Lecture 13. Multi-armed bandits

COMP90051 Statistical Machine Learning

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This lecture

- Stochastic multi-armed bandits
  - Sequential decision making under uncertainty
  - Simplest explore-vs-exploit setting
  - (ε)-greedy
  - UCB algorithm

Exploration vs. Exploitation

Exploration vs. Exploitation

- "Multi-armed bandit" (MAB)
  - Simplest setting for balancing exploration, exploitation
  - Same family of ML tasks as reinforcement learning
- Numerous applications
  - Online advertising
  - Portfolio selection
  - Caching in databases
  - Stochastic search in games (e.g. AlphaGo!)
  - Adaptive A/B testing
  - ....

Stochastic MAB setting

- Possible actions $\{1, \ldots, k\}$ called "arms"
  - Arm i has distribution P_i on bounded rewards with mean μ_i
- In round $t = 1 \ldots T$
  - Play action $i_t \in \{1, \ldots, k\}$ *(possibly randomly)*
  - Receive reward $X_{i_t}(t) \sim P_{i_t}$
- Goal: minimise cumulative regret
  - $\mu^* T - \sum_{t=1}^{T} E\left[X_{i_t}(t)\right]$

    Expected cumulative reward of bandit

    Best expected cumulative reward with hindsight

  where $\mu^* = \max_i \mu_i$
  - Intuition: Do as well as a rule that is simple but has knowledge of the future

Greedy

- At round *t*
  - Estimate value of each arm *i* as average reward observed

$$Q_{t-1}(i) = \begin{cases} \dfrac{\sum_{s=1}^{t-1} X_i(s) 1[i_s = i]}{\sum_{s=1}^{t-1} 1[i_s = i]}, & \text{if } \sum_{s=1}^{t-1} 1[i_s = i] > 0 \\ Q_0, & \text{otherwise} \end{cases}$$

  ... some init constant $Q_0(i) = Q_0$ used until arm *i* has been pulled

  - Exploit, baby, exploit!

$$i_t \in \arg\max_{1 \le i \le k} Q_{t-1}(i)$$

  - Tie breaking randomly

- What do you expect this to do? Effect of init Qs?

ε-Greedy

- At round t
  - Estimate value of each arm i as average reward observed

$$Q_{t-1}(i) = \begin{cases} \frac{\sum_{s=1}^{t-1} X_i(s) 1[i_s = i]}{\sum_{s=1}^{t-1} 1[i_s = i]}, & \text{if } \sum_{s=1}^{t-1} 1[i_s = i] > 0 \\ Q_0, & \text{otherwise} \end{cases}$$

  … some init constant $Q_0(i) = Q_0$ used until arm i has been pulled

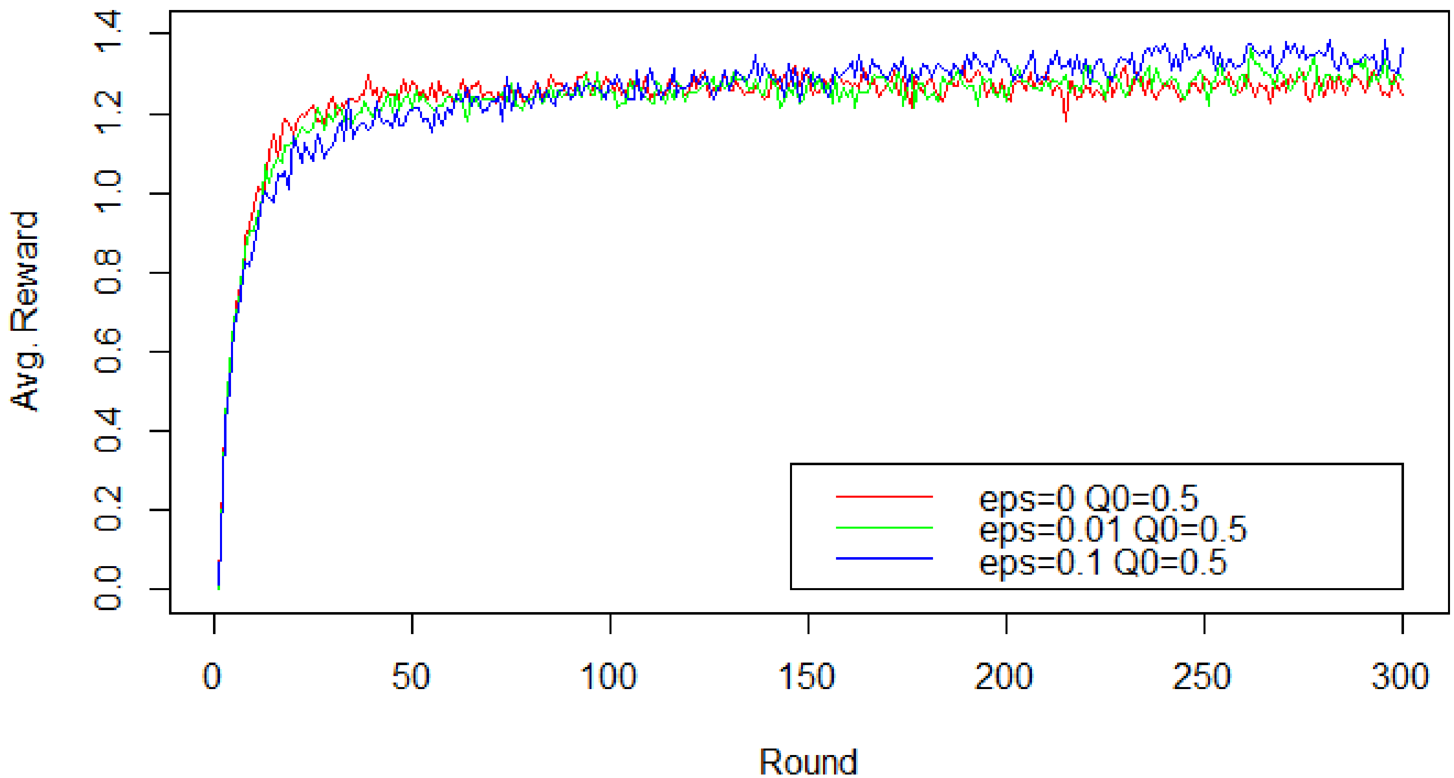
  - Exploit, baby exploit… probably; or possibly explore

$$i_t \sim \begin{cases} \arg\max_{1 \le i \le k} Q_{t-1}(i) & w.p.\ 1-\varepsilon \\ \text{Unif}(\{1, \dots, k\}) & w.p.\ \varepsilon \end{cases}$$

  - Tie breaking randomly

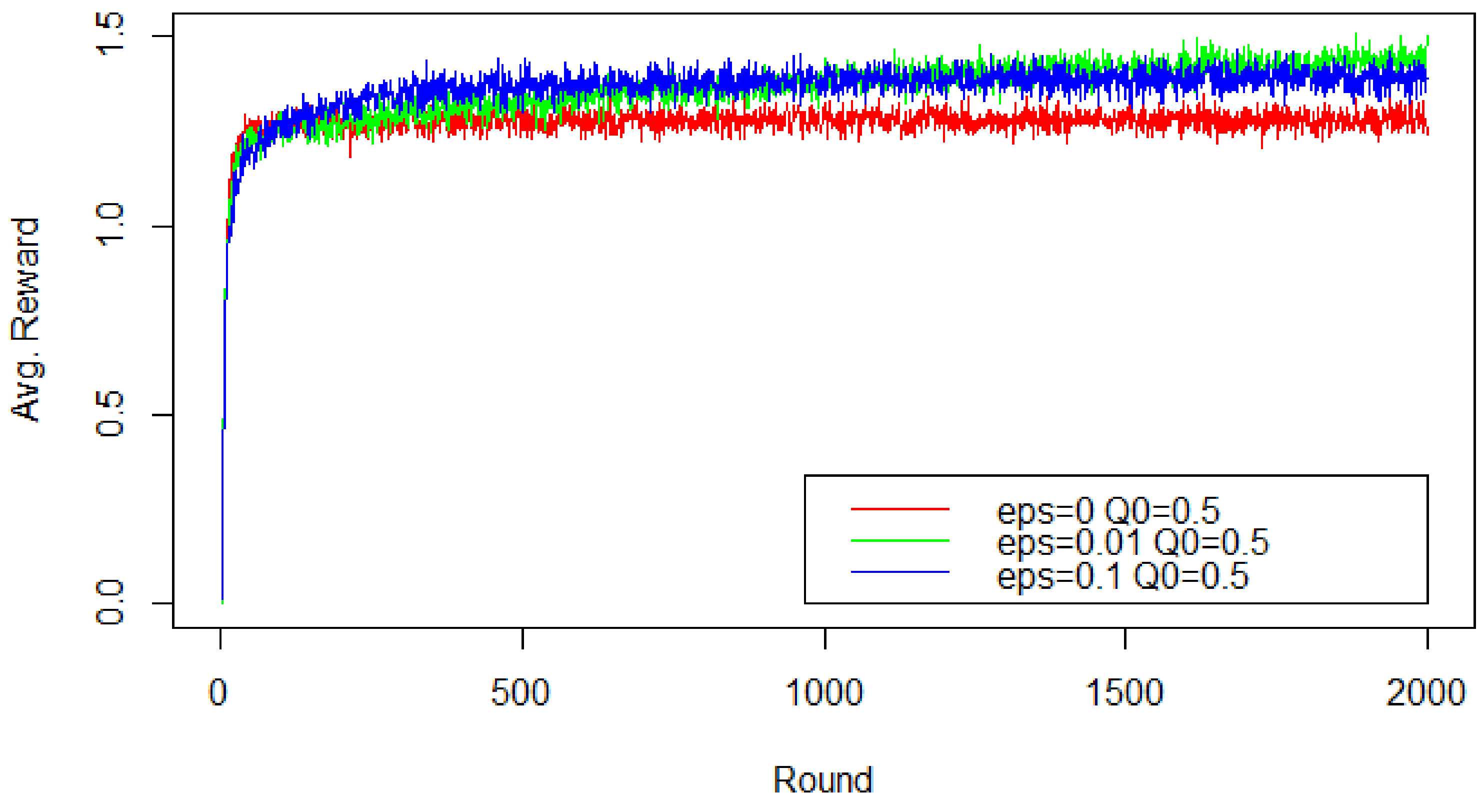
- Hyperparam. ε controls exploration vs. exploitation

Kicking the tyres



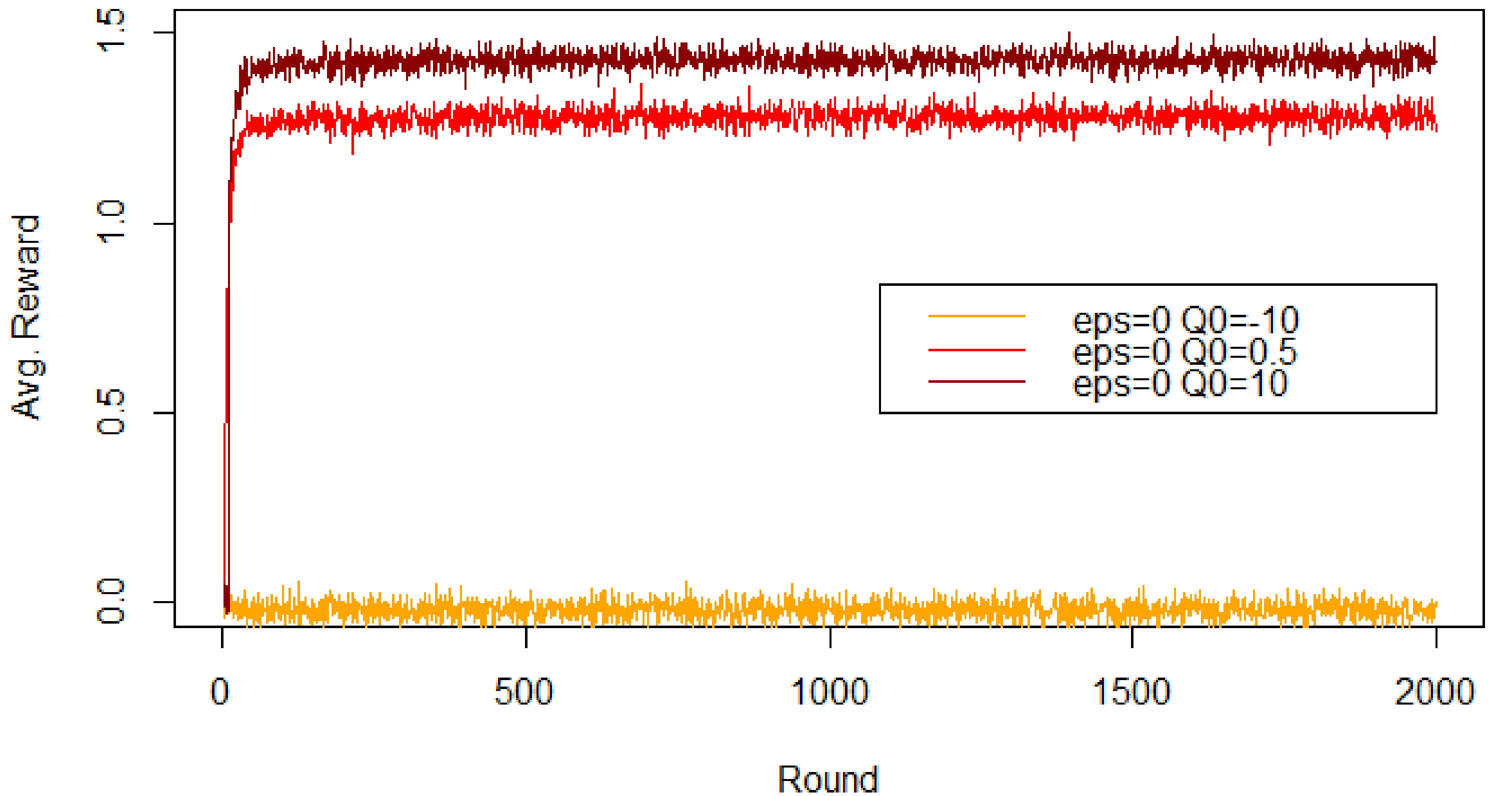
- 10-armed bandit
- Rewards $P_i = Normal(\mu_i, 1)$ with $\mu_i \sim Normal(0,1)$
- Play game for 300 rounds
- Repeat 1,000 games, plot average per-round rewards

Kicking the tyres: More rounds



- Greedy increases fast, but levels off at low rewards
- ε-Greedy does better long-term by exploring
- 0.01-Greedy initially slow (little explore) but eventually superior to 0.1-Greedy (exploits after enough exploration)

Optimistic initialisation improves Greedy



- Pessimism: Init Q's below observable rewards → Only try one arm
- Optimism: Init Q's above observable rewards → Explore arms once
- Middle-ground init Q → Explore arms at most once

But pure greedy never explores an arm more than once

Limitations of ε-Greedy

- While we can improve on basic Greedy with optimistic initialisation and decreasing ε…
- Exploration and exploitation are too “distinct”
  - Exploration actions completely blind to promising arms
  - Initialisation trick only helps with “cold start”
- Exploitation is blind to confidence of estimates
- These limitations are serious in practice

(Upper) confidence interval for Q estimates

- **Theorem**: Hoeffding's inequality
  - Let $X_1, \ldots, X_n$ be i.i.d. random variables in [0,1] mean μ, denote by $\overline{X_n}$ their sample mean
  - For any $\varepsilon \in (0,1)$ with probability at least $1 - \varepsilon$

$$\mu \leq \overline{X_n} + \sqrt{\frac{\log(1/\varepsilon)}{2n}}$$

- Application to $Q_{t-1}(i)$ estimate – also i.i.d. mean*!!*
  - Take $n = N_{t-1}(i) = \sum_{s=1}^{t-1} 1[i_s = i]$ number of *i* plays
  - Then $\overline{X_n} = Q_{t-1}(i)$
  - Critical level $\varepsilon = 1/t$ (Lai & Robbins '85), take $\varepsilon = 1/t^4$

Upper Confidence Bound (UCB) algorithm

- At round t
  - Estimate value of each arm i as average reward observed

$$Q_{t-1}(i) = \begin{cases} \hat{\mu}_{t-1}(i) + \sqrt{\dfrac{2\log(t)}{N_{t-1}(i)}}, & \text{if } \sum_{s=1}^{t-1} 1[i_s = i] > 0 \\ Q_0, & \text{otherwise} \end{cases}$$

…some constant $Q_0(i) = Q_0$ used until arm i has been pulled; where:

$$N_{t-1}(i) = \sum_{s=1}^{t-1} 1[i_s = i] \qquad \hat{\mu}_{t-1}(i) = \frac{\sum_{s=1}^{t-1} X_i(s) 1[i_s = i]}{\sum_{s=1}^{t-1} 1[i_s = i]}$$

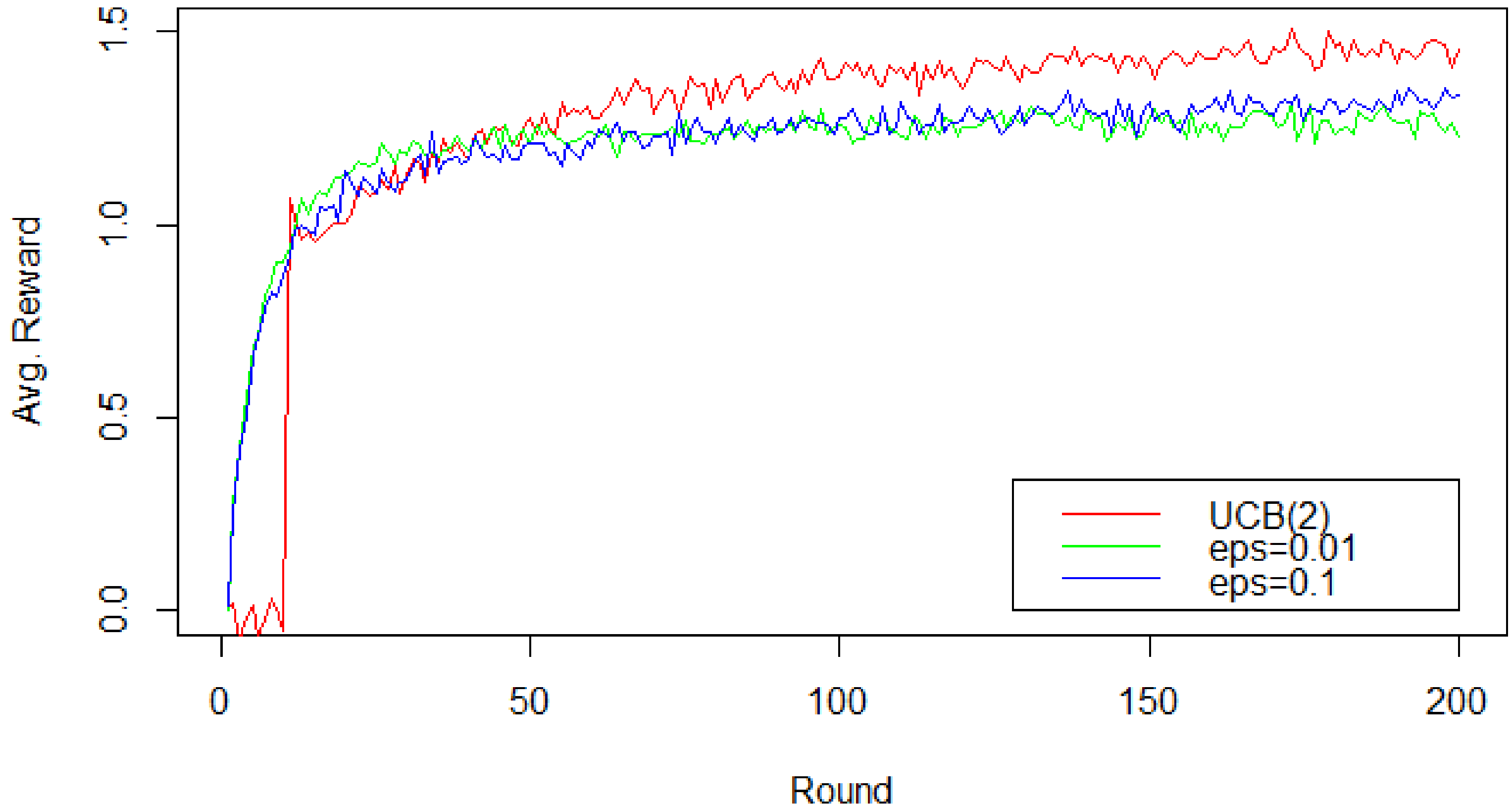
  - "Optimism in the face of uncertainty"

$$i_t \sim \arg\max_{1 \le i \le k} Q_{t-1}(i)$$

…tie breaking randomly

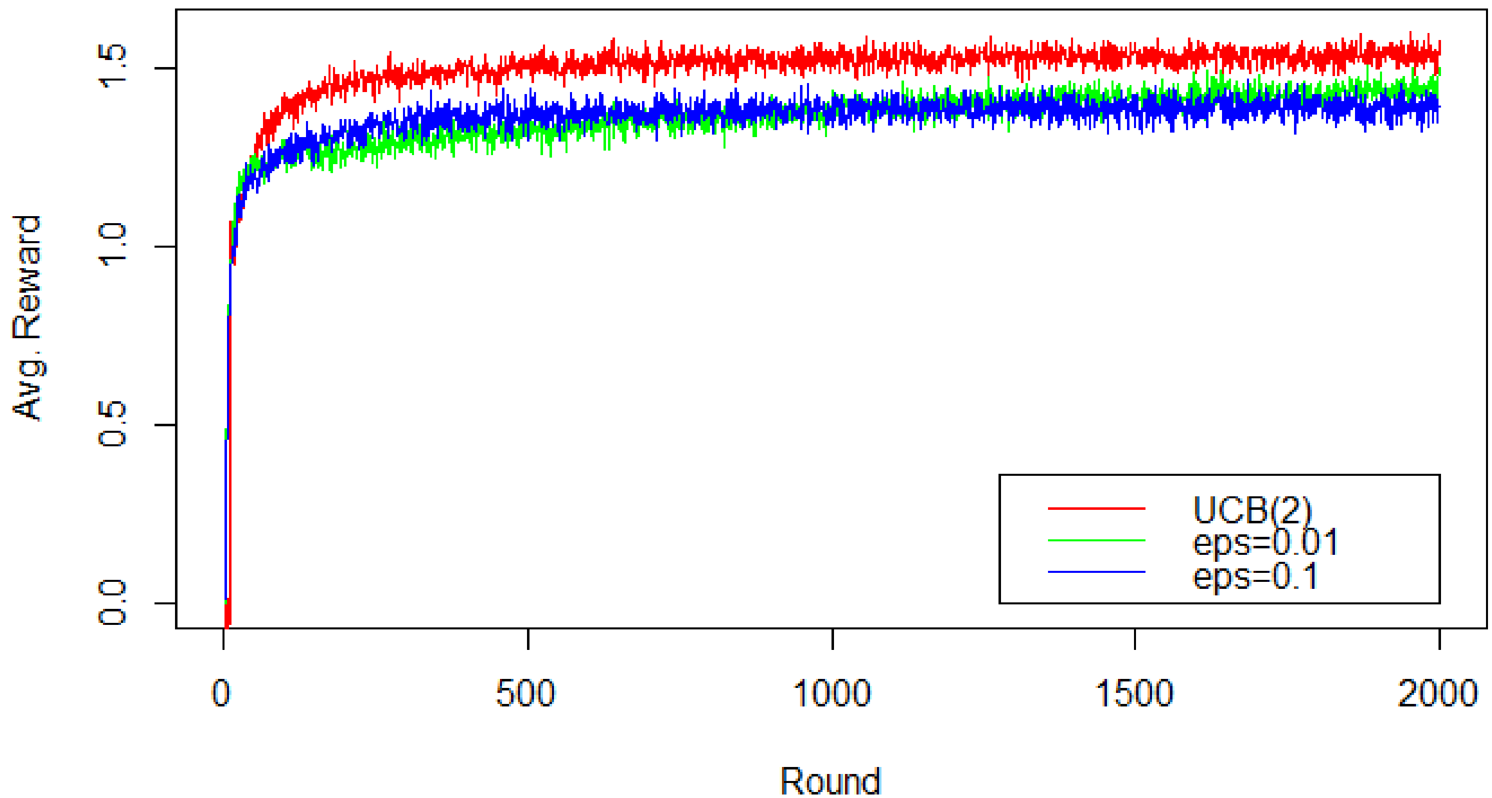
- Addresses several limitations of ε-greedy
- Can "pause" in a bad arm for a while, but eventually find best

Kicking the tyres: How does UCB compare?



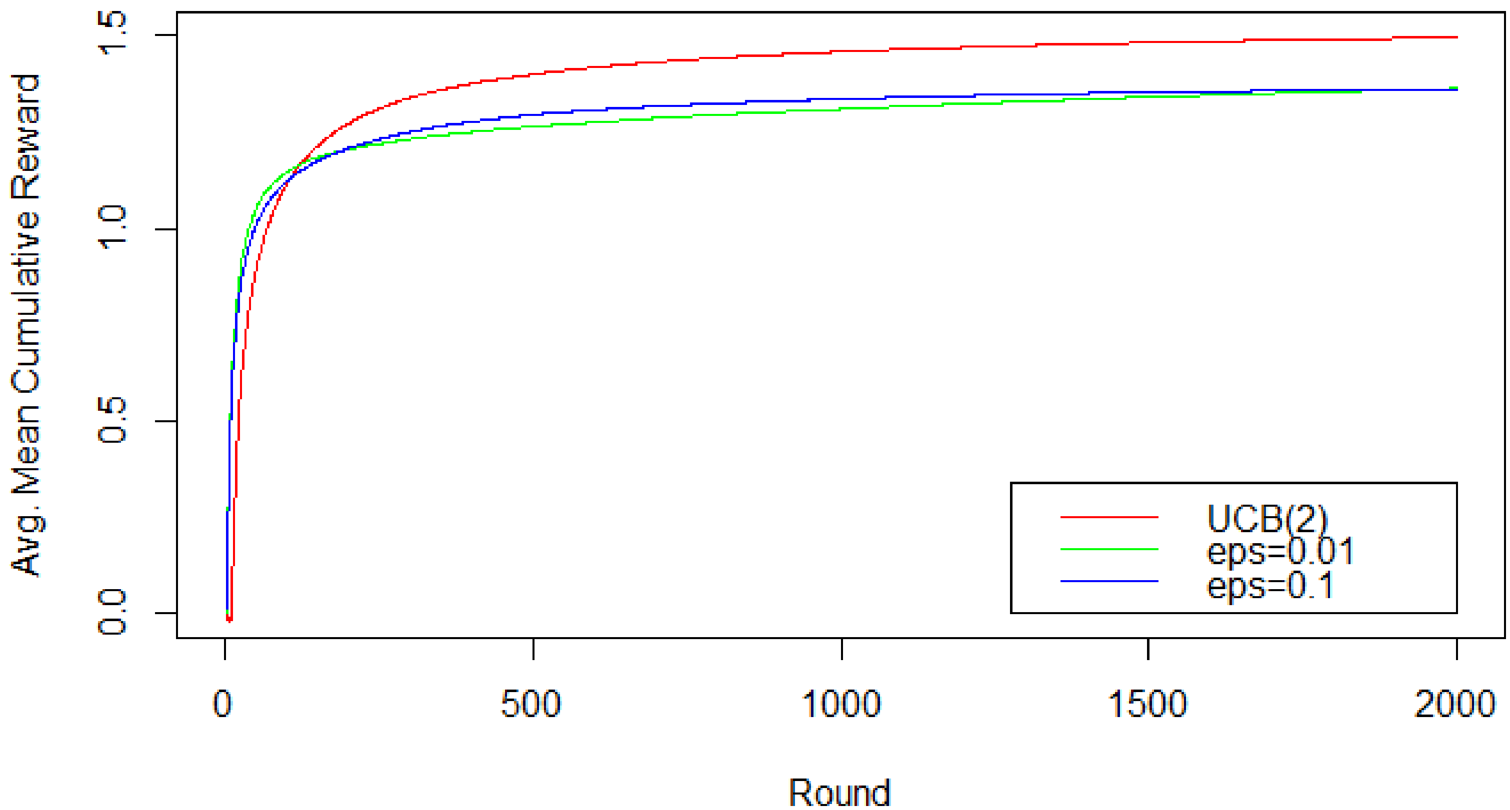
- UCB quickly overtakes the ε-Greedy approaches

Kicking the tyres: How does UCB compare?



- UCB quickly overtakes the ε-Greedy approaches
- Continues to outpace on per round rewards for some time

Kicking the tyres: How does UCB compare?



- UCB quickly overtakes the ε-Greedy approaches
- Continues to outpace on per round rewards for some time
- More striking when viewed as mean cumulative rewards

Notes on UCB

- Theoretical regret bounds, optimal up to multiplicative constant
  - Grows like $\mathrm{O}(\log t)$ i.e. averaged regret goes to zero!
- Tunable $\rho > 0$ exploration hyperparam. replaces "2"

$$Q_{t-1}(i) = \begin{cases} \hat{\mu}_{t-1}(i) + \sqrt{\dfrac{\rho \log(t)}{N_{t-1}(i)}}, & \text{if } \sum_{s=1}^{t-1} 1[i_s = i] > 0 \\ Q_0, & \text{otherwise} \end{cases}$$

  - Captures different ε rates & bounded rewards outside [0,1]
- Many variations e.g. different confidence bounds
- Basis for Monte Carlo Tree Search used in AlphaGo!

This lecture

- Stochastic multi-armed bandits
  - Sequential decision making under uncertainty
  - Simplest explore-vs-exploit setting
  - (ε)-greedy, UCB
- Many applications, variations:
  - Adversarial MAB: rewards not stochastic, but *anything*
  - Contextual bandits: act based on context feature vector
  - Reinforcement learning: more general setting
- Workshops week #8: ensembles
- Next lectures: unsupervised learning