Learning through Experimentation

CS246: Mining Massive Datasets
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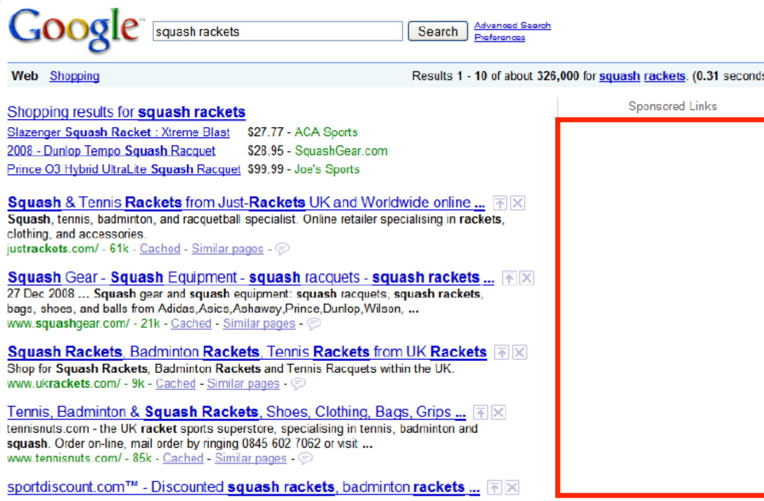
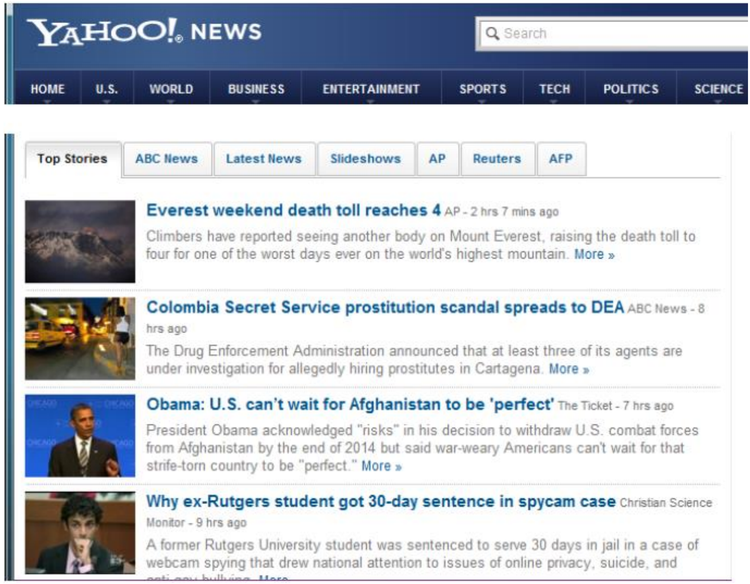
Learning through Experimentation

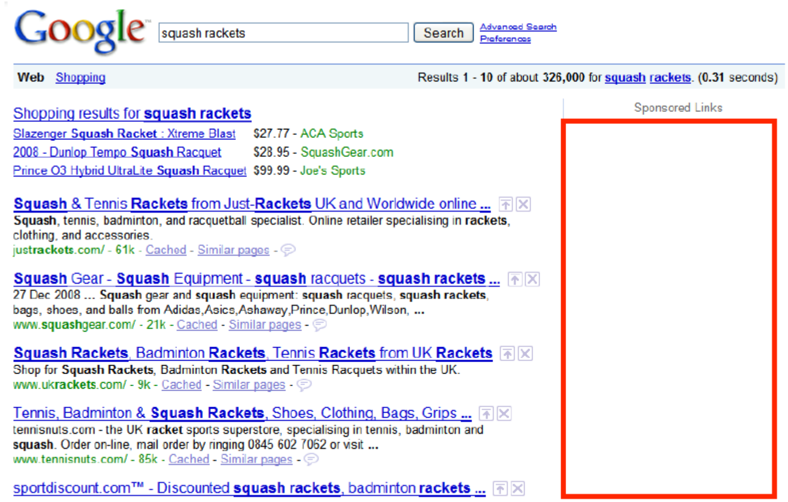
- **Web advertising**
  - We discussed how to match advertisers to queries in real-time
  - **But we did not discuss how to estimate the CTR (Click-Through Rate)**
- **Recommendation engines**
  - We discussed how to build recommender systems
  - **But we did not discuss the cold-start problem**

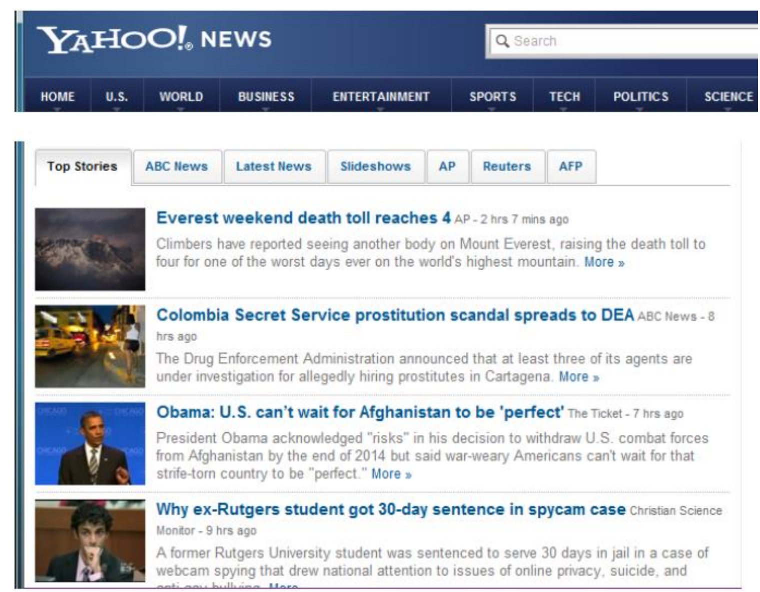




Learning through Experimentation

- What do **CTR** and **cold-start** have in common?
- With every **ad we show/ product we recommend** we gather more data about the **ad/product**
- **Theme: Learning through experimentation**





Example: Web Advertising

- **Google's goal: Maximize revenue**
- **The old way: Pay by impression (CPM)**
  - **Best strategy: Go with the highest bidder**
    - But this ignores the "effectiveness" of an ad
- **The new way: Pay per click! (CPC)**
  - **Best strategy: Go with expected revenue**
  - What's the expected revenue of **ad *a* for query *q***?
  - $\mathbf{E[revenue_{a,q}] = P(click_a \mid q) * amount_{a,q}}$

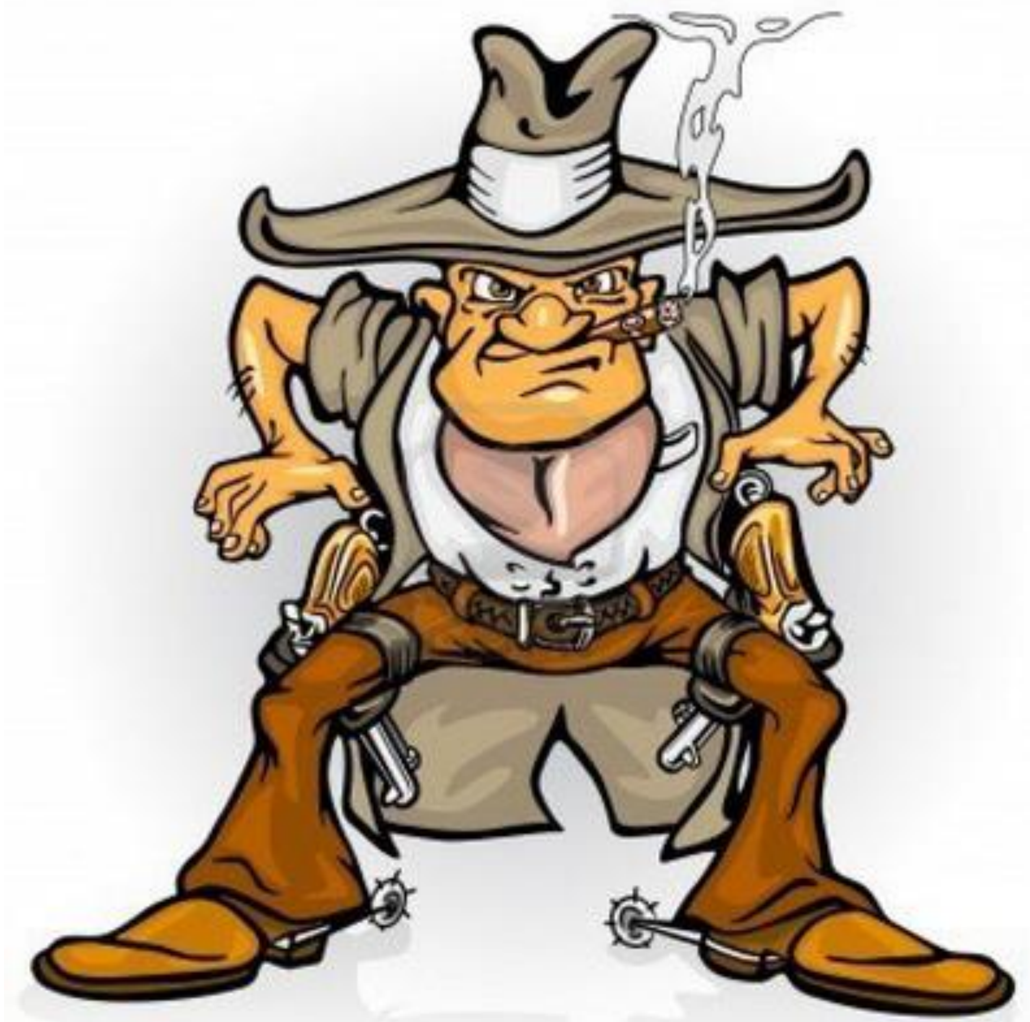
Prob. user will click on ad **a** given that she issues query **q**
(Unknown! Need to gather information)

Bid amount for ad **a** on query **q**
(Known)

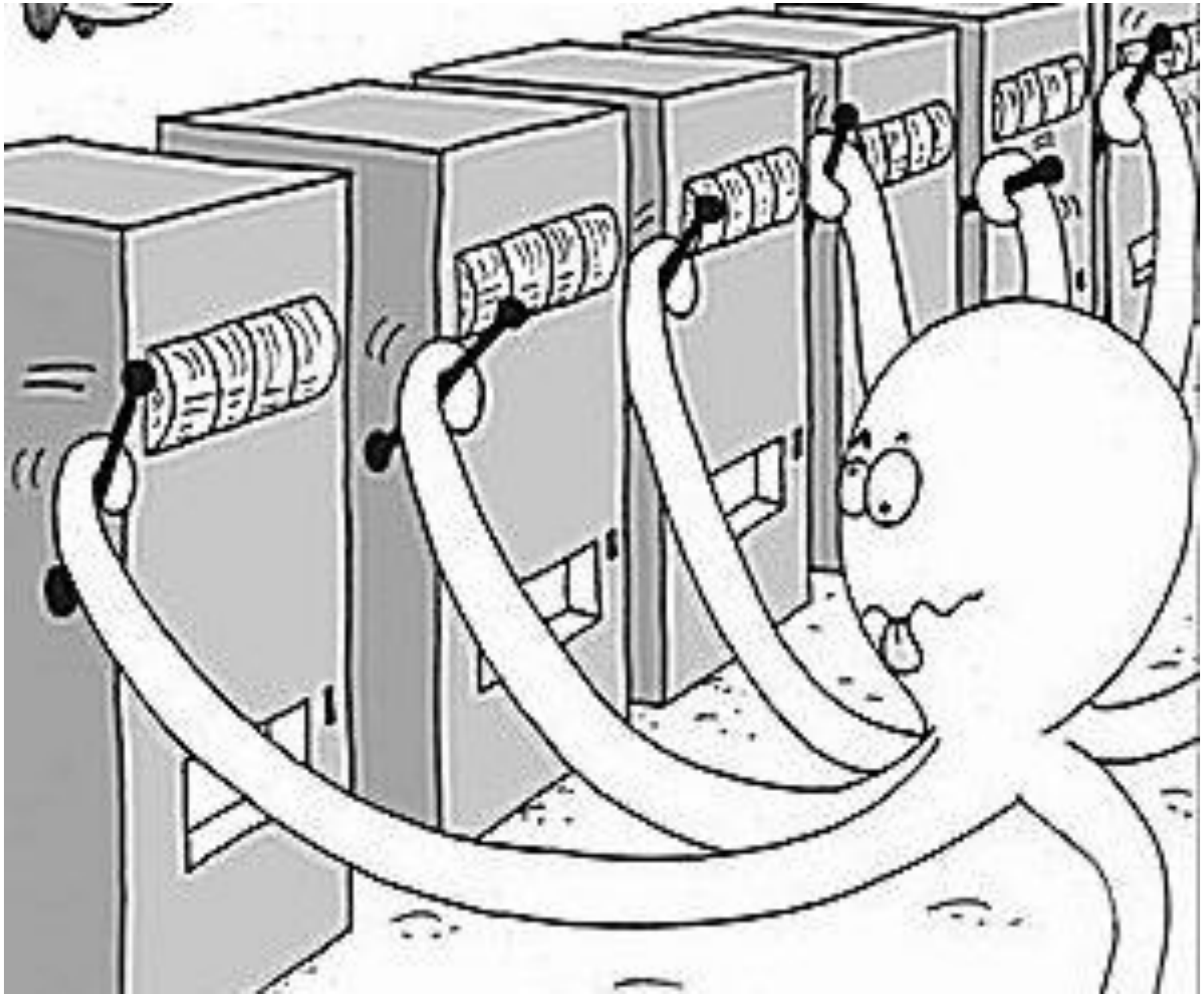
Other Applications

- **Clinical trials:**
  - Investigate effects of different treatments while minimizing adverse effects on patients
- **Adaptive routing:**
  - Minimize delay in the network by investigating different routes
- **Asset pricing:**
  - Figure out product prices while trying to make most money

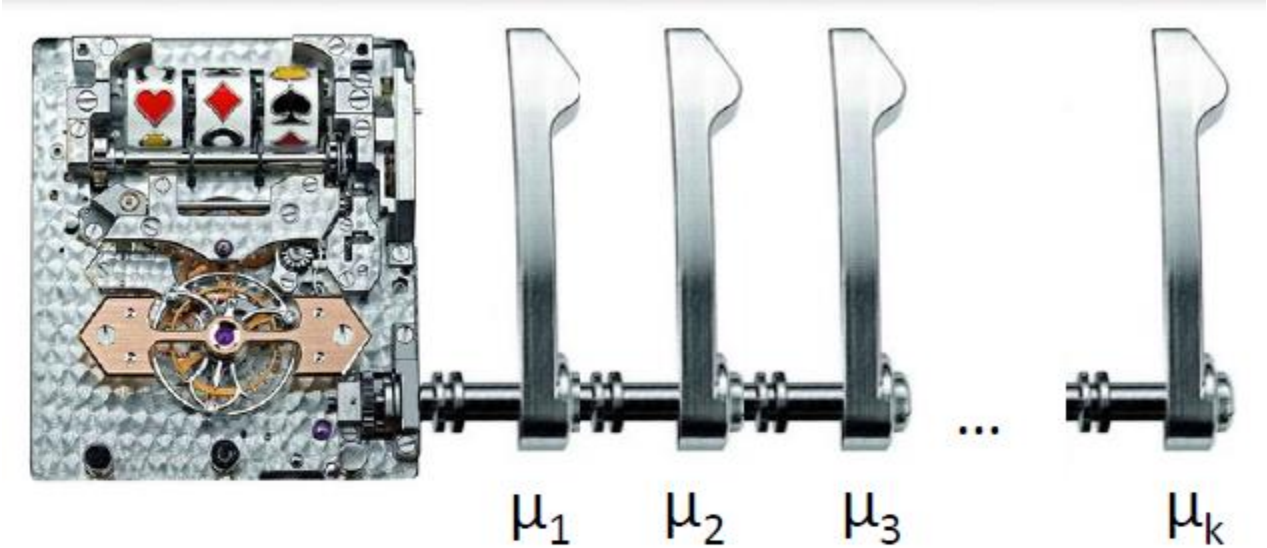
Approach: Bandits



Approach: Multiarmed Bandits

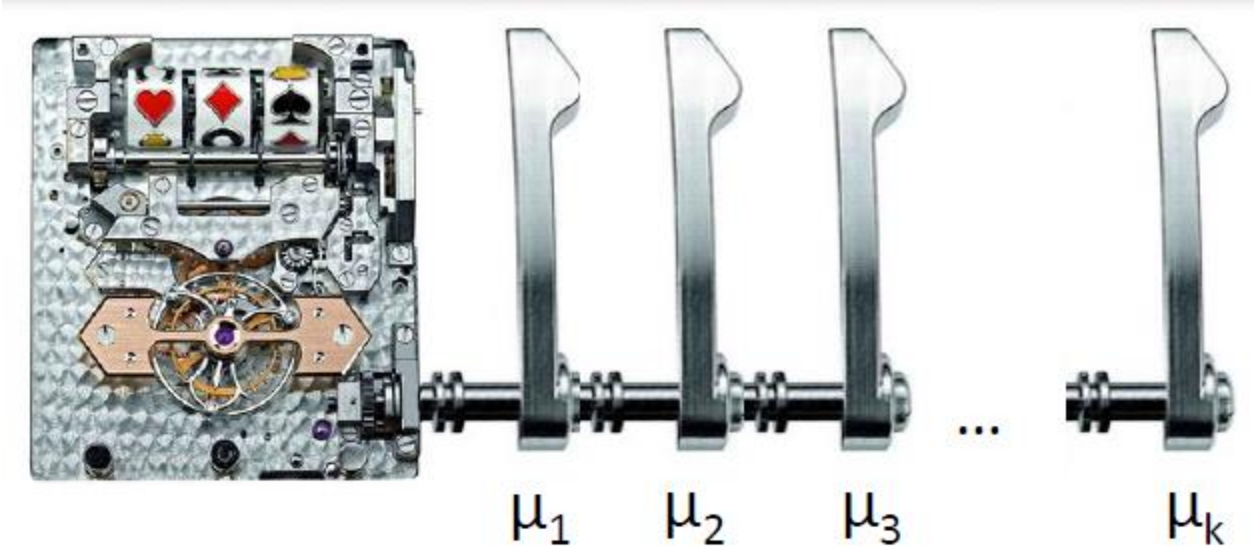


k-Armed Bandit



- **Each arm *a***
  - **Wins** (reward=**1**) with fixed (unknown) prob. $\boldsymbol{\mu_a}$
  - **Loses** (reward=**0**) with fixed (unknown) prob. $\boldsymbol{1-\mu_a}$
- All draws are independent given $\boldsymbol{\mu_1 \ldots \mu_k}$
- **How to pull arms to maximize total reward?**

k-Armed Bandit



- **How does this map to our setting?**
- Each **query** is a **bandit**
- Each **ad** is an **arm**
- **We want to estimate μ_a, the arm's probability of winning (i.e., ad's CTR μ_a)**
- Every time we pull an arm we do an 'experiment'

Stochastic k-Armed Bandit

The setting:

- Set of ***k*** choices (arms)
- Each choice ***a*** is associated with unknown probability distribution P_a supported in **[0,1]**
- We play the game for ***T*** rounds
- In each round ***t***:
  - **(1)** We pick some arm ***a***
  - **(2)** We obtain random sample X_t from P_a
    - Note reward is independent of previous draws
- **Our goal is to maximize** $\sum_{t=1}^{T} X_t$
- **Problem: we don't know** μ_a**!** But every time we pull some arm ***a*** we get to learn a bit about μ_a

Online Optimization

- **Online optimization with limited feedback**

Choices	X_1	X_2	X_3	X_4	X_5	X_6	…
a_1					1	1	
a_2	0		1	0			
…							
a_k		0					

Time

- **Like in online algorithms:**
  - Have to make a choice each time
  - But we only receive information about the chosen action

Solving the Bandit Problem

- **Policy**: a strategy/rule that tells me which arm to pull in each iteration
  - Hopefully policy depends on the history of rewards

- **How to quantify performance of the algorithm? Regret!**

Performance Metric: Regret

- Let $\boldsymbol{\mu_a}$ be the mean reward of $\boldsymbol{P_a}$
- Payoff/reward of **best arm**: $\boldsymbol{\mu^* = \max_a \mu_a}$
- Let $\boldsymbol{i_1, i_2 \dots i_T}$ be the sequence of arms pulled
- Instantaneous **regret** at time $\boldsymbol{t}$: $\boldsymbol{r_t = \mu^* - \mu_{i_t}}$
- **Total regret:**

$$\boldsymbol{R_T = \sum_{t=1}^{T} r_t}$$

- <u>**Typical goal:**</u> **Want a policy (arm allocation strategy) that guarantees:** $\boldsymbol{\frac{R_T}{T} \to 0}$ **as** $\boldsymbol{T \to \infty}$
  - Note: Ensuring $R_T/T \to 0$ is stronger than maximizing payoffs (minimizing regret), as it means that in the limit we discover the true best hand.

Allocation Strategies

- **If we knew the payoffs, which arm would we pull?**

$$\text{Pick} \quad \arg\max_a \mu_a$$

- **What if we only care about estimating payoffs μ_a?**
  - Pick each of k arms equally often: $\frac{T}{k}$
  - **Estimate:** $\widehat{\mu_a} = \frac{k}{T}\sum_{j=1}^{T/k} X_{a,j}$
  - **Regret:** $R_T = \frac{T}{k}\sum_{a=1}^{k}(\mu^* - \widehat{\mu_a})$

$X_{a,j}$ … payoff received when pulling arm a for j-th time

Bandit Algorithm: First try

- Regret is defined in terms of average reward
- So, if we can estimate avg. reward we can minimize regret
- Consider algorithm: *Greedy*
  Take the action with the highest avg. reward
  - **Example:** Consider 2 actions
    - **A1** reward 1 with prob. 0.3
    - **A2** has reward 1 with prob. 0.7
  - Play **A1**, get reward 1
  - Play **A2**, get reward 0
  - Now avg. reward of **A1** will never drop to 0, and we will never play action **A2**

Exploration vs. Exploitation

- **The example illustrates a classic problem in** **decision making:**
  - We need to trade off between **exploration** (gathering data about arm payoffs) and **exploitation** (making decisions based on data already gathered)

- **The Greedy algo does not explore sufficiently**
  - **Exploration:** Pull an arm we never pulled before
  - **Exploitation:** Pull an arm $\boldsymbol{a}$ for which we currently have the highest estimate of $\boldsymbol{\mu_a}$

Optimism

- The problem with our **Greedy** algorithm is that it is **too certain** in the estimate of $\boldsymbol{\mu_a}$
  - When we have seen a single reward of 0 we shouldn't conclude the average reward is 0
- **Greedy can converge to a suboptimal solution!**

New Algorithm: Epsilon-Greedy

Algorithm: Epsilon-Greedy

- **For t=1:T**
  - Set $\boldsymbol{\varepsilon_t = O\left(\frac{1}{t}\right)}$ (that is, ε_t decays over time t as $1/t$)
  - **With prob. $\boldsymbol{\varepsilon_t}$: Explore** by picking an arm chosen uniformly at random
  - **With prob. $\boldsymbol{1-\varepsilon_t}$: Exploit** by picking an arm with highest empirical mean payoff
- **Theorem [Auer et al. '02]**
  For suitable choice of $\boldsymbol{\varepsilon_t}$ it holds that

$$R_T = O(k \log T) \Rightarrow \frac{R_T}{T} = O\left(\frac{k \log T}{T}\right) \to 0$$

k…number of arms

Issues with Epsilon-Greedy

- What are some issues with **Epsilon-Greedy**?
  - **"Not elegant"**: Algorithm explicitly distinguishes between exploration and exploitation
  - **More importantly:** Exploration makes **suboptimal choices** (since it picks any arm equally likely)
- **Idea:** When exploring/exploiting we need to **compare** arms

Comparing Arms

- **Suppose we have done experiments:**
  - **Arm 1**: 1 0 0 1 1 0 0 1 0 1
  - **Arm 2**: 1
  - **Arm 3**: 1 1 0 1 1 1 0 1 1 1
- **Mean arm values:**
  - **Arm 1**: 5/10, **Arm 2**: 1, **Arm 3**: 8/10
- **Which arm would you pick next?**
- **Idea: Don't just look at the mean (that is, expected payoff) but also the confidence!**

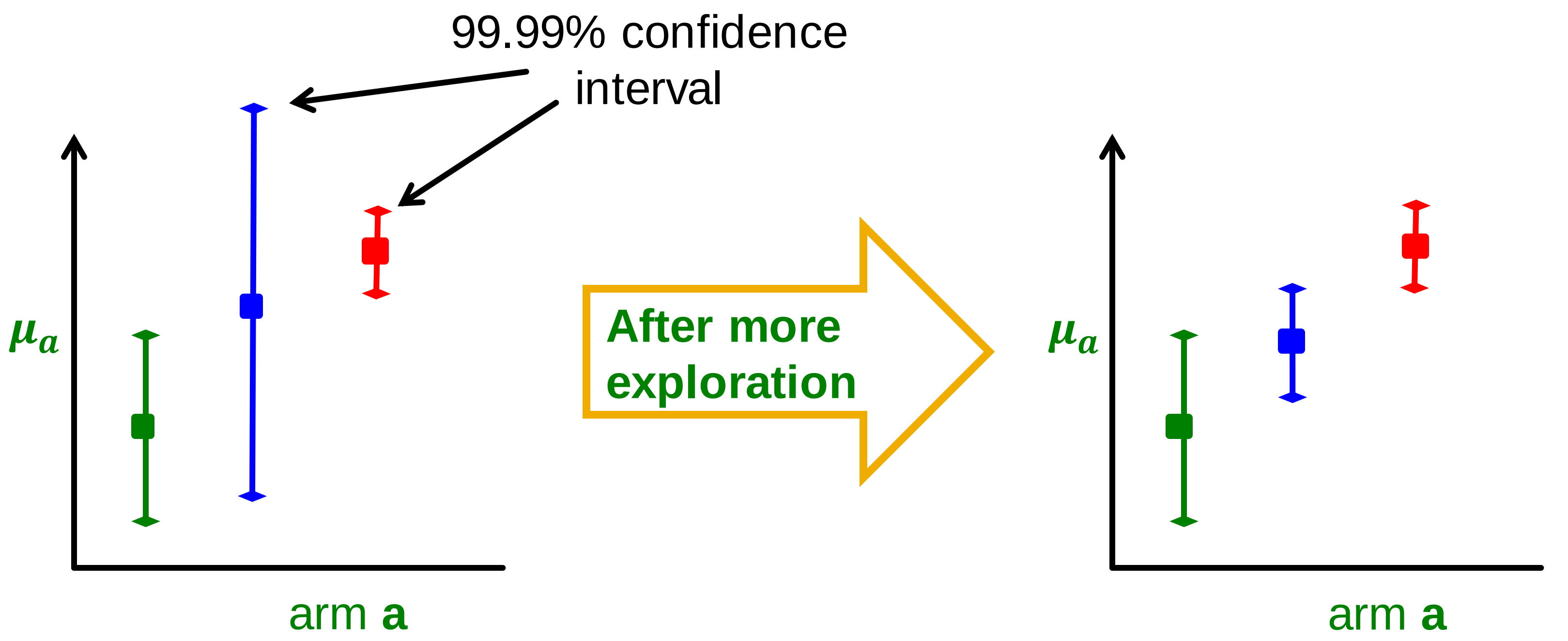
Confidence Intervals (1)

- **A confidence interval is a range of values within which we are sure the mean lies with a certain probability**
  - We could believe $\boldsymbol{\mu_a}$ is within [0.2,0.5] with probability 0.95
  - If we would have tried an action less often, our estimated reward is less accurate so the confidence interval is larger
  - Interval shrinks as we get more information (try the action more often)

Confidence Intervals (2)

- **Assuming we know the confidence intervals**
- **Then, instead of trying the action with the highest mean we can try the action with the highest upper bound on its confidence interval**
- This is called an **optimistic policy**
  - We believe an action is as good as possible given the available evidence

Confidence Based Selection



Calculating Confidence Bounds

Suppose we fix arm *a*:

- Let $X_{a,1} \dots X_{a,m}$ be the payoffs of arm ***a*** in the first ***m*** trials
  - So, $X_{a,1} \dots X_{a,m}$ are **i.i.d.** rnd. vars. taking values in **[0,1]**
- **Mean payoff of arm *a*:** $\mu_a = E[X_{a,\cdot}]$
- **Our estimate:** $\widehat{\mu_{a,m}} = \frac{1}{m}\sum_{\ell=1}^{m} X_{a,\ell}$
- Want to find b such that with high probability $\left|\mu_a - \widehat{\mu_{a,m}}\right| \le b$
  - Want b to be as small as possible (so our estimate is close)
- **Goal: Want to bound** $\mathrm{P}\left(\left|\mu_a - \widehat{\mu_{a,m}}\right| \le b\right)$

Hoeffding's Inequality (1)

Hoeffding's inequality provides an upper bound on the probability that the average deviates from its expected value by more than a certain amount:

- Let $\boldsymbol{X_1} \dots \boldsymbol{X_m}$ be **i.i.d.** rnd. vars. taking values in **[0,1]**
- Let $\boldsymbol{\mu} = \boldsymbol{E}[\boldsymbol{X}]$ and $\widehat{\boldsymbol{\mu_m}} = \frac{\mathbf{1}}{\boldsymbol{m}} \sum_{\boldsymbol{\ell}=\mathbf{1}}^{\boldsymbol{m}} \boldsymbol{X_\ell}$
- **Then:** $\mathbf{P}(|\boldsymbol{\mu} - \widehat{\boldsymbol{\mu_m}}| \geq \boldsymbol{b}) \leq \mathbf{2}\,\boldsymbol{exp}\left(-\mathbf{2}\boldsymbol{b}^{\mathbf{2}}\boldsymbol{m}\right) = \boldsymbol{\delta}$
  - $\boldsymbol{\delta}$**… is the confidence level**

- **To find out the confidence interval $\boldsymbol{b}$ (for a given confidence level $\boldsymbol{\delta}$) we solve:**
  - $2e^{-2b^2m} \leq \delta$ **then** $-2b^2m \leq \ln(\delta/2)$
  - **So:** $\boldsymbol{b} \geq \sqrt{\frac{\ln\left(\frac{2}{\delta}\right)}{2\,m}}$

Hoeffding's Inequality (2)

- $\mathbf{P}(|\mu - \widehat{\mu_m}| \geq b) \leq 2\,exp(-2b^2 m)$ where b **is our upper bound,** m **is number of times we played the action**
- Let's set $b = b(a,T) = \sqrt{2log(T)/m_a}$
- **Then:** $\mathbf{P}(|\mu - \widehat{\mu_m}| \geq b) \leq 2T^{-4}$ **which converges to zero very quickly:**
  - **Notice:**
    - **If we don't play action** a**, its upper bound** b **increases**
      - **This means we never permanently rule out an action no matter how poorly it performs**
    - **Prob. our upper bound is wrong decreases with time** T

UCB1 Algorithm

[Auer et al. '02]
http://www.jmlr.org/papers/volume3/auer02a/auer02a.pdf

- **UCB1 (Upper confidence sampling) algorithm**
  - **Set:** $\widehat{\mu_1} = \cdots = \widehat{\mu_k} = 0$ and $m_1 = \cdots = m_k = 0$
    - $\widehat{\mu_a}$ **is our estimate of payoff of arm** a
    - m_a **is the number of pulls of arm** a **so far**
  - **For** ***t = 1:T***
    - **For each arm** ***a*** **calculate:** $UCB(a) = \widehat{\mu_a} + \alpha\sqrt{\frac{2 \ln t}{m_a}}$

      Upper confidence interval (Hoeffding's inequality)
    - **Pick arm** $j = arg\, max_a\, UCB(a)$
    - **Pull arm** ***j*** **and observe** y_t
    - **Set:** $m_j \leftarrow m_j + 1$ **and** $\widehat{\mu_j} \leftarrow \frac{1}{m_j}\left(y_t + (m_j - 1)\,\widehat{\mu_j}\right)$

α...is a free parameter trading off exploration vs. exploitation

UCB1: Discussion

- $UCB(a) = \widehat{\mu_a} + \alpha\sqrt{\frac{2\ln t}{m_a}}$

$$b \geq \sqrt{\frac{\ln\left(\frac{2}{\delta}\right)}{2\,m}}$$

  - Confidence interval **grows** with the total number of actions t we have taken
  - But **shrinks** with the number of times m_a we have tried arm a
  - This ensures each arm is tried infinitely often but still balances exploration and exploitation
  - α plays the role of δ: $\alpha = f\left(\frac{2}{\delta}\right)$

$$\mathbf{P}(|\mu - \widehat{\mu_m}| \geq b) = \delta$$

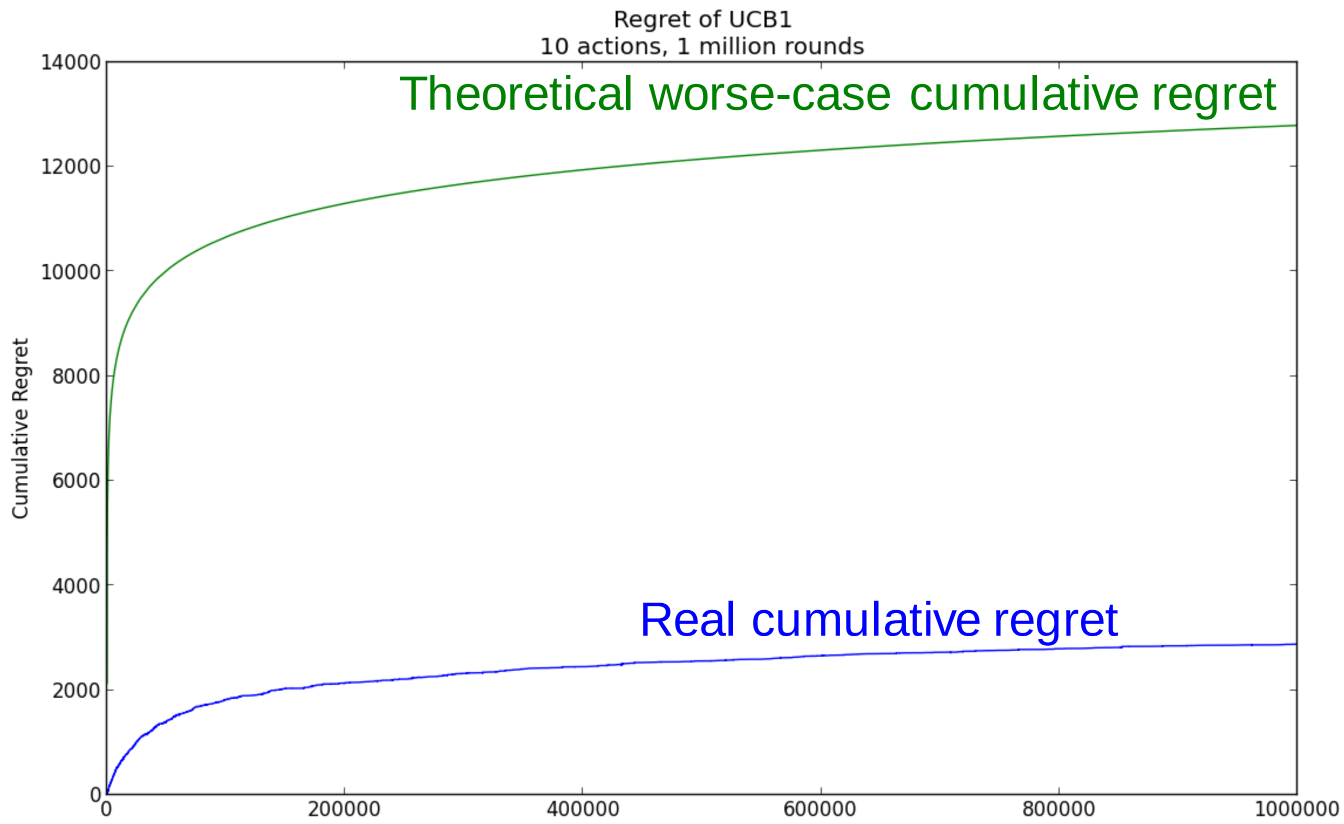
<u>"Optimism in face of uncertainty":</u>
The algorithm believes that it can obtain extra rewards by reaching the unexplored parts of the state space

Summary so far

- ***k***-armed bandit problem as a formalization of the exploration-exploitation tradeoff
- Analog of online optimization (e.g., SGD, BALANCE), but with **limited feedback**
- **Simple algorithms are able to achieve no regret (in the limit)**
  - Epsilon-greedy
  - UCB (Upper Confidence Sampling)

Example

- 10 actions, 1M rounds, uniform [0,1] rewards



Use-case: Pinterest

- **Problem: For new pins/ads we do not have enough signal on how good they are**
  - How likely are people to interact with them?
- **Idea:**
  - Try to maximize the rewards from several unknown slot machines by deciding which machines and the order to play
  - Each pin is regarded as an arm, user engagement are considered as rewards
  - Making tradeoff between exploration and exploitation, avoid keep showing the best known pins and trapping the system into local optima

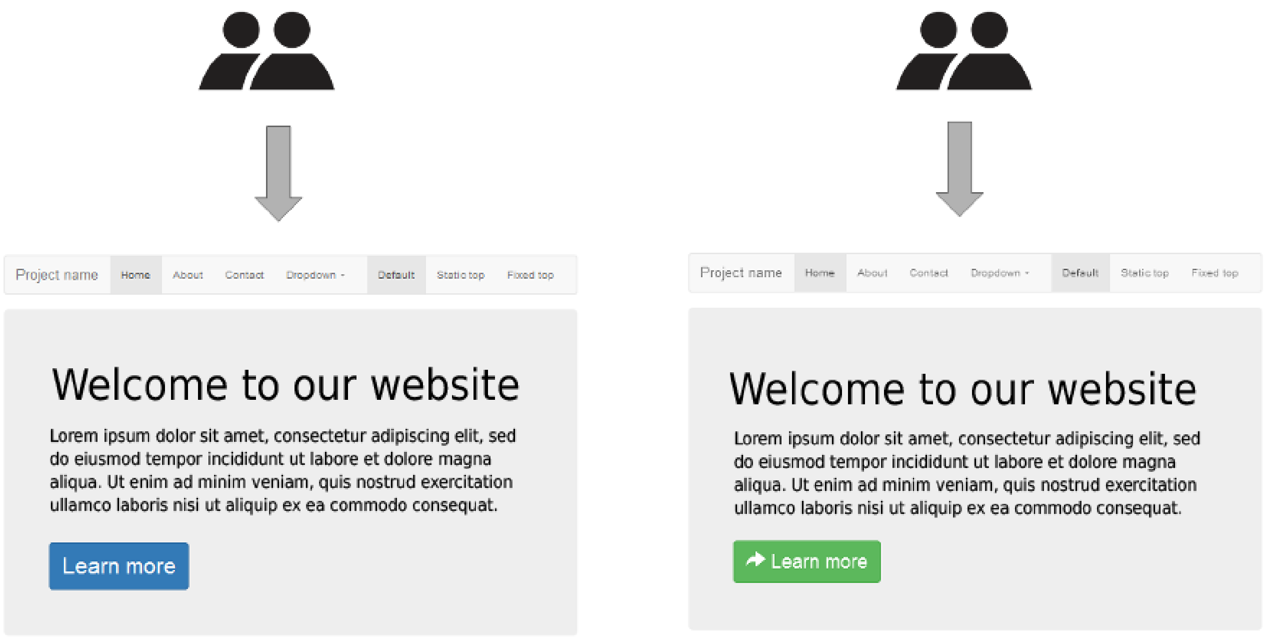
Use-case: Pinterest

- **Solution: Bandit algorithm in round *t***
  - **(1) Algorithm** observes user is seeing a set A of pins/ads
  - **(2)** Based on payoffs from previous trials, algorithm chooses arm $a \in A$ and receives payoff $r_{t,a}$
    - **Note only feedback for the chosen *a* is observed**
  - **(3)** Algorithm improves arm selection strategy with each observation $(a, r_{t,a})$

- **If the score for a pin is low, filter it out**

Use Case: A/B testing

- **A/B testing is a controlled experiment with two variants, A and B**
- Part of the traffic sees variant **A**, part variant **B**



Click rate: 52 % 72 %

Use Case: A/B testing

- **Part of the traffic sees variant A, part variant B**
- Hypothesis test: does variant A outperform variant B? What test to perform?

Assumed Distribution	Example	Standard Test
Gaussian	Average Revenue Per Paying User	Welch's t-test (Unpaired t-test)
Binomial	Click Through Rate	Fisher's exact test
Poisson	Transactions Per Paying User	E-test
Multinomial	Number of each product purchased	Chi-squared test

- If **A** outperforms **B**, we want to stop the experiment as soon as possible

Use Case: A/B testing

- **Imagine you have two versions of the website and you'd like to test which one is better**
  - Version **A** has engagement rate of **5%**
  - Version **B** has engagement rate of **4%**
- **You want to establish with 95% confidence that version A is better**
  - Using t-test, you'd need 22,330 observations (11,165 in each arm) to establish that
- **Can bandits do better?**

Example: Bandits vs. A/B testing

- **How long does it take to discover A > B?**
  - **A/B test:** We need 22,330 observations. Assuming 100 observations/day, we need 223 days
- **The goal is to find the best action (A vs. B)**
- The randomization distribution (traffic to A vs. B) can be updated as the experiment progresses
- **Idea:**
  - Twice per day, examine how each of the variations/arms has performed
  - Adjust the fraction of traffic that each arm will receive going forward
  - An arm that appears to be doing well gets more traffic, and an arm that is clearly underperforming gets less

Thompson Sampling

- **Thompson sampling** assigns sessions to arms in proportion to the probability that each arm is optimal.

- Assume outcome distribution in the set {0,1}
  - The arm either converts or not

- Then we flip a coin with probability θ → Bernoulli distribution!

- To estimate θ, we count up numbers of ones and zeros

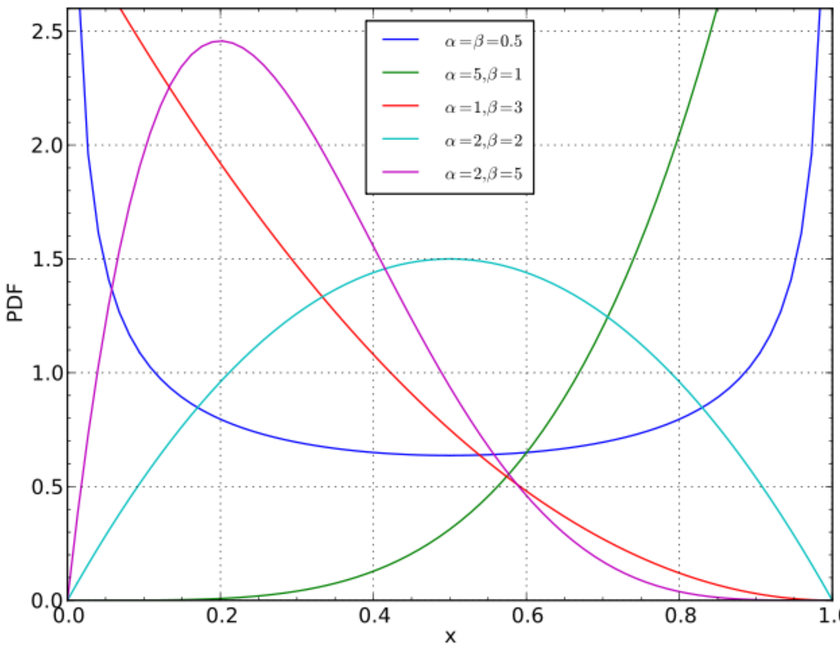
Thompson Sampling: Bernoulli Case

- Given observed 1s and 0s, how do we calculate the distribution of possible values of θ?

- **Let**:
  - $\theta = (\theta_1, \theta_2, \ldots, \theta_k)$ … the vector of conversion rates for arms *1, …, k*.
    - θ_i = #successes / (#successes + #failures)

Beta-Bernoulli Case

- Beta(α,β) → Given a 0's and b 1's, what is the distribution over means?
- Prior → pseudocounts



- Likelihood → observed counts
- Posterior → psuedocounts + observed counts

Thompson Sampling

- **Arm probabilities θ can be computed using sampling:**
  - Each element of θ is an independent random variable from a Beta distribution $(\alpha + successes, \beta + failures)$

Algorithm 2 Thompson sampling for the Bernoulli bandit

Require: α, β prior parameters of a Beta distribution

$S_i = 0, F_i = 0, \quad \forall i.$ {Success and failure counters}

for $t = 1, \ldots, T$ **do**

  for $i = 1, \ldots, K$ **do**

    Draw θ_i according to Beta$(S_i + \alpha, F_i + \beta)$.

  end for

  Draw arm $\hat{\imath} = \arg\max_i \theta_i$ and observe reward r

  if $r = 1$ **then**

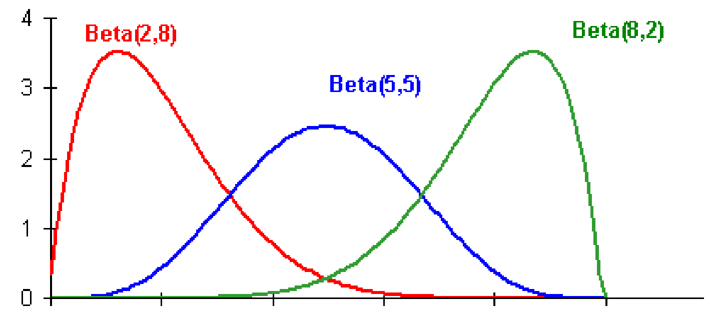
    $S_{\hat{\imath}} = S_{\hat{\imath}} + 1$

  else

    $F_{\hat{\imath}} = F_{\hat{\imath}} + 1$

  end if

end for



Thompson Sampling in General

Thompson Sampling:

- 1. Specify prior (in Beta case often Beta(1,1))
- 2. Sample from each posterior distribution to get estimated mean for each arm
- 3. Pull arm with highest mean
- 4. Repeat step 2 & 3 forever

Back to Our Problem

But, in our case we have to set the amount of traffic. Set it to be proportional to $P(I_a)$:

- **(1)** Simulate many draws from $Beta(\alpha+S_a, \beta + F_a)$:

Time	Arm 1	Arm 2	Arm 3
1	0.54	0.73	0.74
2	0.55	0.66	0.73
3	0.53	0.81	0.80
…			

- **(2) The probability that arm *a*** is optimal is the empirical fraction of rows for which arm *a* had the largest simulated value
- **(3) Set traffic to arm a to be equal to % of wins of arm a**

Reminder: Use Case

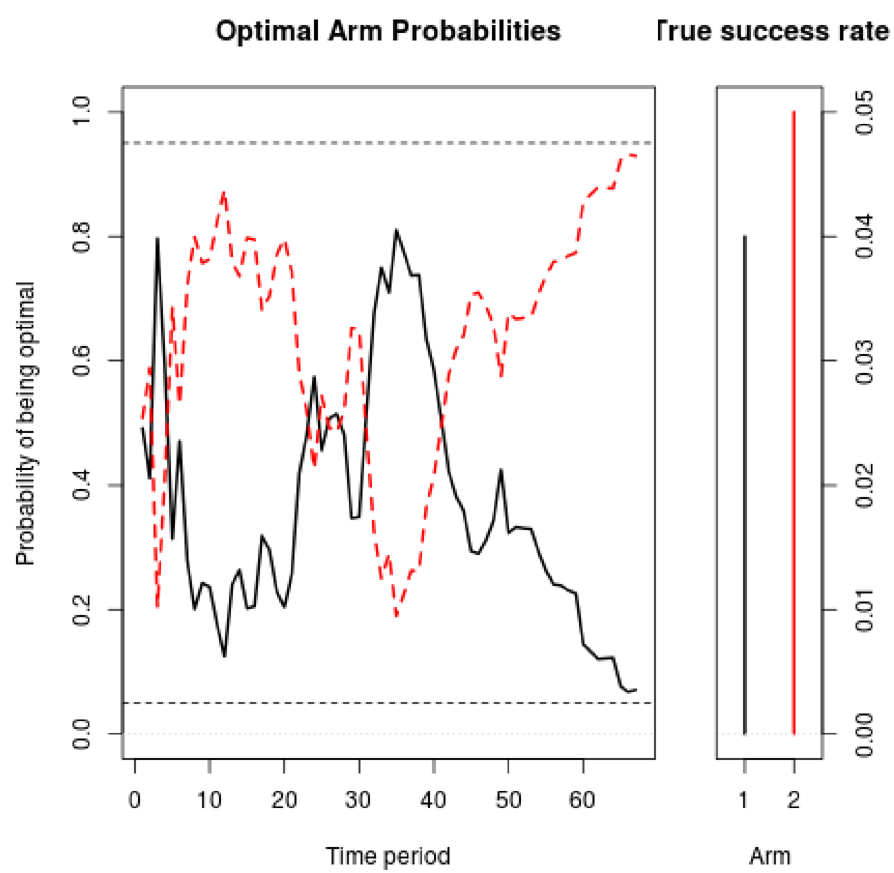
- **Imagine you have two versions of the website and you'd like to test which one is better**
  - Version **A** has engagement rate of **5%**
  - Version **B** has engagement rate of **4%**
- **You want to establish with 95% confidence that version A is better**
  - You'd need 22,330 observations (11,165 in each arm) to establish that
    - Use t-test to establish the sample size
- **Can bandits do better?**

Example

A/B test: We need 22,330 observations. Assuming 100 observations/day, we need 223 days

- On 1st day about 50 sessions are assigned to each arm
- Suppose **A** got really lucky on the first day, and it appears to have a 70% chance of being superior
- Then we assign it 70% of the traffic on the second day, and the variant B gets 30%
- At the end of the 2nd day we accumulate all the traffic we've seen so far (over both days), and recompute the probability that each arm is best

Simulation



- **The experiment finished in 66 days, so it saved you 157 days of testing (66 vs 223)**

Generalization to multiple arms

- **Easy to generalize to multiple arms:**