02465: Introduction to reinforcement learning and control

Exploration and Bandits

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DTU Compute, Technical University of Denmark (DTU)

Lecture Schedule

Dynamical programming

1. The finite-horizon decision problem
   7 February
2. Dynamical Programming
   14 February
3. DP reformulations and introduction to Control
   21 February

Control

4. Discretization and PID control
   28 February
5. Direct methods and control by optimization
   7 March
6. Linear-quadratic problems in control
   14 March
7. Linearization and iterative LQR
   21 March

Reinforcement learning

8. **Exploration and Bandits**
   28 March
9. Bellmans equations and exact planning
   4 April
10. Monte-carlo methods and TD learning
    11 April
11. Model-Free Control with tabular and linear methods
    25 April
12. Eligibility traces
    2 May
13. Deep-Q learning
    9 May

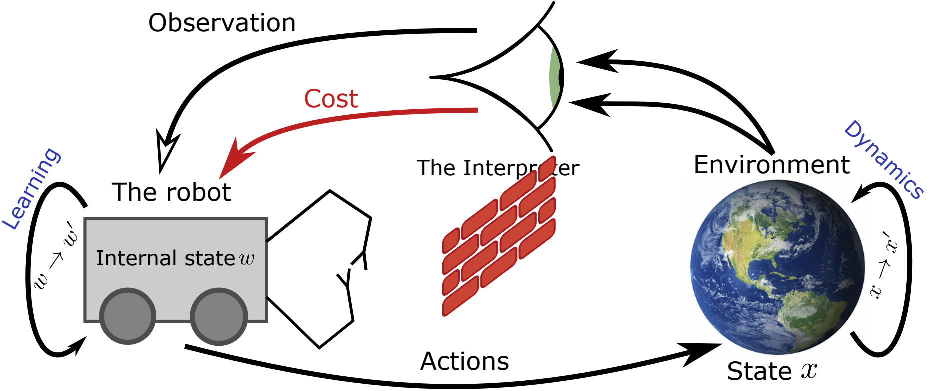
Syllabus: `https://02465material.pages.compute.dtu.dk/02465public`
Help improve lecture by giving feedback on DTU learn

Reading material:

- [SB18, Chapter 1; Chapter 2-2.7; 2.9-2.10] Only as background

Learning Objectives

- Exploration/exploitation problem
- Bandits as a simplified reinforcement learning setting
- Formalizing the bandit problem
- Algorithms for solving the bandit problem

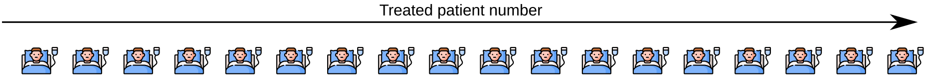


- Dynamics of world not known
- Simultaneously **learn the environment** and **maximize expected reward**
- Balance **exploration** and **exploitation**

Bandit studies this in an idealized setting

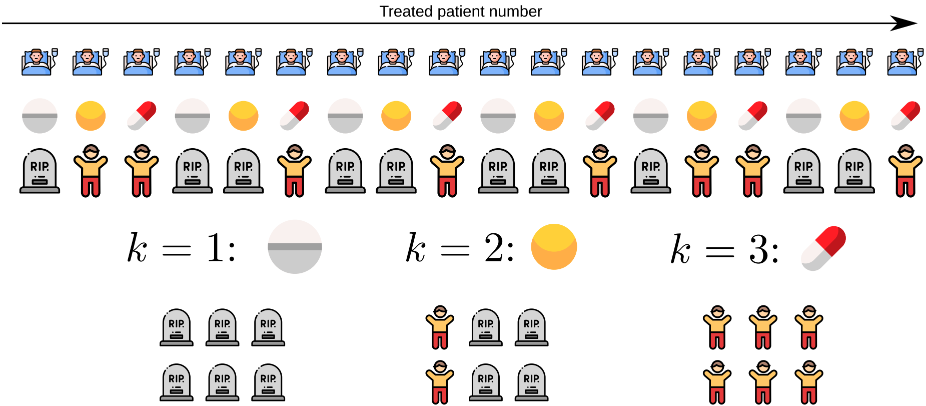
Bandits, examples

- Suppose you have a large number of patients $t = 1, 2, \ldots$ with the same disease
- You have access to k drugs $a = 0, 1, \ldots, k-1$ with different outcome probabilities
- Outcome of treatment is either that the patient recovers, $R_t = 1$, or not $R_t = 0$
- Goal is to maximize $\sum_{t=1}^{T} R_t$



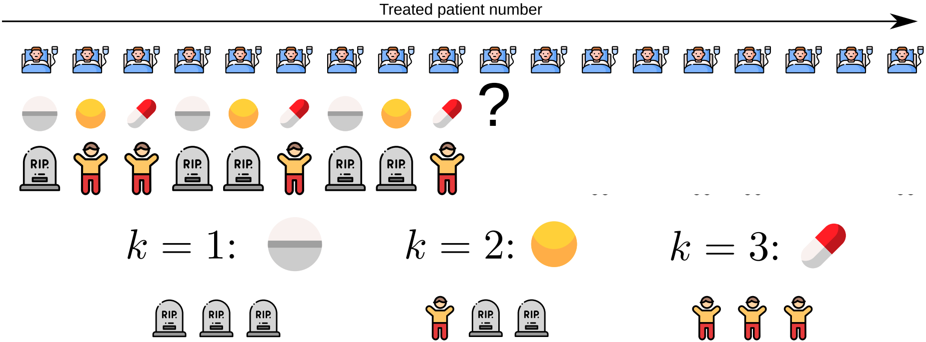
Idea 1: Statistics!

- Divide first T patients into K groups of $S = \frac{T}{K}$ patients
- Administer drugs to each group
- observe results



Bandit approach

- After $t-1$ choices of actions $A_1, \ldots, A_{t-1}$ and observed rewards $R_1, \ldots, R_{t-1}$
- Decide next action A_t to maximize reward
- **Bandit assumption:** Action A_t only affects R_t
  - Personalized medicine
  - Evaluating similar, approved drugs (low risk)
  - SMART trials/JITAIs



Example: An opinion columnist

Suppose you are writing for a major newspaper which relies on social media to get as many reads as possible. You can choose between 5 headlines, and your job is to get as many clicks as possible:

- $k = 0$: "With less destructive nukes on the way, it's time for the left to say good-bye to those annoying non-proliferation treaties. "
- $k = 1$: "Opinion | The upside of nuclear war? Making popcorn without a microwave."
- $k = 2$: "Joe Biden has prevented a nuclear holocaust. But how will that play with suburban moms this fall?"
- $k = 3$: "Opinion | Nuclear war may not be woke. But it's not a war crime."
- $k = 4$: "Opinion | With rising temperatures, would a nuclear winter really be that bad?"

But which one to choose?

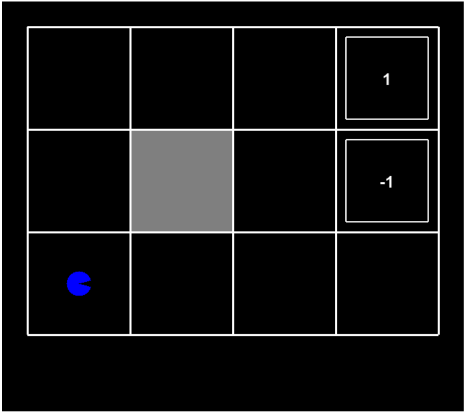
Example: An opinion columnist

- For each exposure $t = 1, 2, ...$ on twitter, selects a headline $A_t = 0, \dots, k-1$
- Observe whether the user clicks the story $R_t \in \{0, 1\}$
- Use this to select the next headline for the next user $A_{t+1} = a$
- **You want to maximize total clicks, knowing the story has a finite lifespan:**

$$\sum_{t=1}^{\text{2-3 days?}} R_t$$

Looking ahead: Reinforcement learning

- In a state s, select optimal action a, then observe what reward we get
- It is like a bandit problem in each state (but more about that in a few weeks)



Many types of bandits

Sequentially take decisions $A_1, A_2, \ldots$ and observe rewards $R_1, R_2, \ldots$

Stationary In a stationary bandit the reward distribution does not change

Nonstationary The environment can change (but not as consequence of our actions)

Contextual You get a bit of information to make your decision

Structured Reward of different arms can be inferred from each other (Bayesian black box optimization)

Stationary bandits

- Action at time step $t = 1, 2, \dots$ is A_t
- Reward is R_t
- Observations available to make action at t:

$$H_t = (A_1, R_1, A_2, R_2, \dots, A_{t-1}, R_{t-1})$$

- Actions are generated from a **policy** π which we learn based on H_t:

$$A_t \sim \pi_t(\cdot)$$

- **Value** of an action is

$$q_*(a) = \mathbb{E}\left[R_t | A_t = a\right], \quad a = 0, \dots, K-1$$

- Optimal strategy at t is to select action with highest value
- Our learned estimate of $q_*(a)$ at time t is $Q_t(a)$

  Exploit Select action a with **highest** estimate of $Q_t(a)$
  Explore Do something else to **learn** more about $Q_t(a)$

- Note bandit methods can be classified according to what they learn about $Q_t(a)$

Bandit objective and definitions

Objective 1: Average reward at time t and total reward up to time T

$$\mathbb{E}_\pi\left[q_*(a_t)\right], \quad \sum_{t=1}^{T} \mathbb{E}_\pi\left[q_*(a_t)\right]$$

Optimal value and optimal action

$$V^* = \max_a \left[q_*(a)\right], \quad a_t^* = \arg\max_a \left[q_*(a)\right]$$

Objective 2: Fraction optimal actions

$$P_\pi(A_t = a_t^*)$$

Gab

$$\Delta_a = V^* - q_*(a)$$

Objective 3: Cumulative regret

$$l_t = \mathbb{E}\left[V^* - q_*\left(a_t\right)\right], \quad L_T = \sum_{t=1}^{T} l_t$$

Goal is to maximize cumulative reward $\leftrightarrow$ minimize total regret

Quiz: What is the regret?

- Reward $R_t = 1$ on win and $R_t = 0$ on loss.
- The win probabilities are shown by horizontal lines
- What is the regret for a policy which always select $a = 3$? $(\pi(a = 3) = 1)$

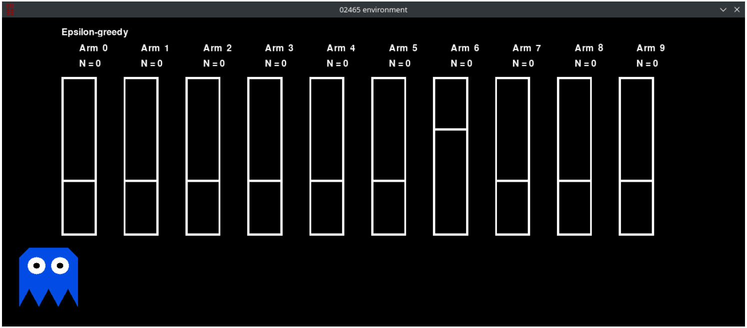
$$l_t = \mathbb{E}\left[V^* - q_*\left(a_t\right)\right], \quad V^* = \max_a \left[q_*(a)\right]$$

a. It is a random quantity (either zero or 1)

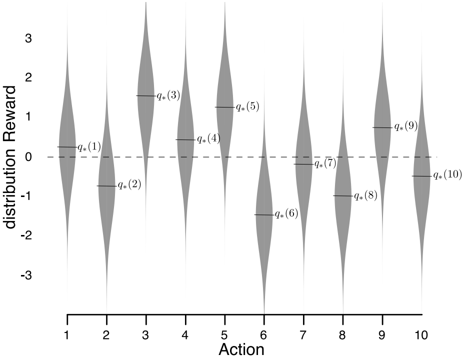
b. It depends on how many actions we have taken

c. It is about $\frac{1}{3}$

d. It is about $-\frac{2}{3}$



The $k = 10$-armed testbed



- Let $k = 10$ and select each $q_*(a) \sim N(\mu = 0, \sigma^2 = 1)$
- for each action a, select reward

$$R_t | a \sim \mathcal{N}(\mu = q_*(a), \sigma^2 = 1)$$

- Let each agent interact for a number of **steps** ~ 1000
- Repeat procedure for 2000 runs to calculate average agent performance

Making it practical: A bandit problem

```python
# bandits.py
class BanditEnvironment(Env):
    def __init__(self, k : int):
        super().__init__()
        self.observation_space = Discrete(1)  # Dummy observation space with a single o
        self.action_space = Discrete(k)       # The arms labelled 0,1,...,k-1.
        self.k = k  # Number of arms


    def reset(self):
        raise NotImplementedError("Implement the reset method")

    def bandit_step(self, a):
        reward = 0 # Compute the reward associated with arm a
        gab = 0 # Compute the gab, by comparing to the optimal arms reward.
        return reward, gab

    def step(self, action):
        reward, gab = self.bandit_step(action)
        info = {'gab': gab}
        return None, reward, False, False, info
```

Action-value method

Idea: approximate $q_*(a)$ by keeping track of $Q_t(a)$

$$Q_t(a) \doteq \frac{\text{sum of rewards when } a \text{ taken prior to } t}{\text{number of times } a \text{ taken prior to } t} = \frac{\sum_{i=1}^{t-1} R_i \cdot \mathbf{1}_{A_i=a}}{\sum_{i=1}^{t-1} \mathbf{1}_{A_i=a}} = \frac{S_t(a)}{N_t(a)}$$

Explore with probability ϵ

- Action selection π
  - With probability ϵ select random action
  - With probabilty $1-\epsilon$ select $a^* = \arg\max_a Q_t(a)$
- As only one entry A_t of Q_t change at a time track number of times a was selected $n = N(a)$:

$$Q_n \doteq \frac{R_1 + R_2 + \cdots + R_{n-1}}{n-1} = \frac{S_n(a)}{N(a)} \tag{1}$$

One can show that:

$$Q_{n+1} = Q_n + \frac{1}{n}\left[R_n - Q_n\right]$$

  - Given observed $a = A_t$, $r = R_t$ update:

Simple action-value bandit algorithm

A simple bandit algorithm

Initialize, for $a = 1$ to k:

$Q(a) \leftarrow 0$

$N(a) \leftarrow 0$

Loop forever:

$$A \leftarrow \begin{cases} \arg\max_a Q(a) & \text{with probability } 1-\varepsilon \quad \text{(breaking ties randomly)} \\ \text{a random action} & \text{with probability } \varepsilon \end{cases}$$

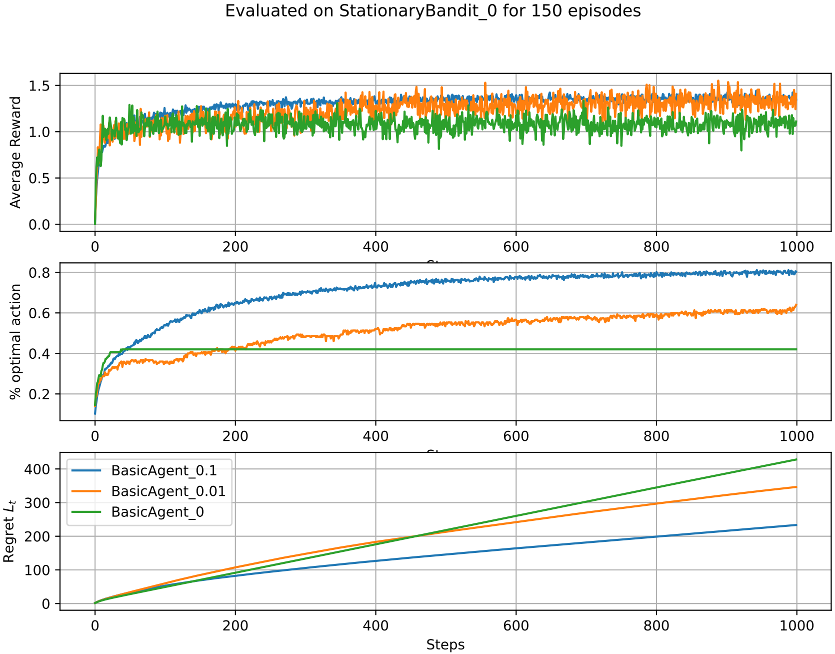
$R \leftarrow bandit(A)$

$N(A) \leftarrow N(A) + 1$

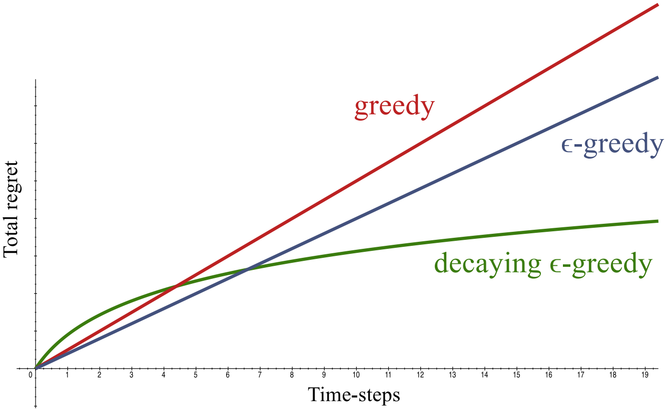
$Q(A) \leftarrow Q(A) + \frac{1}{N(A)}\big[R - Q(A)\big]$

$$Q_{n+1} = Q_n + \frac{1}{n}\Big[R_n - Q_n\Big]$$

Results: action-value bandit



Regret asymptotics



- Fixed-ε algorithms have linear regret
- With decreasing ε it is possible to get sub-linear regret, **but only by assuming we know things about the reward distribution**
  - Theoretically best possible bandit method has logarithmic regret.

Confidence-bound methods

- Estimate an upper confidence bound $\hat{U}_t(a)$ for $q_*(a)$ st.

$$q_*(a) \leq \hat{U}_t(a) + Q_t(a)$$

  with high probability

- Generally
  - If $N_t(a)$ low $\rightarrow \hat{U}_t(a)$ high
  - If $N_t(a)$ high $\rightarrow \hat{U}_t(a)$ low

- Select actions to maximize

$$\arg\max_a \left[\hat{U}_t(a) + Q_t(a)\right]$$

- Intuitively reflects this logic
  - An actions is good if $Q_t(a)$ is high (it just always give good values and deserves **exploitation**)
  - An action is good if we know so little about it ($U_t(a)$ high) that it *might* be good and deserves **exploration**

UCB1

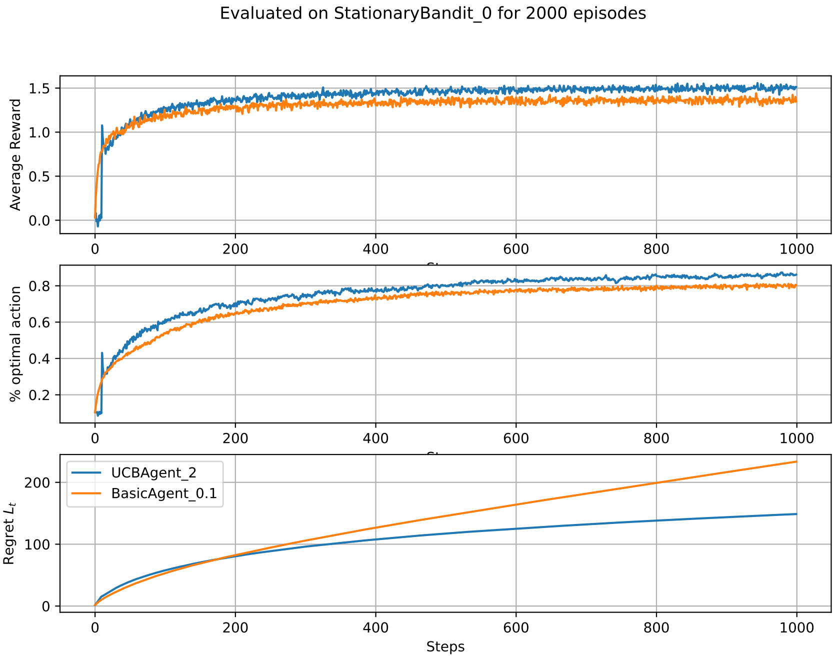
$$A_t = \underset{a}{\operatorname{argmax}} \left[Q_t(a) + c\sqrt{\frac{\ln t}{N_t(a)}} \right]$$

Asymptotic logarithmic regret when $R_t \in [0, 1]$

$$\lim_{t \to \infty} L_t \leq \sum_{a \neq a^*, \Delta_a > 0} \left(\frac{4 \ln t}{\Delta_a} + 2\Delta_a \right)$$

- The variant UCB-normal obtains logarithmic regret on normal reward distributions

Results


Evaluated on StationaryBandit_0 for 2000 episodes
Average Reward
% optimal action
Regret L_t
UCBAgent_2
BasicAgent_0.1
Steps

Quiz: How does UCB explore?

Consider the update rule for UCB1:

$$A_t = \operatorname*{argmax}_a \left[Q_t(a) + c\sqrt{\frac{\ln t}{N_t(a)}} \right]$$

Which one of the following statements is true about UCB1?

a. UCB1 requires that the rewards are positive

b. If one arm give a much higher reward than the other, UCB1 will eventually only select this arm

c. If one arm is much, much worse than the others, UCB1 will eventually stop selecting that arm

d. It is possible to predict which arms UCB1 will select k steps in the future

e. At least one of the upper-confidence estimates $\hat{U}_t(a)$ will converge to 0.

f. Don't know.

Non-stationary bandits

- These is a (hidden) state S_t which evolves as:

$$P(S_{t+1}, R_t | S_t = s, A_t = a) = P(S_{t+1} | S_t = s) P(R_t | S_t = s, A_t = a)$$

- Example: Add normal noise to $q_*(a)$ at each time step
- One idea is to replace $\frac{1}{n}$ with $\alpha_t(a)$ and use scheduling:

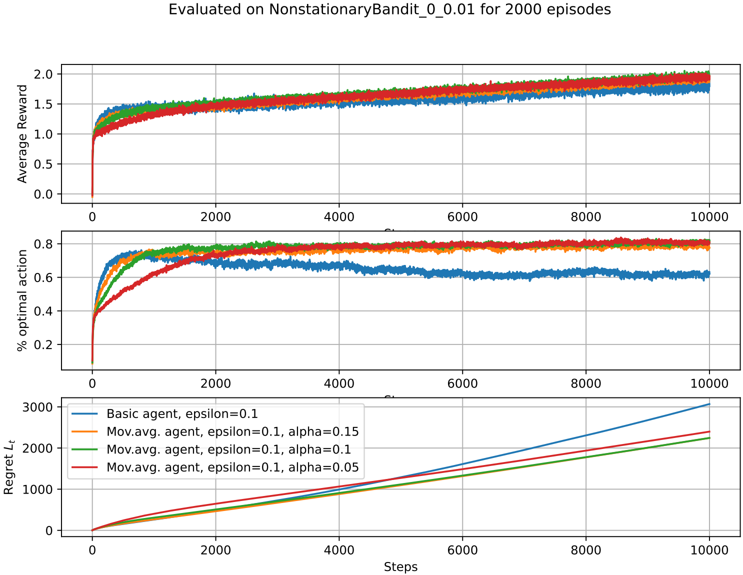
$$\text{Previous update: } Q_{n+1} = Q_n + \frac{1}{n} [R_n - Q_n]$$

$$\text{New update: } Q_{n+1} = Q_n + \alpha [R_n - Q_n]$$

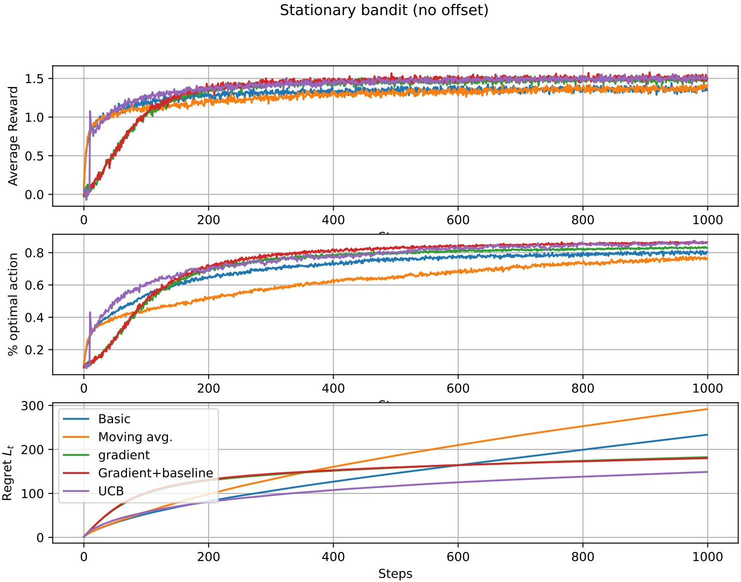
  - Constant α means fast adaption but no convergence
  - Typically chose

$$\sum_{n=1}^{\infty} \alpha_n(a) = \infty \quad \text{and} \quad \sum_{n=1}^{\infty} \alpha_n^2(a) < \infty$$

Results

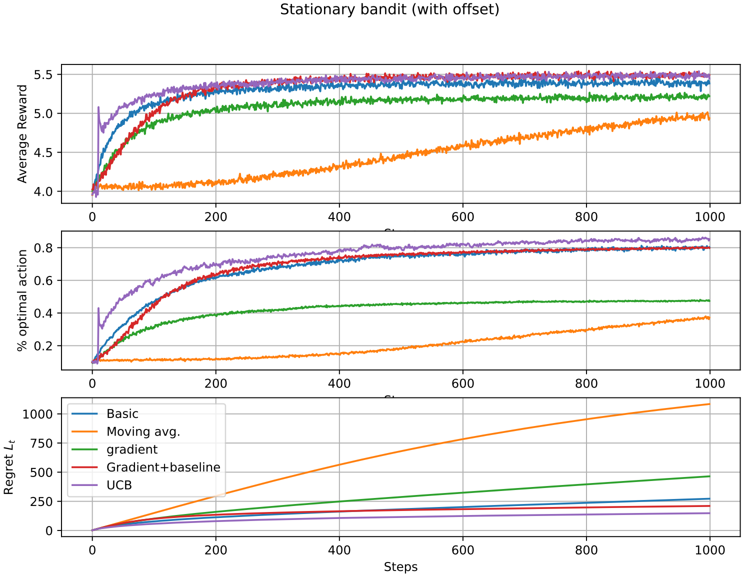

Evaluated on NonstationaryBandit_0_0.01 for 2000 episodes
Average Reward
2.0
1.5
1.0
0.5
0.0
0
2000
4000
6000
8000
10000
% optimal action
0.8
0.6
0.4
0.2
Regret L_t
3000
2000
1000
0
Steps
Basic agent, epsilon=0.1
Mov.avg. agent, epsilon=0.1, alpha=0.15
Mov.avg. agent, epsilon=0.1, alpha=0.1
Mov.avg. agent, epsilon=0.1, alpha=0.05

Results



Stationary bandit (no offset)
Average Reward
1.5
1.0
0.5
0.0
0
200
400
600
800
1000
% optimal action
0.8
0.6
0.4
0.2
Regret L_t
300
200
100
Basic
Moving avg.
gradient
Gradient+baseline
UCB
Steps

Results


Stationary bandit (with offset)
Average Reward
5.5
5.0
4.5
4.0
% optimal action
0.8
0.6
0.4
0.2
Regret L_t
1000
750
500
250
0
200
400
600
800
Basic
Moving avg.
gradient
Gradient+baseline
UCB
Steps

Richard S. Sutton and Andrew G. Barto.
Reinforcement Learning: An Introduction.
The MIT Press, second edition, 2018.
(Freely available online).

Appendix: Probability-matching methods

- Our goal is to find the optimal probability distribution π
- We can parameterize any distribution as

$$\pi(a) = \frac{e^{H_a}}{\sum_{b=1}^{k} e^{H_b}}$$

for a weight-vector $H \in \mathbb{R}^k$

- Optimal π is the one maximizing expected reward

$$\mathbb{E}_\pi \left[R_t\right] = \sum_a \pi_t(a; H) q_*(a) = E(H)$$

- This is a function of H
- Let's just do gradient descent, WCGW?

$$H_{t+1} \leftarrow H_t - \alpha \nabla_H E(H)$$

Gradient bandit: Derivation

$$\frac{\partial}{\partial H} E(H) = \sum_a \pi(a; H) q^*(a) \frac{\partial \log \pi(a; H)}{\partial H} \tag{2}$$

We can sample from $\pi(a)$ and then our environment will give an estimate of $q^*(a)$

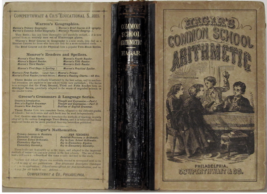
$$\sum_a \pi(a; H) q^*(a) \frac{\partial \log \pi(a; H)}{\partial H} \approx \frac{1}{S} \sum_{s=1}^{S} R_t(a_s) \frac{\partial \log \pi(a_s; H)}{\partial H} \tag{3}$$

- Nobody has told us we cannot use $S = 1$

$$\nabla E(H) \approx R_t \frac{\partial \log \pi(a_t; H)}{\partial H}$$

$$\begin{aligned} H_{t+1}(A_t) &\doteq H_t(A_t) + \alpha R_t (1 - \pi_t(A_t)), && \text{and} \\ H_{t+1}(a) &\doteq H_t(a) - \alpha R_t \pi_t(a), && \text{for all } a \neq A_t \end{aligned}$$

Math facts used in derivation



Kullback-Leibner divergence Given discrete probability distribution p and q:

$$\mathrm{KL}[p; q] = \sum_{i=1}^{n} p(x_i) \log \frac{q(x_i)}{p(x_i)}$$

The logarithm trick for $q(x, \theta) > 0$

$$\frac{\partial}{\partial\theta} \int q(x,\theta) f(x) dx = \int q(x,\theta) \frac{\partial \log q(x,\theta)}{\partial\theta} f(x) dx$$

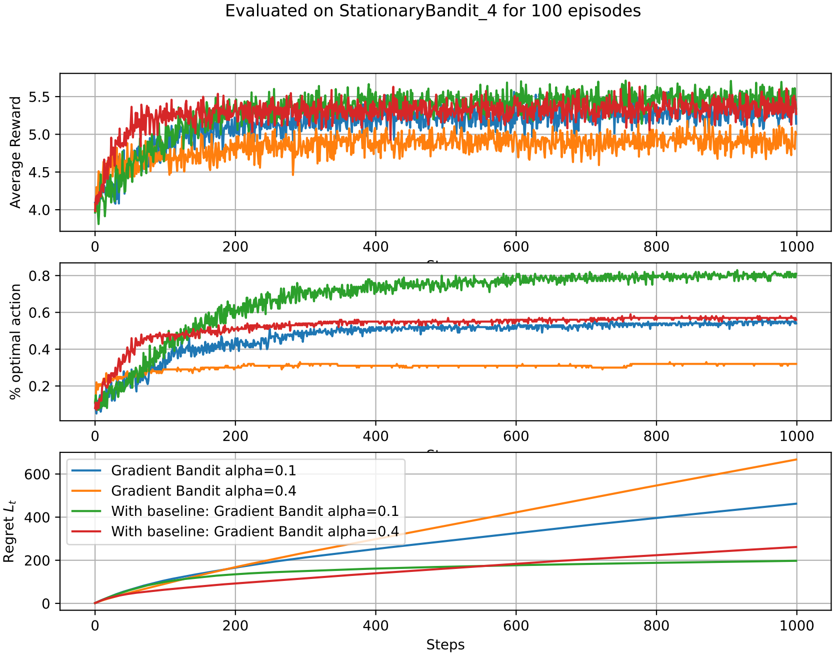
Gradient bandits

- Let $\bar{R}_t$ be the average reward over $0, \ldots, t-1$
- Update weights as

$$\begin{aligned} H_{t+1}(A_t) &\doteq H_t(A_t) + \alpha \left(R_t - \bar{R}_t\right)\left(1 - \pi_t(A_t)\right), && \text{and} \\ H_{t+1}(a) &\doteq H_t(a) - \alpha \left(R_t - \bar{R}_t\right)\pi_t(a), && \text{for all } a \neq A_t \end{aligned}$$

- Why? **legal** because they do not change the gradient, **sensible** because they can reduce variance/promote exploration
- To my knowledge, no theoretical analysis exists
- This gradient-trick is basis of **policy gradient** methods for reinforcement learning

Results


Evaluated on StationaryBandit_4 for 100 episodes
Average Reward
% optimal action
Regret L_t
Steps
Gradient Bandit alpha=0.1
Gradient Bandit alpha=0.4
With baseline: Gradient Bandit alpha=0.1
With baseline: Gradient Bandit alpha=0.4