

# Lecture 13: Multi-Armed Bandits

## CS486/686 Intro to Artificial Intelligence

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# Outline

- Exploration/exploitation tradeoff
- Regret
- Multi-armed bandits
  - $\epsilon$ -greedy strategies
  - Upper confidence bounds
  - Thompson sampling

# Exploration/Exploitation Tradeoff

- Fundamental problem of RL due to the active nature of the learning process
- Consider one-state RL problems known as **bandits**

# Stochastic Bandits

- Formal definition:
  - Single state:  $S = \{s\}$
  - $A$ : set of actions (also known as **arms**)
  - Space of rewards (often re-scaled to be  $[0,1]$ )
- **No transition function to be learned** since there is a single state
- We simply need to **learn the stochastic** reward function

# Origin and Applications

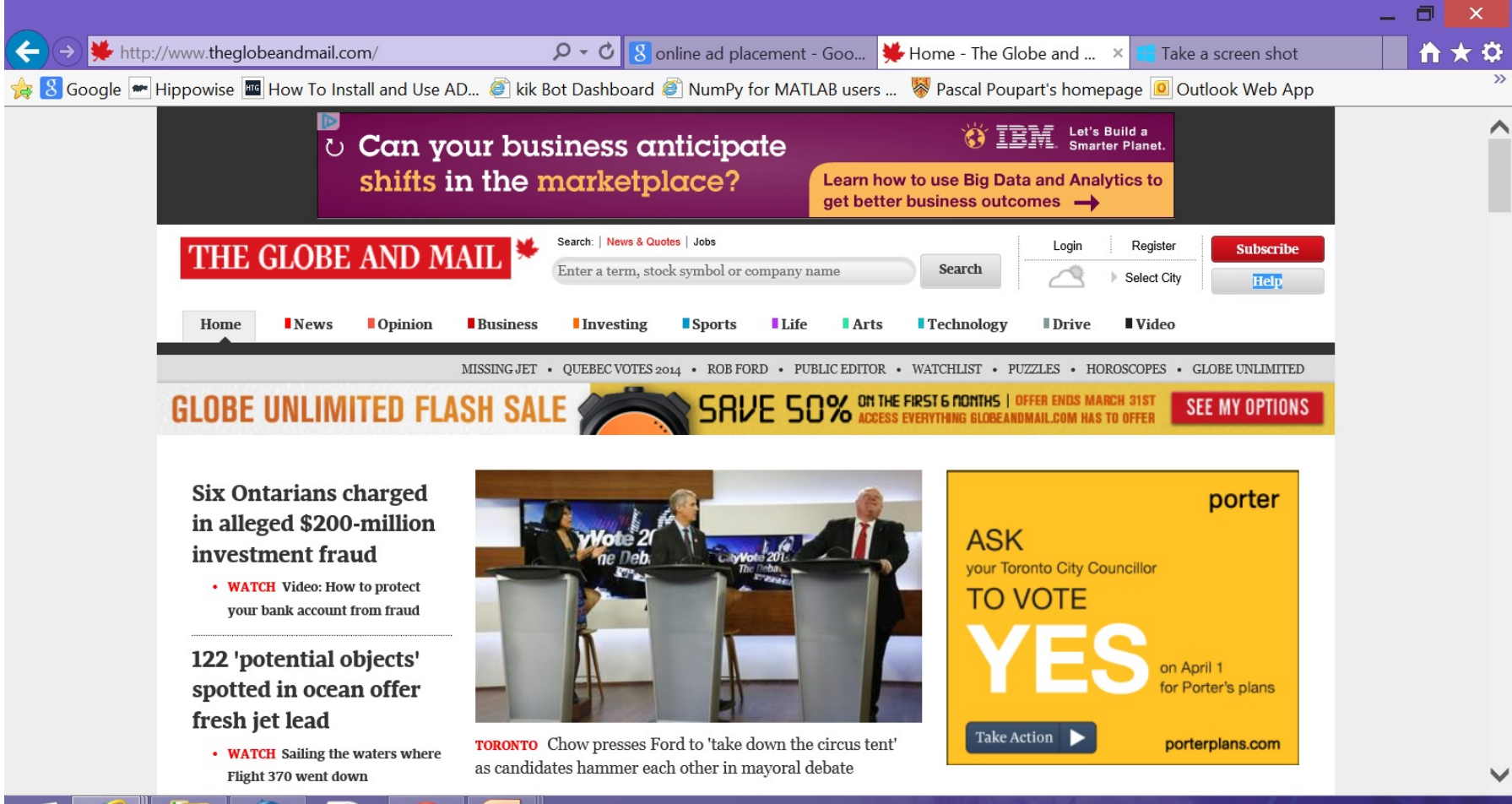
- “bandit” comes from gambling where slot machines can be thought as one-armed bandits.



## Applications

- **Marketing** (ad placement, recommender systems)
- **Loyalty programs** (personalized offers)
- **Pricing** (airline seat pricing, cargo shipment pricing, food pricing)
- **Optimal design** (web design, interface personalization)
- **Networks** (routing)

# Online Ad Placement



# Online Ad Optimization

- Problem: **which ad should be presented?**
- Answer: present ad with highest payoff

$$\text{payoff} = \text{clickThroughRate} \times \text{payment}$$

- Click through rate: probability that user clicks on ad
- Payment: \$\$ paid by advertiser
  - Amount determined by an auction

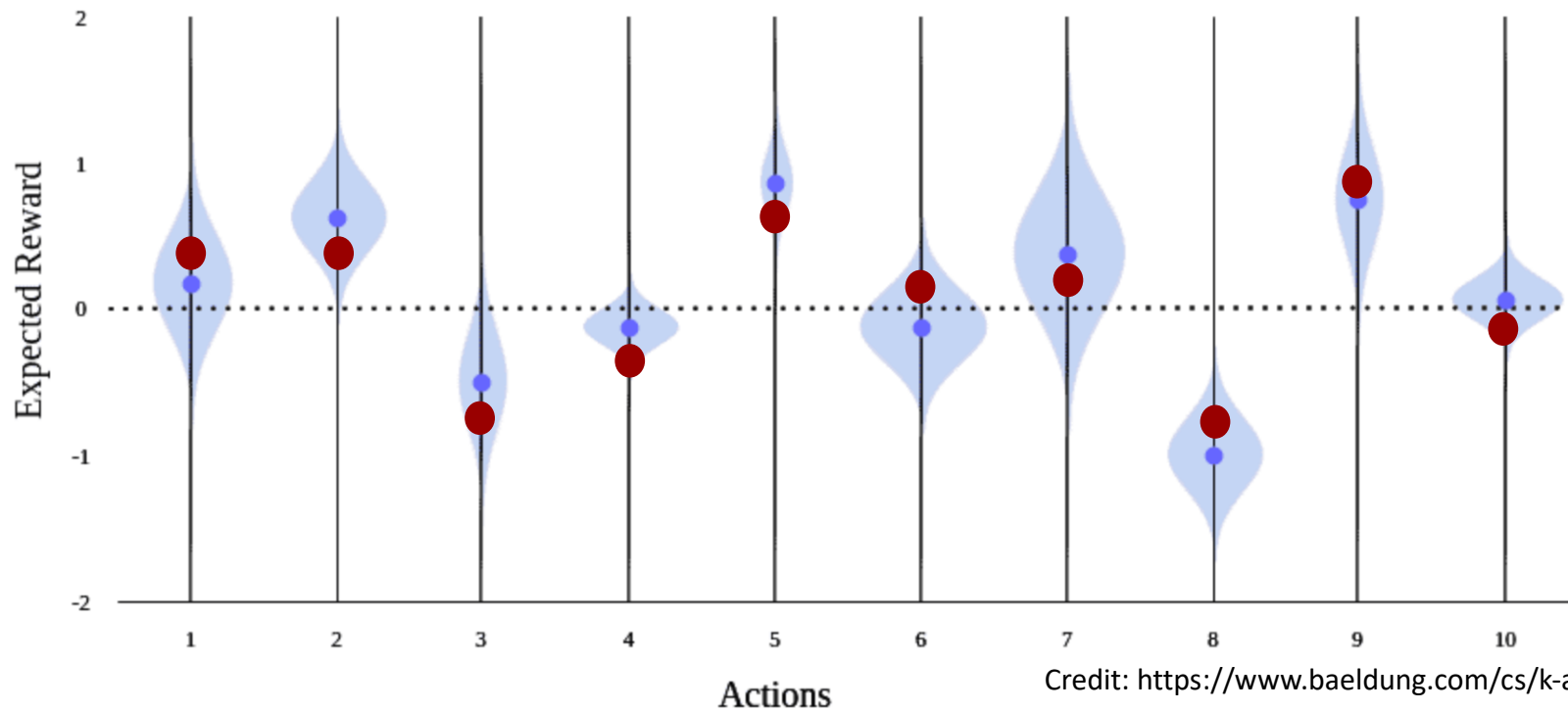
# Simplified Problem

- Assume payment is 1 unit for all ads
- Need to estimate click through rate
- Formulate as a bandit problem:
  - Arms: the set of possible ads
  - Rewards: 0 (no click) or 1 (click)
- In what order should ads be presented to maximize revenue?
  - How should we balance exploitation and exploration?



# Uncertainty Quantification

- Distribution of rewards:  $\Pr(r|a)$
- Expected reward:  $R(a) = E(r|a)$
- Empirical average reward:  $\tilde{R}(a) = \frac{1}{n} \sum_t^n r_t$



Credit: <https://www.baeldung.com/cs/k-armed-bandit-problem>

# Simple Heuristics

- **Greedy strategy**: select the arm with the highest average so far
  - May get stuck due to lack of exploration
- **$\epsilon$ -greedy**: select an arm at random with probability  $\epsilon$  and otherwise do a greedy selection
  - Convergence rate depends on choice of  $\epsilon$

# Regret

- Let  $R(a)$  be the unknown average reward of  $a$
- Let  $r^* = \max_a R(a)$  and  $a^* = \operatorname{argmax}_a R(a)$

- Denote by  $loss(a)$  the **expected regret** of  $a$

$$loss(a) = r^* - R(a)$$

- Denote by  $Loss_n$  the **expected cumulative regret** for  $n$  time steps

$$Loss_n = \sum_{t=1}^n loss(a_t)$$

# Theoretical Guarantees

- When  $\epsilon$  is constant, then
  - For large enough  $t$ :  $\Pr(a_t \neq a^*) \approx \epsilon$
  - Expected cumulative regret:  $Loss_n \approx \sum_{t=1}^n \epsilon = O(n)$ 
    - Linear regret
- When  $\epsilon_t \propto 1/t$ 
  - For large enough  $t$ :  $\Pr(a_t \neq a^*) \approx \epsilon_t = O\left(\frac{1}{t}\right)$
  - Expected cumulative regret:  $Loss_n \approx \sum_{t=1}^n \frac{1}{t} = O(\log n)$ 
    - Logarithmic regret

# Empirical Mean

- Problem: how far is the empirical mean  $\tilde{R}(a)$  from the true mean  $R(a)$ ?
- If we knew that  $|R(a) - \tilde{R}(a)| \leq bound$ 
  - Then we would know that  $R(a) < \tilde{R}(a) + bound$
  - And we could select the arm with best  $\tilde{R}(a) + bound$
- Overtime, additional data will allow us to refine  $\tilde{R}(a)$  and compute a tighter *bound*.

# Positivism in the Face of Uncertainty

- Suppose that we have an oracle that returns an **upper bound**  $UB_n(a)$  on  $R(a)$  for each arm based on  $n$  trials of arm  $a$ .
- Suppose the upper bound returned by this oracle converges to  $R(a)$  in the limit:
  - i.e.,  $\lim_{n \rightarrow \infty} UB_n(a) = R(a)$
- **Optimistic algorithm**
  - At each step, **select**  $\operatorname{argmax}_a UB_n(a)$

# Convergence

- **Theorem:** An optimistic strategy that always selects  $\operatorname{argmax}_a UB_n(a)$  will converge to  $a^*$
- Proof by contradiction:
  - Suppose that we converge to suboptimal arm  $a$  after infinitely many trials.
  - Then  $R(a) = UB_\infty(a) \geq UB_\infty(a') = R(a') \forall a'$
  - But  $R(a) \geq R(a') \forall a'$  contradicts our assumption that  $a$  is suboptimal.

# Probabilistic Upper Bound

- Problem: We can't compute an upper bound with certainty since we are sampling
- However, we can obtain measures  $f$  that are upper bounds most of the time
  - i.e.,  $\Pr(R(a) \leq f(a)) \geq 1 - \delta$
  - Example: Hoeffding's inequality

$$\Pr \left( R(a) \leq \tilde{R}(a) + \sqrt{\frac{\log\left(\frac{1}{\delta}\right)}{2n_a}} \right) \geq 1 - \delta$$

where  $n_a$  is the number of trials for arm  $a$



# Upper Confidence Bound (UCB)

- Set  $\delta_n = 1/n^4$  in Hoeffding's bound
- Choose  $a$  with highest Hoeffding bound

UCB( $h$ )

$V \leftarrow 0, n \leftarrow 0, n_a \leftarrow 0 \quad \forall a$

Repeat until  $n = h$

Execute  $\operatorname{argmax}_a \tilde{R}(a) + \sqrt{\frac{2 \log n}{n_a}}$

Receive  $r$

$V \leftarrow V + r$

$\tilde{R}(a) \leftarrow \frac{n_a \tilde{R}(a) + r}{n_a + 1}$

$n \leftarrow n + 1, n_a \leftarrow n_a + 1$

Return  $V$

# UCB Convergence

- **Theorem:** Although Hoeffding's bound is probabilistic, **UCB converges.**
- **Idea:** As  $n$  increases, the term  $\sqrt{\frac{2 \log n}{n_a}}$  increases, ensuring that all arms are tried infinitely often
- Expected cumulative regret:  $Loss_n = O(\log n)$ 
  - **Logarithmic regret**

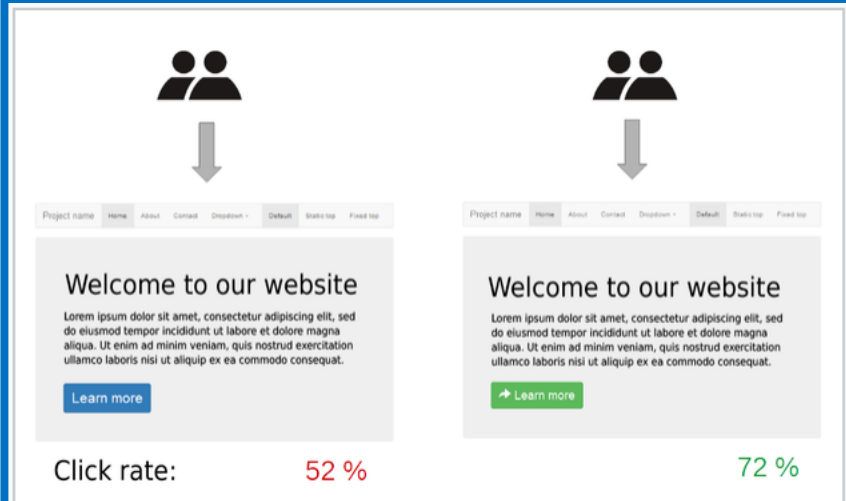
# Extension of A/B Testing

- **A/B Testing:** randomized experiment with 2 variants
  - Select best variant after completion of experiment

## Example: email marketing

- "Offer ends this Saturday! Use code A" (response rate: 5%)
- "Offer ends soon! Use code B" (response rate: 3%)

- **Multi-armed bandits:** form of **continual A/B testing**



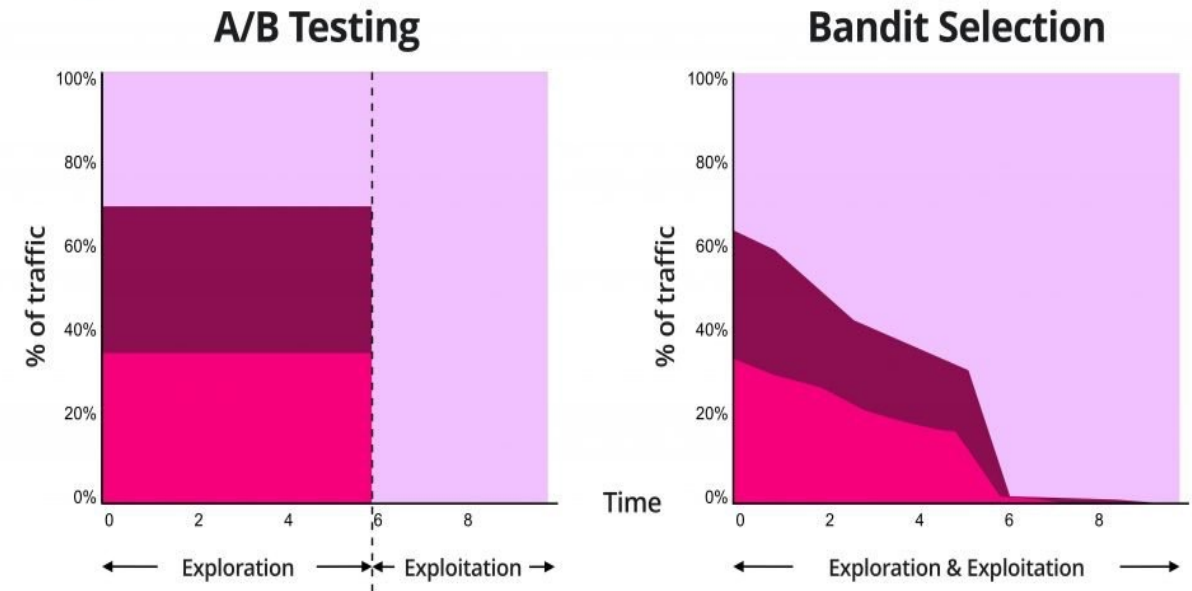
Example of A/B testing on a website. By randomly serving visitors two versions of a website that differ only in the design of a single button element, the relative efficacy of the two designs can be measured.

# Multi-Armed Bandit

Components	Formal Def	Marketing
Actions (arms)	$a \in A$	{A, B, C}
Rewards	$r \in \mathbb{R}$	{0, 1}
Reward model	$\Pr(r a)$	unknown
Horizon	$h \in \mathbb{N}$ or $\infty$	$h = \infty$



Credit: Shubhankar Gupta (vwo.com)



Variation **A**  
High CTR

Variation **B**  
Medium CTR

Variation **C**  
Low CTR

# Bayesian Learning

- Notation:
  - $r^a$ : random variable for  $a$ 's rewards
  - $\Pr(r^a; \theta)$ : unknown distribution (parameterized by  $\theta$ )
  - $R(a) = E[r^a]$ : unknown average reward
- Idea:
  - Express uncertainty about  $\theta$  by a prior  $\Pr(\theta)$
  - Compute posterior  $\Pr(\theta | r_1^a, r_2^a, \dots, r_n^a)$  based on samples  $r_1^a, r_2^a, \dots, r_n^a$  observed for  $a$  so far.
- **Bayes theorem:**

$$\Pr(\theta | r_1^a, r_2^a, \dots, r_n^a) \propto \Pr(\theta) \Pr(r_1^a, r_2^a, \dots, r_n^a | \theta)$$

# Distributional Information

- Posterior over  $\theta$  allows us to estimate

- Distribution over next reward  $r^a$

$$\Pr(r^a | r_1^a, r_2^a, \dots, r_n^a) = \int_{\theta} \Pr(r^a; \theta) \Pr(\theta | r_1^a, r_2^a, \dots, r_n^a) d\theta$$

- Distribution over  $R(a)$  when  $\theta$  includes the mean

$$\Pr(R(a) | r_1^a, r_2^a, \dots, r_n^a) = \Pr(\theta | r_1^a, r_2^a, \dots, r_n^a) \text{ if } \theta = R(a)$$

- To guide exploration:

- UCB:  $\Pr(R(a) \leq \text{bound}(r_1^a, r_2^a, \dots, r_n^a)) \geq 1 - \delta$
- Bayesian techniques:  $\Pr(R(a) | r_1^a, r_2^a, \dots, r_n^a)$

# Coin Example

- Consider two biased coins  $C_1$  and  $C_2$

$$R(C_1) = \Pr(C_1 = \textit{head})$$

$$R(C_2) = \Pr(C_2 = \textit{head})$$

- Problem:
  - Maximize # of heads in  $k$  flips
  - Which coin should we choose for each flip?

# Bernoulli Variables

- $r^{C_1}, r^{C_2}$  are Bernoulli variables with domain  $\{0,1\}$
- Bernoulli distributions are parameterized by their mean
  - i.e.,  $\Pr(r^{C_1}; \theta_1) = \theta_1 = R(C_1)$   
 $\Pr(r^{C_2}; \theta_2) = \theta_2 = R(C_2)$

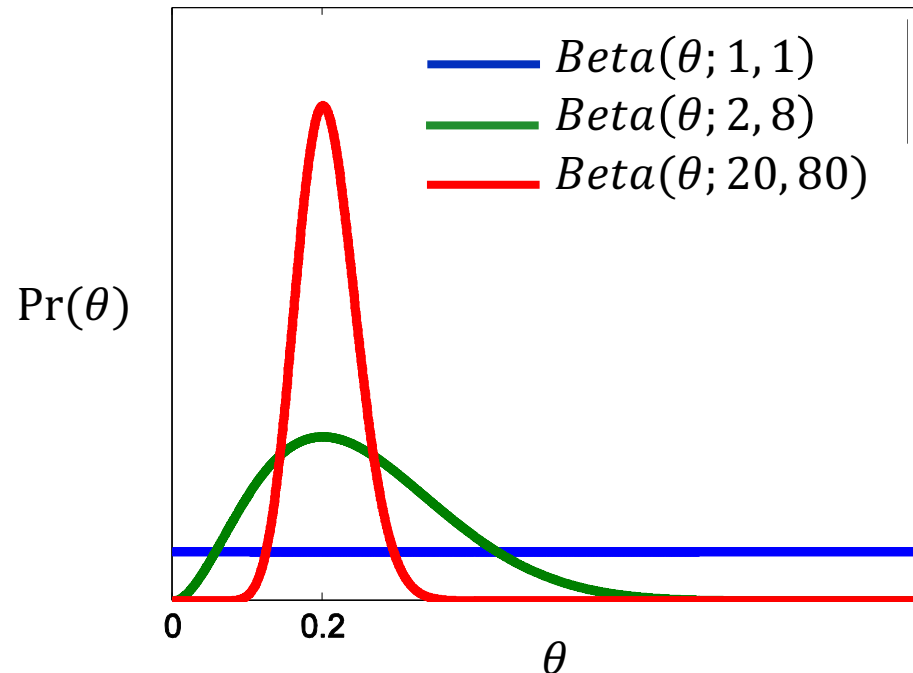


# Beta Distribution

- Let the prior  $\Pr(\theta)$  be a Beta distribution

$$\text{Beta}(\theta; \alpha, \beta) \propto \theta^{\alpha-1} (1 - \theta)^{\beta-1}$$

- $\alpha - 1$ : # of heads
- $\beta - 1$ : # of tails
- $E[\theta] = \alpha / (\alpha + \beta)$



# Belief Update

- Prior:  $\Pr(\theta) = \text{Beta}(\theta; \alpha, \beta) \propto \theta^{\alpha-1} (1 - \theta)^{\beta-1}$
- Posterior after coin flip:

$$\begin{aligned}\Pr(\theta|\text{head}) &\propto \Pr(\theta) \Pr(\text{head}|\theta) \\ &\propto \theta^{\alpha-1} (1 - \theta)^{\beta-1} \theta \\ &= \theta^{(\alpha+1)-1} (1 - \theta)^{\beta-1} \propto \text{Beta}(\theta; \alpha + 1, \beta)\end{aligned}$$

$$\begin{aligned}\Pr(\theta|\text{tail}) &\propto \Pr(\theta) \Pr(\text{tail}|\theta) \\ &\propto \theta^{\alpha-1} (1 - \theta)^{\beta-1} (1 - \theta) \\ &= \theta^{\alpha-1} (1 - \theta)^{(\beta+1)-1} \propto \text{Beta}(\theta; \alpha, \beta + 1)\end{aligned}$$

# Thompson Sampling

- Idea:
  - Sample several potential average rewards:  
 $\hat{R}(a) \sim \Pr(R(a) | r_1^a, \dots, r_n^a)$  for each  $a$
  - Execute  $\operatorname{argmax}_a \hat{R}(a)$
- Coin example
  - $\Pr(R(a) | r_1^a, \dots, r_n^a) = \text{Beta}(\theta_a; \alpha_a, \beta_a)$   
where  $\alpha_a - 1 = \#heads$  and  $\beta_a - 1 = \#tails$

# Thompson Sampling (Bernoulli rewards)

## ThompsonSampling( $h$ )

Initialize  $\alpha_a \leftarrow 1, \beta_a \leftarrow 1 \quad \forall a$

Repeat  $h$  times

Sample  $\hat{R}(a) \sim \text{Beta}(R(a) | \alpha_a, \beta_a) \quad \forall a$

$a^* \leftarrow \operatorname{argmax}_a \hat{R}(a)$

Execute  $a^*$  and receive  $r$

if  $r = 1$  then  $\alpha_{a^*} \leftarrow \alpha_{a^*} + 1$

else  $\beta_{a^*} \leftarrow \beta_{a^*} + 1$

# Analysis

- Thompson sampling converges to best arm
- Theory:
  - Expected cumulative regret:  $O(\log n)$
  - On par with UCB and  $\epsilon$ -greedy
- Practice:
  - Thompson Sampling often outperforms UCB and  $\epsilon$ -greedy