Reinforcement Learning: Multi-Armed Bandits

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Reinforcement Learning

- Learning by trial and error
- Inspired by the behavior of animals (including humans!)
- ► The exploration-exploitation trade-off
- Many applications: robotics, games, advertising, content recommendation, medicine, etc.



Outline

- 1. Multi-armed bandits
- 2. Main algorithms
- 3. Performance analysis
- 4. Extensions
- 5. A case study: AlphaGo

Multi-armed bandits

- ▶ A class of RL problems where the agent does **not** modify its environment
- At time t = 1, 2, ..., the agent selects an **action** a_t in some **finite** set A and receives some **reward** r_t
- ▶ The rewards of action $a \in A$ are i.i.d. with some **unknown** distribution $p(\cdot|a)$, with expectation

$$q(a) = \mathrm{E}(r|a) = \sum_{r} rp(r|a)$$

The objective is to find and to exploit the best action(s) on observing the rewards

Example: A/B testing

- Objective: find the best version of a Web site
- Action = show version A or B
- ► Reward (binary) = click / no click

Example: Obama 2008 campaign





Time horizon

The objective is to maximize the cumulative reward over some (possibly unknown) time horizon T:

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

- ▶ If action a is always selected, the cumulative reward is approximately Tq(a) for large T
- Maximum reward (per action):

$$q^* = \max_a q(a)$$

► Best action(s)

$$a^* = \arg\max_a q(a)$$

Performance metrics

1. Cumulative regret (gap to optimal reward)

$$R = q^*T - \sum_{t=1}^T r_t$$

2. Precision (proportion of optimal actions)

$$P = \frac{1}{T} \sum_{t=1}^{T} 1_{\{a_t = a^*\}}$$

Performance metrics (in expectation)

Let $N_t(a)$ be # of times action a has been selected up to time t

1. **Cumulative regret** (expected gap to optimal reward)

$$\mathrm{E}(R) = q^{\star}T - \sum_{t=1}^{T} \mathrm{E}(r_t)$$

$$= \sum_{a \in A} (q^{\star} - q(a)) \mathrm{E}(N_T(a))$$

Precision (expected proportion of optimal actions)

$$E(P) = \frac{1}{T} \sum_{t=1}^{I} P(a_t = a^*)$$
$$= \frac{E(N_T(a^*))}{T}$$

Action	a	b	С
Expected reward	1	9	10

Policy A

Action | a | b | c

Distribution | 10% + 40% + 50%Regret (per action) = 1.3, Precision = 0.5

Policy B					
Action	a	b	С		
Distribution	20%	20%	60%		
legret (per actio	(n) = 2,	Precis	sion = 0	0.6	

Efficiency

► Efficient algorithm = sublinear regret

$$\frac{\mathrm{E}(R)}{T} \to 0$$
 when $T \to +\infty$

Since

$$\mathrm{E}(R) = \sum_{a \in A} (q^{\star} - q(a)) \mathrm{E}(N_{T}(a))$$

this implies

$$\forall a \neq a^{\star}, \quad \frac{\mathrm{E}(N_T(a))}{T} \to 0$$

and

$$P \rightarrow 1$$

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Variables

Keep for each action a:

- ightharpoonup R(a) = cumulative reward of action a
- ightharpoonup N(a) = number of selections of action a
- \rightarrow estimation of the value of action a:

$$Q(a) = \frac{R(a)}{N(a)}$$

Start for each action a with:

- $ightharpoonup R(a) \leftarrow 0$
- $ightharpoonup N(a) \leftarrow 0$
- \rightarrow the initial value of Q(a) is undefined!

A first algorithm

Greedy algorithm

Repeat:

- ▶ $a \leftarrow \arg \max_a Q(a)$ (random tie breaking)
- $ightharpoonup r \leftarrow \text{reward}(a)$
- $ightharpoonup R(a) \leftarrow R(a) + r$
- $ightharpoonup N(a) \leftarrow N(a) + 1$
- $Q(a) \leftarrow \frac{R(a)}{N(a)}$

Note: The initial value of Q(a) plays a key role!

→ Be **optimistic** in case of uncertainty

A second algorithm

ε -greedy algorithm

Parameter: ε

Repeat:

- ▶ $r \leftarrow \text{reward}(a)$
- $ightharpoonup R(a) \leftarrow R(a) + r$
- \triangleright $N(a) \leftarrow N(a) + 1$
- $\qquad \qquad Q(a) \leftarrow \frac{R(a)}{N(a)}$

An adaptive algorithm

Adaptive-greedy algorithm

Parameter: c

Repeat for $t = 1, 2, \dots$

$$\triangleright \varepsilon \leftarrow \frac{c}{c+t}$$

- $a \leftarrow \begin{cases} \text{random action} & \text{with probability } \varepsilon \\ \text{arg max}_a Q(a) & \text{with probability } 1 \varepsilon \end{cases}$
- $ightharpoonup r \leftarrow \text{reward}(a)$
- $ightharpoonup R(a) \leftarrow R(a) + r$
- $ightharpoonup N(a) \leftarrow N(a) + 1$
- $\qquad \qquad Q(a) \leftarrow \tfrac{R(a)}{N(a)}$

Upper confident bound

Idea = **bonus** for uncertainty

UCB algorithm

Parameter: c

Repeat for $t = 1, 2, \ldots$

▶
$$a \leftarrow \arg\max_{a} (Q(a) + c\sqrt{\frac{\log t}{N(a)}})$$

$$ightharpoonup r \leftarrow \text{reward}(a)$$

$$ightharpoonup R(a) \leftarrow R(a) + r$$

$$ightharpoonup N(a) \leftarrow N(a) + 1$$

$$Q(a) \leftarrow \frac{R(a)}{N(a)}$$

(Auer, Cesa-Bianchi & Fischer 2002)

Bayesian algorithm

Idea = replace uncertainty by... randomness!

Thompson sampling

Initialize, for all actions a:

▶ P(a) ← prior on Q(a)

Repeat:

- ▶ for all actions a, $Q(a) \leftarrow \text{sample}(P(a))$
- ▶ $a \leftarrow \arg\max_a Q(a)$
- $ightharpoonup r \leftarrow \text{reward}(a)$
- ▶ $P(a) \leftarrow \text{update}(r)$

Proposed by Thompson in... 1933!

Thompson sampling: binary rewards

► Prior = uniform distribution

$$p(q) = 1_{(0,1)}(q)$$

Writing

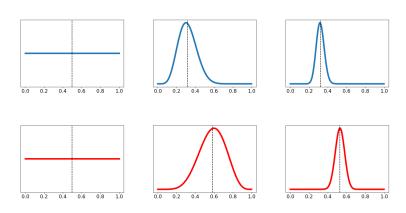
$$p(r|q) = q^{r}(1-q)^{1-r}, \quad r = 0, 1,$$

the posterior distribution follows from Bayes' rule:

$$p(q|r_1,...,r_N) = \frac{p(r_1,...,r_N|q)p(q)}{p(r_1,...,r_N)} \\ \propto q^{r_1+...+r_N} (1-q)^{N-(r_1+...+r_N)}$$

► This is a **Beta distribution** with parameters s + 1, N - s + 1, with $s = r_1 + ... + r_N$

- ightharpoonup True parameters = 0.3 and 0.5
- ▶ Beta distribution after N = 0, 10, 100 tries of each:



Thompson sampling: normal rewards

Prior = standard normal distribution

$$p(q) = \frac{1}{\sqrt{2\pi}}e^{-\frac{1}{2}q^2}$$

Since

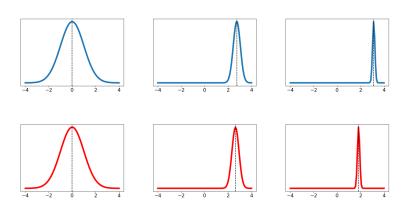
$$p(r|q) = \frac{1}{\sqrt{2\pi}}e^{-\frac{1}{2}(r-q)^2},$$

the posterior distribution follows from Bayes' rule:

$$p(q|r_1,...,r_N) = \frac{p(r_1,...,r_N|q)p(q)}{p(r_1,...,r_N)} \\ \propto e^{-\frac{N+1}{2}(q-\frac{1}{N+1}(r_1+...+r_N))^2}$$

► This is a **normal distribution** with mean $\frac{1}{N+1}(r_1 + ... + r_N)$ and variance $\frac{1}{N+1}$

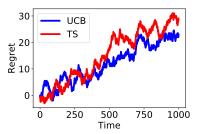
- ► True parameters = 3 and 2 (variance 1)
- ▶ Normal distribution after N = 0, 10, 100 tries:



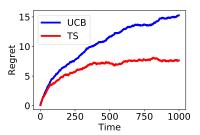
Outline

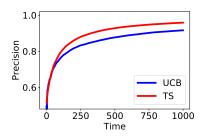
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- Binary rewards
- ▶ Parameters = 0.3 and 0.5

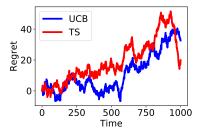


- ► Binary rewards
- ► Parameters = 0.3 and 0.5
- ▶ 200 independent runs

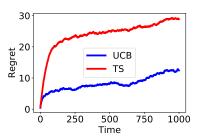


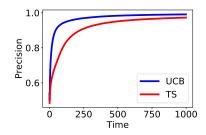


- Normal rewards
- ▶ Parameters = 2 and 3 (variance 1)



- Normal rewards
- ▶ Parameters = 2 and 3 (variance 1)
- ▶ 200 independent runs





Efficiency of UCB and TS

Expected regret:

$$E(R) = O(\log T) \rightarrow$$
sublinear

► For **binary rewards**, the multiplicative constant is:

$$\sum_{a \neq a^{\star}} \frac{1}{q^{\star} - q(a)} \quad \text{for UCB}$$

$$\sum_{a \neq a^{\star}} \frac{q^{\star} - q(a)}{D(q(a)||q^{\star})} \quad \text{for TS}$$

→ highest cost due to **quasi-optimal** actions!

Lower bound (binary rewards)

- A fundamental bound valid for any algorithm with sublinear regret (Lai & Robbins 1985)
- ▶ For any suboptimal action $a \neq a^*$,

$$\liminf_{T \to +\infty} \frac{N_T(a)}{\log T} \ge \frac{1}{D(q(a)||q^*)}$$

In particular,

$$\liminf_{T \to +\infty} \frac{\mathrm{E}(R)}{\log T} \ge \sum_{a \ne a^*} \frac{q^* - q(a)}{D(q(a)||q^*)}$$

 \rightarrow TS is **optimal**

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Contextual bandits

- ► Some **context** associated with each action (e.g., information on user for advertising)
- At time t = 1, 2, ..., choose **action** a_t based on **state** s_t (context) and get **reward** r_t that depends on both a_t and s_t
- Case of linear bandits:

$$q(a) = < \theta(a), s > \theta(a), s \in \mathbb{R}^d$$

Need to learn both $\theta(a)$ for each action a and a^* LinUCB algorithm combines linear regression and UCB

Adaptive bandits

- Assume some slowly varying environment
- ▶ **Discounted UCB**: Select the action *a*^t maximizing:

$$Q(a) + c\sqrt{\frac{1}{N(a)}\log\frac{1-\gamma^t}{1-\gamma}}$$

then update for all actions:

$$R(a) \leftarrow \gamma R(a) + r \mathbb{1}_{\{a_t = a\}}$$
 $N(a) \leftarrow \gamma N(a) + \mathbb{1}_{\{a_t = a\}}$
 $Q(a) \leftarrow \frac{R(a)}{N(a)}$

and $\gamma < 1$ is the discount factor

Adversarial bandits

- Assume the rewards are arbitrary sequences, chosen by some adversary
- ▶ Regret is for the **worst-case** scenario (minimax regret):

$$\min_{a} \max_{r} E(R)$$

where the regret is now

$$R = \max_{a} \sum_{t=1}^{T} r_{t,a} - \sum_{t=1}^{T} r_{t,a_t}$$

Exp3 (Exponential-weight algorithm for Exploration and Exploitation) → random selection of action a with prob. $\propto w(a)$, adapted through $w(a) \leftarrow w(a)e^{\eta r}$

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Brief history

Go has long been considered as the **ultimate game**, showing the superiority of humans over machines...

- ▶ In 2015, AlphaGo beats a human professional
- ▶ In 2016, AlphaGo beats the world champion Lee Sedol 4-1
- ▶ In 2017, AlphaGo Zero beats AlphaGo 100-0
- 2 months later, AlphaZero beats the world-champion prog.
 Stockfish (chess), Elmo (shogi) and AlphaGo Zero (go)



AlphaGo Zero

Based on Monte-Carlo Tree Search with

- bandit algorithm for opportunistic exploration
- deep learning for reward estimation



 $3^{19\times19}$ states $\approx 10^{172}$

Monte-Carlo Tree Search

Built from each state (the **root** of the tree) to choose the action, through simulations (e.g., 1600 runs in AlphaGo)

Based on 4 steps:

- ▶ **Selection:** select a leaf starting from the root
 - ightarrow bandit algorithm
- **Expansion:** expand this leaf with all possible actions
- ► Simulation: estimate the outcome of the game from the leaf
 → replaced by the neural net in AlphaGo
- Backpropagation: update the returns on the path from the leaf back to the root

Bandit algorithm in AlphaGo

Store in each branch of the tree:

- ightharpoonup R(s,a), cumulative reward of s after action a
- \triangleright N(s, a), number of selections of action a in state s
- ► *P*(*s*, *a*), prior prob. of action *a* in state *s* (given by the neural net)

Select **action** a that maximizes Q(s, a) + cU(s, a) with:

$$Q(s,a) = \frac{R(s,a)}{N(s,a)}, \quad U(s,a) = P(s,a) \frac{\sqrt{N(s)}}{1 + N(s,a)}$$

After 1600 runs, select for the root, say s_0 , the action a with probability $\pi(a) \propto N(s_0, a)^{1/\tau}$ (for some parameter $\tau > 0$) and discard the tree except the **subtree** under action a

Neural network

Input = game state + short history

- ▶ black = $8 \times 19 \times 19$
- white $= 8 \times 19 \times 19$
- ▶ total $\approx 6\,000$ bits

Output = moves (policy) + outcome (value)

- ▶ move probabilities \in [0, 1] $^{19\times19}$
- win probability $\in [0, 1]$

Architecture = deep CNN

- 40 layers
- $ho \approx 184\,000$ neurons

Training the neural net

Self play

- ► The best current player (= best neural net) plays 25 000 games against itself
- ightharpoonup Each game is stored, with the move prob. π and the outcome

$\textbf{Training} \rightarrow \mathsf{new} \; \mathsf{player}$

- ▶ 1000 epochs
- ► Each epoch = 2 048 states from the last 500 000 games
- ▶ Loss = KL on π + MSE on outcome $\in \{0,1\}$ + regularization

Competition

- Play 400 games of best current player vs. new player
- ▶ Decide that the new player is the best player if it wins at least 55% of the games

References

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