CS 747, Autumn 2022: Lecture 3

Shivaram Kalyanakrishnan

Department of Computer Science and Engineering Indian Institute of Technology Bombay

Autumn 2022

Shivaram Kalyanakrishnan (2022)

- The exploration-exploitation dilemma
- Definitions: Bandit, Algorithm
- *e*-greedy algorithms
- Evaluating algorithms: Regret
- Achieving sub-linear regret
- A lower bound on regret

- The exploration-exploitation dilemma
- Definitions: Bandit, Algorithm
- *e*-greedy algorithms
- Evaluating algorithms: Regret
- Achieving sub-linear regret
- A lower bound on regret
- UCB, KL-UCB algorithms
- Thompson Sampling algorithm
- Concentration bounds

- The exploration-exploitation dilemma
- Definitions: Bandit, Algorithm
- *c*-greedy algorithms
- Evaluating algorithms: Regret
- Achieving sub-linear regret
- A lower bound on regret
- UCB, KL-UCB algorithms
- Thompson Sampling algorithm
- Concentration bounds
- Analysis of UCB
- Understanding Thompson Sampling
- Other bandit problems

- The exploration-exploitation dilemma
- Definitions: Bandit, Algorithm
- e-greedy algorithms
- Evaluating algorithms: Regret
- Achieving sub-linear regret
- A lower bound on regret
- UCB, KL-UCB algorithms
- Thompson Sampling algorithm
- Concentration bounds
- Analysis of UCB
- Understanding Thompson Sampling
- Other bandit problems

Upper Confidence Bounds = UCB (Auer et al., 2002) - At time t, for every arm *a*, define $ucb_a^t = \hat{p}_a^t + \sqrt{\frac{2 \ln(t)}{u_a^t}}$.

- \hat{p}_{a}^{t} is the empirical mean of rewards from arm a.
- u_a^t the number of times a has been sampled at time t.



Upper Confidence Bounds = UCB (Auer et al., 2002) - At time t, for every arm *a*, define $ucb_a^t = \hat{p}_a^t + \sqrt{\frac{2 \ln(t)}{u_a^t}}$.

- \hat{p}_{a}^{t} is the empirical mean of rewards from arm a.
- u_a^t the number of times a has been sampled at time t.
- Pull an arm *a* for which ucb_a^t is maximum.



Upper Confidence Bounds = UCB (Auer et al., 2002)

- At time t, for every arm *a*, define $\operatorname{ucb}_a^t = \hat{p}_a^t + \sqrt{\frac{2\ln(t)}{u_a^t}}$.
- \hat{p}_a^t is the empirical mean of rewards from arm a.
- u_a^t the number of times *a* has been sampled at time *t*.
- Pull an arm a for which ucb^t_a is maximum.



Upper Confidence Bounds = UCB (Auer et al., 2002)

- At time t, for every arm *a*, define $\operatorname{ucb}_a^t = \hat{p}_a^t + \sqrt{\frac{2\ln(t)}{u_a^t}}$.
- \hat{p}_a^t is the empirical mean of rewards from arm a.
- u_a^t the number of times *a* has been sampled at time *t*.
- Pull an arm a for which ucb_a^t is maximum.



Achieves regret of $O(\log(T))$: optimal dependence on T.

 Identical to UCB algorithm on previous slide, except for a different definition of the upper confidence bound.

 Identical to UCB algorithm on previous slide, except for a different definition of the upper confidence bound.

 $\mathsf{ucb-kl}_a^t = \max\{q \in [\hat{p}_a^t, 1] \text{ s. t. } u_a^t \mathsf{KL}(\hat{p}_a^t, q) \le \ln(t) + c \ln(\ln(t))\}, \text{ where } c \ge 3.$

 Identical to UCB algorithm on previous slide, except for a different definition of the upper confidence bound.

ucb-kl^t_a = max{ $q \in [\hat{p}_a^t, 1]$ s. t. $u_a^t KL(\hat{p}_a^t, q) \le \ln(t) + c \ln(\ln(t))$ }, where $c \ge 3$. Equivalently, ucb-kl^t_a is the solution $q \in [\hat{p}_a^t, 1]$ to $KL(\hat{p}_a^t, q) = \frac{\ln(t) + c \ln(\ln(t))}{u_a^t}$.

 Identical to UCB algorithm on previous slide, except for a different definition of the upper confidence bound.

 $ucb-kl_a^t = \max\{q \in [\hat{p}_a^t, 1] \text{ s. t. } u_a^t \mathcal{KL}(\hat{p}_a^t, q) \le \ln(t) + c \ln(\ln(t))\}, \text{ where } c \ge 3.$

Equivalently, ucb-kl^t_a is the solution $q \in [\hat{p}_a^t, 1]$ to $KL(\hat{p}_a^t, q) = \frac{\ln(t) + c \ln(\ln(t))}{u_a^t}$.

KL-UCB algorithm: at step *t*, pull $\operatorname{argmax}_{a \in A} \operatorname{ucb-kl}_{a}^{t}$.

 Identical to UCB algorithm on previous slide, except for a different definition of the upper confidence bound.

ucb-kl^t_a = max{ $q \in [\hat{p}_{a}^{t}, 1]$ s. t. $u_{a}^{t} KL(\hat{p}_{a}^{t}, q) \leq \ln(t) + c \ln(\ln(t))$ }, where $c \geq 3$. Equivalently, ucb-kl^t_a is the solution $q \in [\hat{p}_{a}^{t}, 1]$ to $KL(\hat{p}_{a}^{t}, q) = \frac{\ln(t) + c \ln(\ln(t))}{u_{a}^{t}}$. KL-UCB algorithm: at step t, pull $\operatorname{argmax}_{a \in A}$ ucb-kl^t_a.

- Observe that $KL(\hat{p}_a^t, q)$ monotonically increases with q, and
 - $KL(\hat{p}_{a}^{t},\hat{p}_{a}^{t})=0;$
 - $KL(\hat{p}_a^t, 1) = \infty.$

Easy to compute ucb- kl_a^t numerically (for example through binary search).

 Identical to UCB algorithm on previous slide, except for a different definition of the upper confidence bound.

ucb-kl^t_a = max{ $q \in [\hat{p}_{a}^{t}, 1]$ s. t. $u_{a}^{t} KL(\hat{p}_{a}^{t}, q) \leq \ln(t) + c \ln(\ln(t))$ }, where $c \geq 3$. Equivalently, ucb-kl^t_a is the solution $q \in [\hat{p}_{a}^{t}, 1]$ to $KL(\hat{p}_{a}^{t}, q) = \frac{\ln(t) + c \ln(\ln(t))}{u_{a}^{t}}$. KL-UCB algorithm: at step t, pull $\operatorname{argmax}_{a \in A}$ ucb-kl^t_a.

- Observe that $KL(\hat{p}_a^t, q)$ monotonically increases with q, and
 - $KL(\hat{p}_{a}^{t},\hat{p}_{a}^{t})=0;$
 - $KL(\hat{p}_a^t, 1) = \infty.$

Easy to compute ucb- kl_a^t numerically (for example through binary search).

• ucb-kl^t_a is a tighter confidence bound than ucb^t_a.

 Identical to UCB algorithm on previous slide, except for a different definition of the upper confidence bound.

ucb-kl^t_a = max{ $q \in [\hat{p}_{a}^{t}, 1]$ s. t. $u_{a}^{t}KL(\hat{p}_{a}^{t}, q) \leq \ln(t) + c\ln(\ln(t))$ }, where $c \geq 3$. Equivalently, ucb-kl^t_a is the solution $q \in [\hat{p}_{a}^{t}, 1]$ to $KL(\hat{p}_{a}^{t}, q) = \frac{\ln(t) + c\ln(\ln(t))}{u_{a}^{t}}$. KL-UCB algorithm: at step t, pull $\operatorname{argmax}_{a \in A}$ ucb-kl^t_a.

- Observe that $KL(\hat{p}_a^t, q)$ monotonically increases with q, and
 - $KL(\hat{p}_{a}^{t},\hat{p}_{a}^{t})=0;$
 - $KL(\hat{p}_a^t, 1) = \infty.$

Easy to compute ucb- kl_a^t numerically (for example through binary search).

ucb-kl^t_a is a tighter confidence bound than ucb^t_a.
 Regret of KL-UCB asymptotically matches Lai and Robbins' lower bound!

- 1. UCB, KL-UCB algorithms
- 2. Thompson Sampling algorithm
- 3. Concentration bounds

Background: Beta Distribution

• Beta(α , β) defined on [0, 1]. Two parameters: α and β .

Mean =
$$\frac{\alpha}{\alpha + \beta}$$
; Variance = $\frac{\alpha\beta}{(\alpha + \beta)^2(\alpha + \beta + 1)}$.



Background: Beta Distribution

• Beta(α , β) defined on [0, 1]. Two parameters: α and β .



- At time t, let arm a have s_a^t successes (1's/heads) and f_a^t failures (0's/tails).

- At time t, let arm a have s_a^t successes (1's/heads) and f_a^t failures (0's/tails).
- $Beta(s_a^t + 1, f_a^t + 1)$ represents a "belief" about the true mean of arm *a*.
- Mean = $\frac{s_a^t+1}{s_a^t+t_a^t+2}$; variance = $\frac{(s_a^t+1)(t_a^t+1)}{(s_a^t+t_a^t+2)^2(s_a^t+t_a^t+3)}$.



- At time t, let arm a have s_a^t successes (1's/heads) and f_a^t failures (0's/tails).
- $Beta(s_a^t + 1, f_a^t + 1)$ represents a "belief" about the true mean of arm *a*.
- Mean = $\frac{s_a^t+1}{s_a^t+t_a^t+2}$; variance = $\frac{(s_a^t+1)(t_a^t+1)}{(s_a^t+t_a^t+2)^2(s_a^t+t_a^t+3)}$.
- Computational step: For every arm a, draw a sample (in agent's mind) $x_a^t \sim Beta(s_a^t + 1, f_a^t + 1).$
- Sampling step: Pull (in real world) arm *a* for which x_a^t is maximum.



- At time t, let arm a have s_a^t successes (1's/heads) and f_a^t failures (0's/tails).
- $Beta(s_a^t + 1, f_a^t + 1)$ represents a "belief" about the true mean of arm *a*.
- Mean = $\frac{s_a^t+1}{s_a^t+t_a^t+2}$; variance = $\frac{(s_a^t+1)(t_a^t+1)}{(s_a^t+t_a^t+2)^2(s_a^t+t_a^t+3)}$.
- Computational step: For every arm a, draw a sample (in agent's mind) $x_a^t \sim Beta(s_a^t + 1, f_a^t + 1).$
- Sampling step: Pull (in real world) arm *a* for which x_a^t is maximum.



- At time t, let arm a have s_a^t successes (1's/heads) and f_a^t failures (0's/tails).
- $Beta(s_a^t + 1, f_a^t + 1)$ represents a "belief" about the true mean of arm *a*.
- Mean = $\frac{s_a^t+1}{s_a^t+t_a^t+2}$; variance = $\frac{(s_a^t+1)(t_a^t+1)}{(s_a^t+t_a^t+2)^2(s_a^t+t_a^t+3)}$.
- Computational step: For every arm a, draw a sample (in agent's mind) $x_a^t \sim Beta(s_a^t + 1, f_a^t + 1).$
- Sampling step: Pull (in real world) arm *a* for which x_a^t is maximum.

Achieves optimal regret (Kaufmann et al., 2012); is excellent in practice (Chapelle and Li, 2011).



- 1. UCB, KL-UCB algorithms
- 2. Thompson Sampling algorithm
- 3. Concentration bounds

• Let X be a random variable bounded in [0, 1], with $\mathbb{E}[X] = \mu$;

- Let X be a random variable bounded in [0, 1], with $\mathbb{E}[X] = \mu$;
- Let $u \ge 1$;
- Let x_1, x_2, \ldots, x_u be i.i.d. samples of X; and

- Let X be a random variable bounded in [0, 1], with $\mathbb{E}[X] = \mu$;
- Let $u \ge 1$;
- Let x_1, x_2, \ldots, x_u be i.i.d. samples of X; and
- Let \bar{x} be the mean of these samples (an *empirical* mean):

$$\bar{x} = \frac{1}{u} \sum_{i=1}^{u} x_i.$$

- Let X be a random variable bounded in [0, 1], with $\mathbb{E}[X] = \mu$;
- Let *u* ≥ 1;
- Let x_1, x_2, \ldots, x_u be i.i.d. samples of X; and
- Let \bar{x} be the mean of these samples (an *empirical* mean):

$$\bar{x} = \frac{1}{u} \sum_{i=1}^{u} x_i$$

• Then, for or any fixed $\epsilon > 0$, we have

$$\mathbb{P}\{ar{x} \ge \mu + \epsilon\} \le e^{-2u\epsilon^2}, ext{ and } \ \mathbb{P}\{ar{x} \le \mu - \epsilon\} \le e^{-2u\epsilon^2}.$$

- Let X be a random variable bounded in [0, 1], with $\mathbb{E}[X] = \mu$;
- Let *u* ≥ 1;
- Let x_1, x_2, \ldots, x_u be i.i.d. samples of X; and
- Let \bar{x} be the mean of these samples (an *empirical* mean):

$$\bar{x} = \frac{1}{u} \sum_{i=1}^{u} x_i$$

• Then, for or any fixed $\epsilon > 0$, we have

$$\mathbb{P}\{\bar{x} \ge \mu + \epsilon\} \le e^{-2u\epsilon^2}, \text{ and}$$

 $\mathbb{P}\{\bar{x} \le \mu - \epsilon\} \le e^{-2u\epsilon^2}.$

• Note the bounds are trivial for large ϵ , since $\bar{x} \in [0, 1]$.

For given mistake probability δ and tolerance ε, how many samples u₀ of X do we need to guarantee that with probability at least 1 − δ, the empirical mean x̄ will not exceed the true mean µ by ε or more?

For given mistake probability δ and tolerance ε, how many samples u₀ of X do we need to guarantee that with probability at least 1 − δ, the empirical mean x̄ will not exceed the true mean μ by ε or more?

 $u_0 = \lfloor \frac{1}{2\epsilon^2} \ln(\frac{1}{\delta}) \rfloor$ pulls are sufficient, since Hoeffding's Inequality gives

 $\mathbb{P}\{\bar{\mathbf{x}} \geq \mu + \epsilon\} \leq \mathbf{e}^{-2u_0\epsilon^2} \leq \delta.$

For given mistake probability δ and tolerance ε, how many samples u₀ of X do we need to guarantee that with probability at least 1 − δ, the empirical mean x̄ will not exceed the true mean μ by ε or more?

 $u_0 = \lfloor \frac{1}{2\epsilon^2} \ln(\frac{1}{\delta}) \rfloor$ pulls are sufficient, since Hoeffding's Inequality gives

$$\mathbb{P}\{\bar{\mathbf{x}} \geq \mu + \epsilon\} \leq \mathbf{e}^{-2u_0\epsilon^2} \leq \delta.$$

We have *u* samples of *X*. How do we fill up this blank?:
 With probability at least 1 − δ, the empirical mean x̄ exceeds the true mean μ by at most ϵ₀ = _____.

For given mistake probability δ and tolerance ε, how many samples u₀ of X do we need to guarantee that with probability at least 1 − δ, the empirical mean x̄ will not exceed the true mean μ by ε or more?

 $u_0 = \lfloor \frac{1}{2\epsilon^2} \ln(\frac{1}{\delta}) \rfloor$ pulls are sufficient, since Hoeffding's Inequality gives

$$\mathbb{P}\{\bar{\mathbf{x}} \geq \mu + \epsilon\} \leq \mathbf{e}^{-2u_0\epsilon^2} \leq \delta.$$

• We have u samples of X. How do we fill up this blank?: With probability at least $1 - \delta$, the empirical mean \bar{x} exceeds the true mean μ by at most $\epsilon_0 =$ _____.

We can write $\epsilon_0 = \sqrt{\frac{1}{2u} \ln(\frac{1}{\delta})}$; by Hoeffding's Inequality:

$$\mathbb{P}\{\bar{\mathbf{x}} \geq \mu + \epsilon_0\} \leq \mathbf{e}^{-2u(\epsilon_0)^2} \leq \delta.$$

• Suppose *X* is a random variable bounded in [*a*, *b*]. Can we still apply Hoeffding's Inequality?

• Suppose *X* is a random variable bounded in [*a*, *b*]. Can we still apply Hoeffding's Inequality?

Yes. Assume u; x_1, x_2, \ldots, x_u ; ϵ as defined earlier.

• Suppose *X* is a random variable bounded in [*a*, *b*]. Can we still apply Hoeffding's Inequality?

Yes. Assume u; x_1, x_2, \ldots, x_u ; ϵ as defined earlier.

Consider $Y = \frac{X-a}{b-a}$; for $1 \le i \le u$, $y_i = \frac{x_i-a}{b-a}$; $\bar{y} = \frac{1}{u} \sum_{i=1}^{u} y_i$.

• Suppose X is a random variable bounded in [a, b]. Can we still apply Hoeffding's Inequality?

Yes. Assume u; $x_1, x_2, ..., x_u$; ϵ as defined earlier. Consider $Y = \frac{X-a}{b-a}$; for $1 \le i \le u$, $y_i = \frac{x_i-a}{b-a}$; $\bar{y} = \frac{1}{u} \sum_{i=1}^{u} y_i$. Since Y is bounded in [0, 1], we get

$$\mathbb{P}\{\bar{\mathbf{x}} \ge \mu + \epsilon\} = \mathbb{P}\left\{\bar{\mathbf{y}} \ge \frac{\mu - a}{b - a} + \frac{\epsilon}{b - a}\right\} \le e^{-\frac{2u\epsilon^2}{(b - a)^2}}, \text{ and}$$
$$\mathbb{P}\{\bar{\mathbf{x}} \le \mu - \epsilon\} = \mathbb{P}\left\{\bar{\mathbf{y}} \le \frac{\mu - a}{b - a} - \frac{\epsilon}{b - a}\right\} \le e^{-\frac{2u\epsilon^2}{(b - a)^2}}.$$

A "KL" Inequality

- Let X be a random variable bounded in [0, 1], with $\mathbb{E}[X] = \mu$;
- Let *u* ≥ 1;
- Let x_1, x_2, \ldots, x_u be i.i.d. samples of X; and
- Let \bar{x} be the mean of these samples (an *empirical* mean):

$$\bar{x} = \frac{1}{u} \sum_{i=1}^{u} x_i.$$

A "KL" Inequality

- Let X be a random variable bounded in [0, 1], with $\mathbb{E}[X] = \mu$;
- Let *u* ≥ 1;
- Let x_1, x_2, \ldots, x_u be i.i.d. samples of X; and
- Let \bar{x} be the mean of these samples (an *empirical* mean):

$$\bar{x} = \frac{1}{u} \sum_{i=1}^{u} x_i$$

• Then, for or any fixed $\epsilon \in [0, 1 - \mu]$, we have

$$\mathbb{P}\{ar{\pmb{x}} \geq \mu + \epsilon\} \leq \pmb{e}^{-\textit{uKL}(\mu + \epsilon, \mu)},$$

and for or any fixed $\epsilon \in [\mathbf{0}, \mu],$ we have

$$\mathbb{P}\{ar{\pmb{x}} \leq \mu - \epsilon\} \leq \pmb{e}^{-\textit{uKL}(\mu - \epsilon, \mu)},$$

where for $p, q \in [0, 1]$, $KL(p, q) \stackrel{\text{\tiny def}}{=} p \ln(\frac{p}{q}) + (1 - p) \ln(\frac{1 - p}{1 - q})$.

Some Observations

The KL inequality gives a tighter upper bound:
 For *p*, *q* ∈ [0, 1],

$$\mathit{KL}(\rho,q) \geq 2(
ho-q)^2 \implies e^{-\mathit{u}\mathit{KL}(\rho,q)} \leq e^{-2\mathit{u}(
ho-q)^2}$$

- Both bounds are instances of "Chernoff bounds", of which there are many more forms.
- Similar bounds can also be given when *X* has infinite support (such as a Gaussian), but might need additional assumptions.

- 1. UCB, KL-UCB algorithms
- 2. Thompson Sampling algorithm
- 3. Concentration bounds