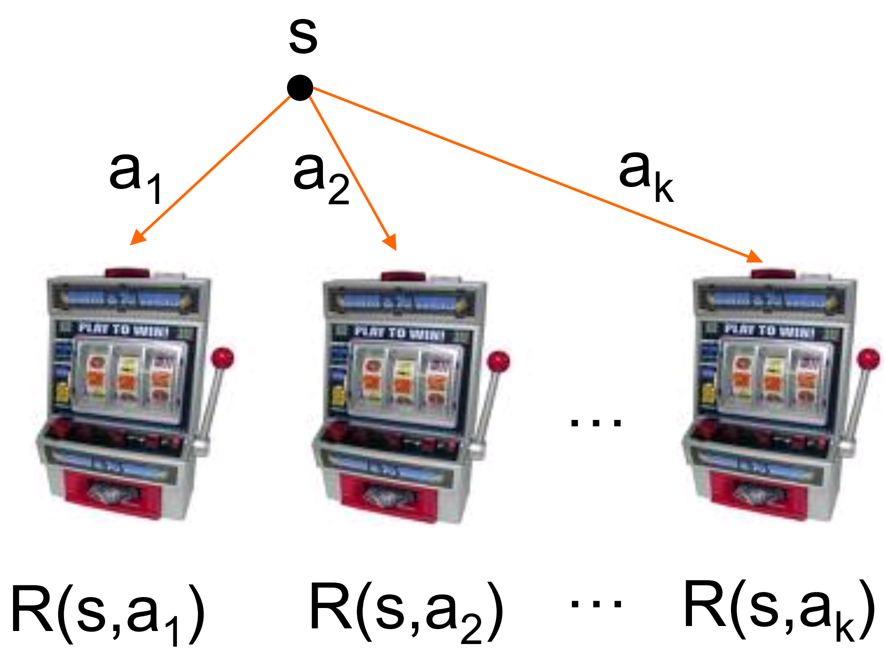
If $w \geq \left(\frac{R_{\max}}{\varepsilon}\right)^2 \ln\frac{k}{\delta}$ then for all arms simultaneously

$$\left| E[R(s,a_i)] - \frac{1}{w}\sum_{j=1}^{w} r_{ij} \right| \leq \varepsilon$$

with probability at least $1-\delta$

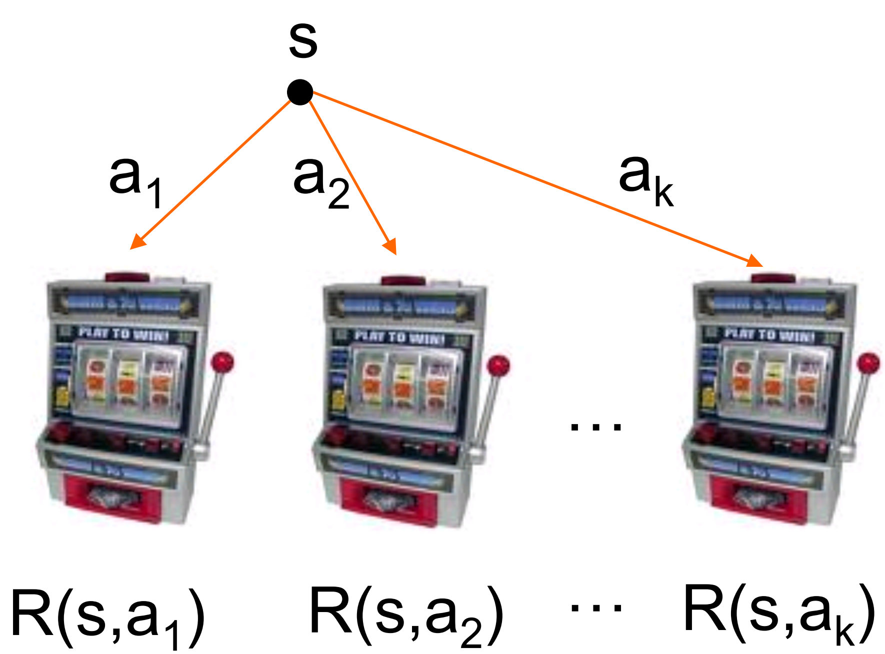
- That is, estimates of all actions are ε – accurate with probability at least 1- δ
- Thus selecting estimate with highest value is approximately optimal with high probability, or PAC

Simulator Calls for UniformBandit



- Total simulator calls for PAC: $k \cdot w = \left(\frac{R_{\max}}{\varepsilon} \right)^2 k \ln \frac{k}{\delta}$
  - So we have an **efficient** PAC algorithm
  - Can we do better than this?

Non-Uniform Sampling



- If an arm is really bad, we should be able to eliminate it from consideration early on
- **Idea:** try to allocate more pulls to arms that appear more promising

Median Elimination Algorithm

Even-Dar, E., Mannor, S., & Mansour, Y. (2002). PAC bounds for multi-armed bandit and Markov decision processes. In *Computational Learning Theory*

Median Elimination

A = set of all arms

For i = 1 to …..

    Pull each arm in A $\mathbf{w_i}$ times

    m = median of the average rewards of the arms in A

    A = A – {arms with average reward less than m}

    If |A| = 1 then return the arm in A

Eliminates half of the arms each round.

How to set the $\mathbf{w_i}$ to get PAC guarantee?

Median Elimination (proof not covered)

- Theoretical values used by Median Elimination:

$$w_i = \frac{4}{\epsilon_i^2} \ln \frac{3}{\delta_i} \qquad \epsilon_i = \left(\frac{3}{4}\right)^{i-1} \cdot \frac{\epsilon}{4} \qquad \delta_i = \frac{\delta}{2^i}$$

Theorem: Median Elimination is a PAC algorithm and uses a number of pulls that is at most $O\left(\frac{k}{\varepsilon^2} \ln \frac{1}{\delta}\right)$

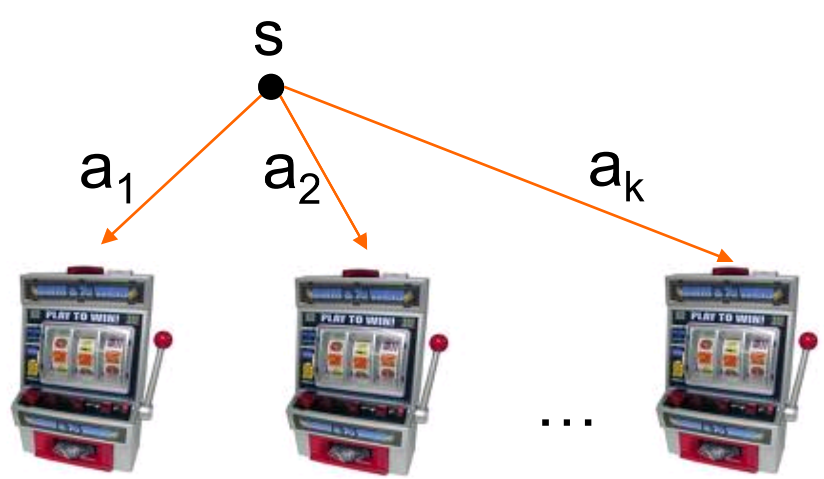
Compare to $O\left(\frac{k}{\varepsilon^2} \ln \frac{k}{\delta}\right)$ for UniformBandit

PAC Summary

- Median Elimination uses O(log(k)) fewer pulls than Uniform
  - Known to be asymptotically optimal (no PAC algorithm can use fewer pulls in worst case)
- PAC objective is sometimes awkward in practice
  - Sometimes we are not given a budget on pulls
  - Sometimes we can't control how many pulls we get
  - Selecting ϵ and δ can be quite arbitrary
- Cumulative & simple regret partly address this

Cumulative Regret Objective

- **Problem:** find arm-pulling strategy such that the expected total reward at time *n* is close to the best possible (one pull per time step)
  - Optimal (in expectation) is to pull optimal arm *n* times
  - UniformBandit is poor choice --- waste time on bad arms
  - Must balance **exploring** machines to find good payoffs and **exploiting** current knowledge



Cumulative Regret Objective

- Theoretical results are often about "expected cumulative regret" of an arm pulling strategy.

- **Protocol:** At time step n the algorithm picks an arm a_n based on what it has seen so far and receives reward r_n *(a_n and r_n are random variables)*.

- **Expected Cumulative Regret ($\boldsymbol{E[Reg_n]}$):** difference between optimal expected cummulative reward and expected cumulative reward of our strategy at time n

$$E[Reg_n] = n \cdot R^* - \sum_{i=1}^{n} E[r_n]$$

UCB Algorithm for Minimizing Cumulative Regret

Auer, P., Cesa-Bianchi, N., & Fischer, P. (2002). Finite-time analysis of the multiarmed bandit problem. *Machine learning*, *47*(2), 235-256.

- Q(a) : average reward for trying action a (in our single state *s*) so far
- n(a) : number of pulls of arm a so far
- Action choice by UCB after n pulls:

$$a_n = \arg\max_a Q(a) + \sqrt{\frac{2 \ln n}{n(a)}}$$

- Assumes rewards in [0,1]. We can always normalize given a bounded reward assumption

UCB: Bounded Sub-Optimality

$$a_n = \arg\max_a Q(a) + \sqrt{\frac{2\ln n}{n(a)}}$$

Value Term:
favors actions that looked good historically

Exploration Term:
actions get an exploration bonus that grows with ln(n)

Expected number of pulls of sub-optimal arm **a** is bounded by:

$$\frac{8}{\Delta_a^2}\ln n$$

where Δ_a is the sub-optimality of arm **a**

Doesn't waste much time on sub-optimal arms, unlike uniform!

UCB Performance Guarantee
[Auer, Cesa-Bianchi, & Fischer, 2002]

Theorem: The expected cumulative regret of UCB $\boldsymbol{E}[\boldsymbol{Reg_n}]$ after *n* arm pulls is bounded by O(log *n*)

- Is this good?

Yes. The average per-step regret is $O\left(\frac{\log(n)}{n}\right)$

Theorem: No algorithm can achieve a better expected regret (up to constant factors)

What Else ….

- UCB is great when we care about cumulative regret
- But, sometimes all we care about is finding a good arm quickly
- This is similar to the PAC objective, but:
  - The PAC algorithms required precise knowledge of or control of # pulls
  - We would like to be able to stop at any time and get a good result with some guarantees on expected performance
- “Simple regret” is an appropriate objective in these cases

Simple Regret Objective

- **Protocol:** At time step n the algorithm picks an "exploration" arm a_n to pull and observes reward r_n and also picks an arm index it thinks is best j_n *($a_n,\ j_n\ and\ r_n$ are random variables)*.
  - If interrupted at time n the algorithm returns j_n.

- **Expected Simple Regret ($\boldsymbol{E[SReg_n]}$):** difference between R^* and expected reward of arm j_n selected by our strategy at time n

$$E[SReg_n] = R^* - E[R(a_{j_n})]$$

Simple Regret Objective

- What about UCB for simple regret?
  - Intuitively we might think UCB puts too much emphasis on pulling the best arm
  - After an arm starts looking good, we might be better off trying figure out if there is indeed a better arm

Theorem: The expected simple regret of UCB after *n* arm pulls is upper bounded by $O(n^{-c})$ for a constant c.

Seems good, but we can do much better in theory.

Incremental Uniform (or Round Robin)

Bubeck, S., Munos, R., & Stoltz, G. (2011). Pure exploration in finitely-armed and continuous-armed bandits. Theoretical Computer Science, 412(19), 1832-1852

Algorithm:

- At round n pull arm with index (k mod n) + 1
- At round n return arm (if asked) with largest average reward

Theorem: The expected simple regret of Uniform after *n* arm pulls is upper bounded by O(e^{-cn}) for a constant c.

- This bound is exponentially decreasing in n!

  Compared to polynomially for UCB O(n^{-c}).

Can we do better?

Tolpin, D. & Shimony, S, E. (2012). MCTS Based on Simple Regret. *AAAI Conference on Artificial Intelligence.*

Algorithm ϵ-Greedy **:** (parameter $0 < \epsilon < 1$)

- At round n, with probability ϵ pull arm with best average reward so far, otherwise pull one of the other arms at random.
- At round n return arm (if asked) with largest average reward

Theorem: The expected simple regret of ϵ-Greedy for $\epsilon = 0.5$ after *n* arm pulls is upper bounded by O(e^{-cn}) for a constant c that is larger than the constant for Uniform (this holds for "large enough" n).

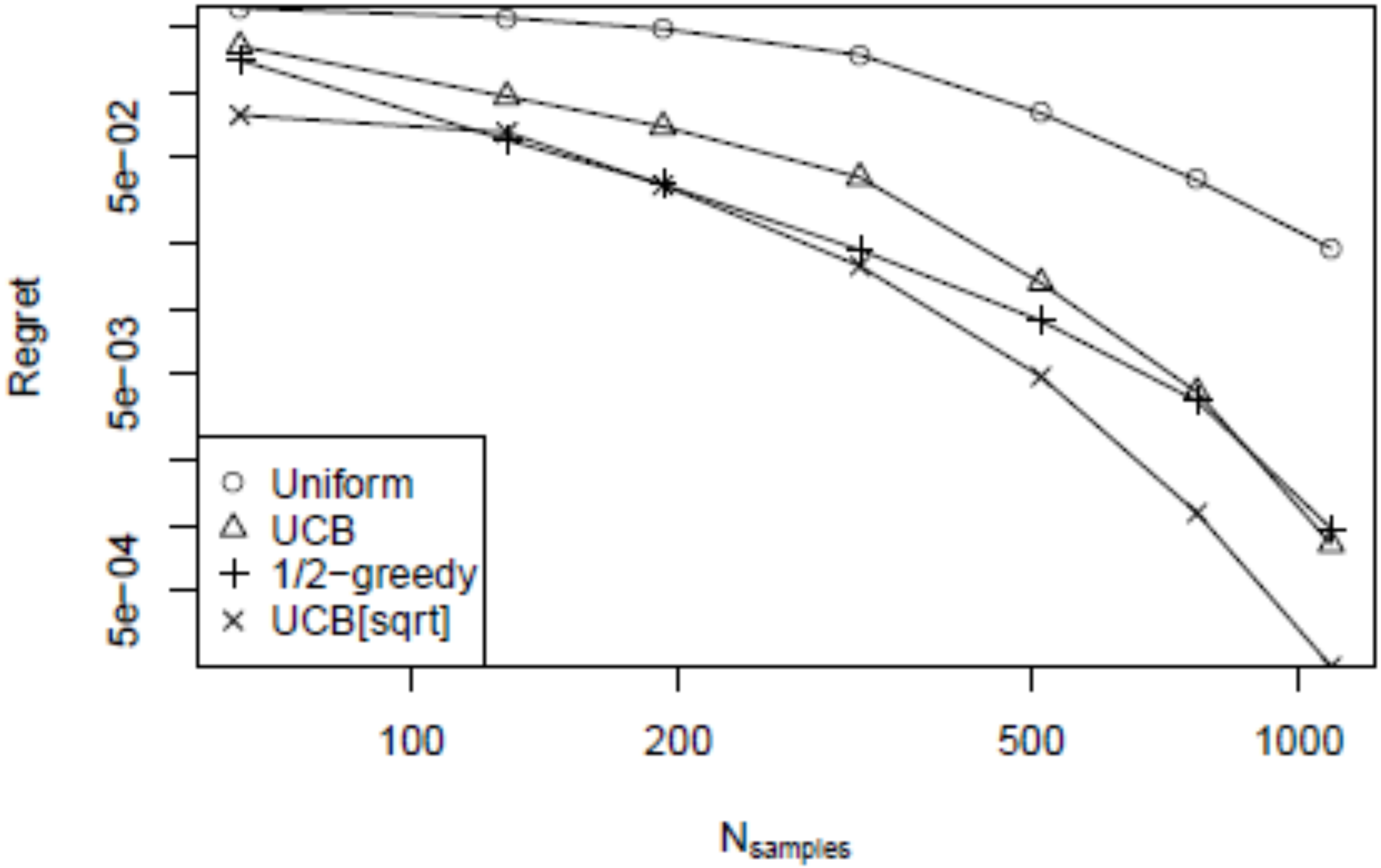
Summary of Bandits in Theory

- PAC Objective:
  - **UniformBandit** is a simple PAC algorithm
  - **MedianElimination** improves by a factor of log(k) and is optimal up to constant factors
- Cumulative Regret:
  - **Uniform** is very bad!
  - **UCB** is optimal (up to constant factors)
- Simple Regret:
  - **UCB** shown to reduce regret at polynomial rate
  - **Uniform** reduces at an exponential rate
  - **0.5-Greedy** may have even better exponential rate

Theory vs. Practice

- The established theoretical relationships among bandit algorithms have often been useful in predicting empirical relationships.
- But not always ….

Theory vs. Practice



b. regret vs. number of samples