Lecture20: Multi-Armed Bandits
CS486/686 Intro to Artificial Intelligence

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Outline

- Exploration/exploitation tradeoff
- Regret
- Multi-armed bandits
  - Frequentist approaches
    - ϵ-greedy strategies
    - Upper confidence bounds
  - Bayesian bandits
    - 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])
  - Finite/Infinite horizons
  - Average reward setting ($\gamma = 1$)
- No transition function to be learned since there is a single state
- We simply need to learn the **stochastic** reward function

Origin

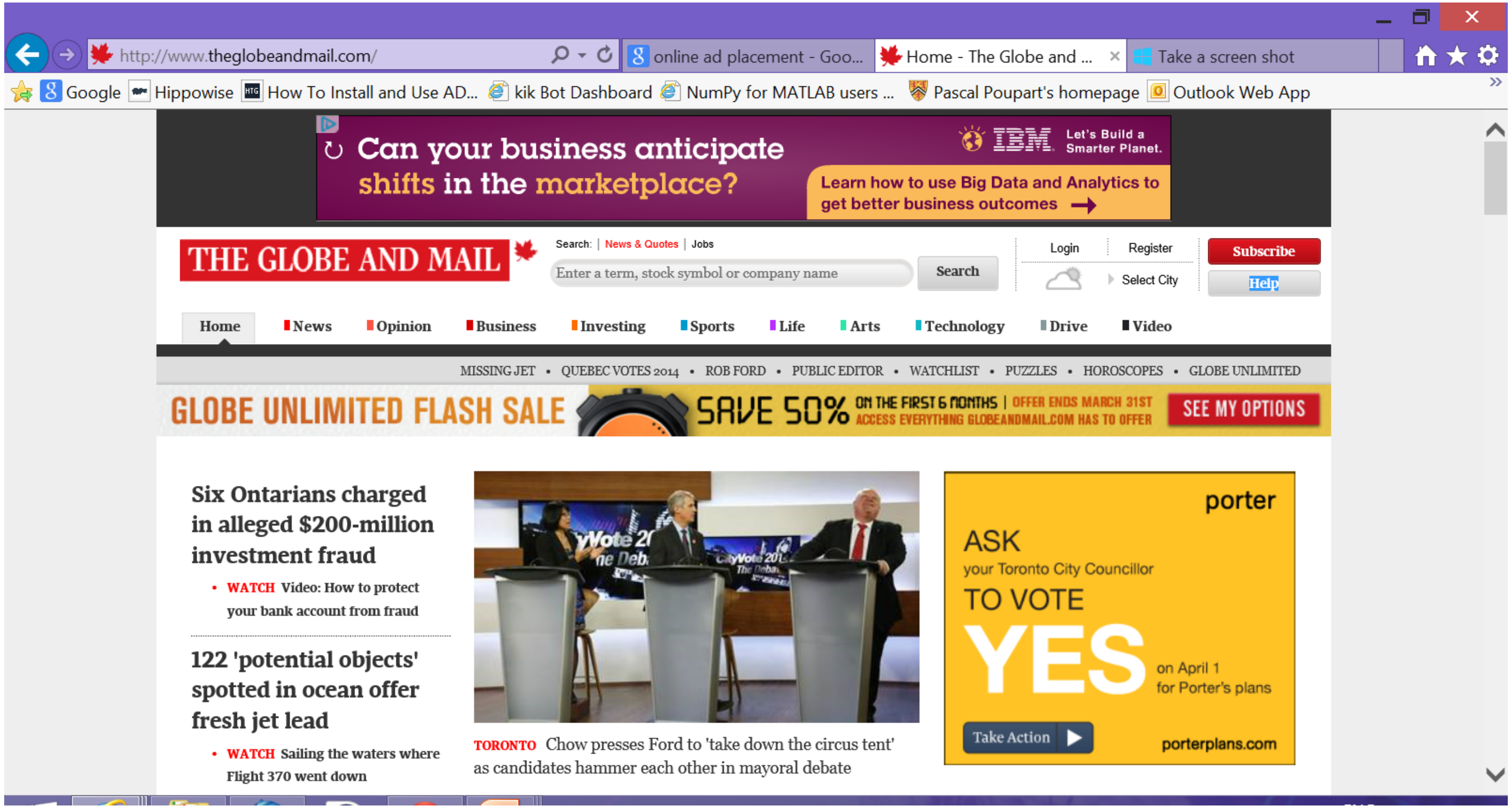
- The term bandit comes from gambling where slot machines can be thought as one-armed bandits.

- Problem: which slot machine should we play at each turn when their payoffs are not necessarily the same and initially unknown?

Examples

- Design of experiments (Clinical Trials)
- Online ad placement
- Web page personalization
- Recommender systems
- Networks (packet routing)

Online Ad Placement



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Online Ad Optimization

- Problem: which ad should be presented?

- Answer: present ad with highest payoff

$$payoff = clickThroughRate \times payment$$

  - 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?

Simple yet Difficult Problem

- Simple: description of the problem is short
- Difficult: no known tractable optimal solution

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Simple Heuristics

- Greedy strategy: select the arm with the highest average so far
  - May get stuck due to lack of exploration

- ϵ-greedy: select an arm at random with probability ϵ and otherwise do a greedy selection
  - Convergence rate depends on choice of ϵ

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Regret

- Let $R(a)$ be the **true (unknown) expected reward** of a
- Let $r^* = \max_a R(a)$ and $a^* = argmax_a\, R(a)$

- 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 ϵ is constant, then
  - For large enough t: $Pr(a_t \neq a^*) \approx \epsilon$
  - Expected cumulative regret: $Loss_n \approx \sum_{t=1}^{n} \epsilon \times 1 + (1-\epsilon) \times 0 = \sum_{t=1}^{n} \epsilon = O(n)$
    - 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 $\left| R(a) - \tilde{R}(a) \right| \leq bound$
  - Then we would know that $R(a) \leq \tilde{R}(a) + bound$
  - 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., $\lim_{n \to \infty} UB_n(a) = R(a)$

- Optimistic algorithm
  - At each step, select $\arg\max_a UB_n(a)$

Convergence

- Theorem: An optimistic strategy that always selects $\text{argmax}_a UB_n(a)$ 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., $\Pr\big(R(a) \leq f(a)\big) \geq 1 - \delta$
  - 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 $\text{argmax}_a \ \tilde{R}(a) + \sqrt{\frac{2\log n}{n_a}}$
  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

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Multi-Armed Bandits

- Problem:
  - N bandits with unknown average reward $R(a)$
  - Which arm a should we play at each time step?
  - Exploitation/exploration tradeoff
- Common frequentist approaches:
  - ϵ-greedy
  - Upper confidence bound (UCB)

- Alternative Bayesian approaches
  - Thompson sampling
  - Gittins indices

Bayesian Learning

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

- Bayes theorem:

$$\Pr\left(\theta \middle| r_1^a, r_2^a, \ldots, r_n^a\right) \propto \Pr(\theta)\Pr(r_1^a, r_2^a, \ldots, r_n^a | \theta)$$

Distributional Information

- Posterior over θ allows us to estimate
  - Distribution over next reward r^a

$$Pr(r^a_{n+1} \,|\, r^a_1, r^a_2, \ldots, r^a_n) = \int_\theta Pr(r^a_{n+1}; \theta) Pr(\theta \,|\, r^a_1, r^a_2, \ldots, r^a_n) d\theta$$

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

$$\Pr\left(R(a) \middle| r^a_1, r^a_2, \ldots, r^a_n\right) = \Pr\left(\theta \middle| r^a_1, r^a_2, \ldots, r^a_n\right) \text{ if } \theta = R(a)$$

- To guide exploration:
  - UCB: $\Pr\left(R(a) \leq bound(r^a_1, r^a_2, \ldots, r^a_n)\right) \geq 1 - \delta$
  - Bayesian techniques: $\Pr\left(R(a) \,|\, r^a_1, r^a_2, \ldots, r^a_n\right)$

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Coin Example

- Consider two biased coins C_1 and C_2

  $R(C_1) = \Pr(C_1 = head)$

  $R(C_2) = \Pr(C_2 = head)$

- 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., $\Pr\left(r^{C_1};\theta_1\right) = \theta_1 = R\left(C_1\right)$

    $\Pr\left(r^{C_2};\theta_2\right) = \theta_2 = R(C_2)$

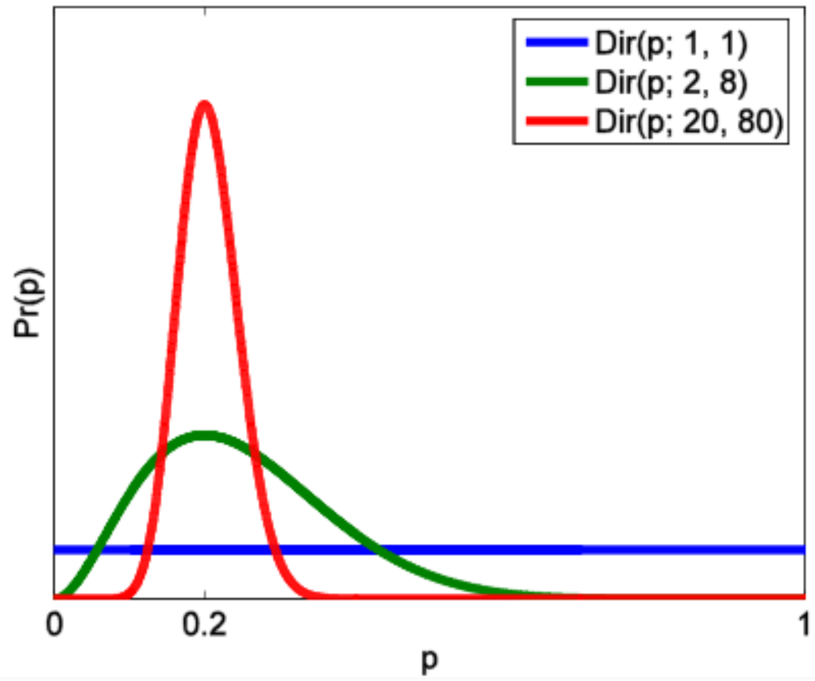
Beta Distribution

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

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

- $\alpha - 1$: # of heads
- $\beta - 1$: # of tails

- $E[\theta] = \alpha/(\alpha + \beta)$



Belief Update

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

$$\Pr\left(\theta \middle| head\right) \propto \quad \Pr(\theta) \quad \Pr\left(head \middle| \theta\right)$$

$$\propto \theta^{\alpha-1}(1-\theta)^{\beta-1} \quad \theta$$

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

$$\Pr(\theta | tail) \propto \quad \Pr(\theta) \quad \Pr(tail | \theta)$$

$$\propto \theta^{\alpha-1}(1-\theta)^{\beta-1} \quad (1-\theta)$$

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

Thompson Sampling

- Idea:
  - Sample several potential average rewards:
    $R_1(a), \ldots R_k(a) \sim \Pr(R(a) \mid r_1^a, \ldots, r_n^a)$ for each a
  - Estimate empirical average $\hat{R}(a) = \frac{1}{k}\sum_{i=1}^{k} R_i(a)$
  - Execute $argmax_a \, \hat{R}(a)$
- Coin example
  - $\Pr\left(R(a) \middle| r_1^a, \ldots, r_n^a\right) = \text{Beta}\left(\theta_a; \alpha_a, \beta_a\right)$
    where $\alpha_a - 1 = \#heads$ and $\beta_a - 1 = \#tails$

Thompson Sampling Algorithm Bernoulli Rewards

ThompsonSampling(h)

$V \leftarrow 0$

For $n = 1$ to h

Sample $R_1(a), \ldots, R_k(a) \sim \Pr(R(a)) \quad \forall a$

$\hat{R}(a) \leftarrow \frac{1}{k} \sum_{i=1}^{k} R_i(a) \quad \forall a$

$a^* \leftarrow \text{argmax}_\text{a} \; \hat{R}(a)$

Execute a^* and receive r

$V \leftarrow V + r$

Update $\Pr(R(a^*))$ based on r

Return V

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Comparison

Thompson Sampling

- Action Selection

  $$a^* = \text{argmax}_{\text{a}} \hat{R}(a)$$

- Empirical mean

  $$\hat{R}(a) = \frac{1}{k} \sum_{i=1}^{k} R_i(a)$$

- Samples

  $$R_j(a) \sim Pr(R(a) \mid r_1^a, \ldots, r_n^a)$$

  $$r_i^a \sim \Pr(r^a; \theta)$$

- Some exploration

Greedy Strategy

- Action Selection

  $$a^* = \text{argmax}_{\text{a}} \tilde{R}(a)$$

- Empirical mean

  $$\tilde{R}(a) = \frac{1}{n} \sum_{i=1}^{n} r_i^a$$

- Samples

  $$r_i^a \sim \Pr(r^a; \theta)$$

- No exploration

Sample Size

- In Thompson sampling, amount of data n and sample size k regulate amount of exploration
- As n and k increase, $\hat{R}(a)$ becomes less stochastic, which reduces exploration
  - As $n \uparrow$, $Pr(R(a) \mid r_1^a, \ldots, r_n^a)$ becomes more peaked
  - As $k \uparrow$, $\hat{R}(a)$ approaches $\mathbb{E}[R(a) \mid r_1^a, \ldots, r_n^a]$
- The stochasticity of $\hat{R}(a)$ ensures that all actions are chosen with some probability

Analysis

- Thompson sampling converges to best arm
- Theory:
  - Expected cumulative regret: $O(\log n)$
  - On par with UCB and ϵ-greedy
- Practice:
  - Sample size k often set to 1

Summary

- Stochastic bandits
  - Exploration/exploitation tradeoff
  - ϵ-greedy and UCB
    - Theory: logarithmic expected cumulative regret
- In practice:
  - UCB often performs better than ϵ-greedy
  - Many variants of UCB improve performance

- Bayesian Bandits
  - Thompson Sampling