Reinforcement Learning

Lecture 9 : Bandit tools for Reinforcement Learning

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From bandit to RL

Solve a multi-armed bandit problem
$=$ maximize rewards in a MDP with one state

The bandit world

- several principles for exploration/exploitation
- efficient algorithms (UCB, Thompson Sampling)
- with regret guarantees

RL algorithms so far

- ϵ-greedy exploration
- algorithms with (sometimes) convergence guarantees that are not very efficient

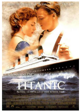
vs. (more) efficient algorithms with little theoretical understanding

Question : can we be inspired by bandit algorithms to

- propose new RL algorithms
- ... with theoretical guarantees ?

Outline

A more general bandit problem



In each time step t :

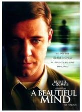
- a *context* $x_t \in \mathcal{X}$ is observed
  (e.g. the history of user t, characteristics of the movies)
- an arm $a_t \in \mathcal{A}_t$ is chosen by the algorithm
  (e.g. a movie in the catalog which is currently available)
- a reward $r_t = f(x_t, a_t) + \varepsilon_t$ is observed

Observations :

→ the mean rewards depends on the chosen arm AND on the context

→ the context plays the role of a *state*
(however the next state does not necessarily depend on our actions)

A more general bandit problem



user t : characteristic vector $u_t \in \mathbb{R}^p$

movie a : characteristic vector $x_a \in \mathbb{R}^{p'}$

➜ build a user-movie feature vector $x_{a,t} \in \mathbb{R}^d$

In each time step :

- the agent chooses an "arm" $x_t \in \mathcal{X}_t = \{(x_{a,t})_{a \in \mathcal{A}_t}\} \subseteq \mathbb{R}^d$
- and gets a reward $r_t = f(x_t) + \varepsilon_t$

where $f : \mathbb{R}^d \to \mathbb{R}$ is a regression function and $\mathbb{E}[\varepsilon_t | \mathcal{F}_{t-1}] = 0$.

Contextual linear bandits

In each round t, the agent

- receives a (finite) set of arms $\mathcal{X}_t \subseteq \mathbb{R}^d$
- chooses an arm $x_t \in \mathcal{X}_t$
- gets a reward $r_t = \theta_\star^\top x_t + \varepsilon_t$

where

- $\theta_\star \in \mathbb{R}^d$ is an unknown regression vector
- ε_t is a centered noise, independent from past data

Assumption : σ^2- sub-Gaussian noise

$$\forall \lambda \in \mathbb{R}, \ \mathbb{E}\left[e^{\lambda X}\right] \leq e^{\frac{\lambda^2 \sigma^2}{2}}$$

e.g., Gaussian noise, bounded noise.

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where

- $\theta_\star \in \mathbb{R}^d$ is an unknown regression vector
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(Pseudo)-regret for contextual bandit

maximizing expected total reward $\leftrightarrow$ minimizing the expectation of

$$\mathcal{R}_T = \sum_{t=1}^{T} \left(\max_{x \in \mathcal{X}_t} \theta_\star^\top x - \theta_\star^\top x_t \right)$$

→ in each round, comparison to a possibly different optimal action !

Tools for solving linear bandits

Algorithms will rely on estimates / confidence regions / posterior distributions for $\theta_\star \in \mathbb{R}^d$.

- design matrix (with regularization parameter $\lambda > 0$)

$$B_t^\lambda = \lambda I_d + \sum_{s=1}^{t} x_s x_s^\top$$

- regularized least-square estimate

$$\hat{\theta}_t^\lambda = \left(B_t^\lambda\right)^{-1} \left(\sum_{s=1}^{t} r_t x_t \right)$$

- estimate of the expected reward of an arm $x \in \mathbb{R}^d$: $x^\top \hat{\theta}_t^\lambda$

➜ sufficient for Follow the Leader, but not for smarter algorithms !

A Bayesian view on Linear Regression

Bayesian model :

- likelihood : $r_t = \theta_\star^\top x_t + \varepsilon_t$
- prior : $\theta_\star \sim \mathcal{N}(0, \kappa^2 \mathrm{I}_d)$

Assuming further that the noise is Gaussian : $\varepsilon_t \sim \mathcal{N}(0, \sigma^2)$, the posterior distribution of $\theta_\star$ has a closed form :

$$\theta_\star | x_1, r_1, \dots, x_t, r_t \ \sim \ \mathcal{N}\left(\hat{\theta}_t^\lambda, \sigma^2 \left(B_t^\lambda\right)^{-1}\right)$$

with

- $B_t^\lambda = \lambda \mathrm{I}_d + \sum_{s=1}^t x_s x_s^\top$
- $\hat{\theta}_t^\lambda = \left(B_t^\lambda\right)^{-1} \left(\sum_{s=1}^t r_s x_s\right)$ is the regularized least square estimate

with a regularization parameter $\lambda = \frac{\sigma^2}{\kappa^2}$.

Thompson Sampling for Linear Bandits

Recall the Thompson Sampling principle :

> "draw a possible model from the posterior distribution and act optimally in this sampled model"

Thompson Sampling in linear bandits

In each round $t+1$,

$$
\begin{aligned}
\tilde{\theta}_t &\sim \mathcal{N}\left(\hat{\theta}_t^\lambda, \sigma^2 \left(B_t^\lambda\right)^{-1}\right) \\
x_{t+1} &= \underset{x \in \mathcal{X}_{t+1}}{\operatorname{argmax}}\ x^\top \tilde{\theta}_t
\end{aligned}
$$

Numerical complexity : one needs to draw a sample from a multivariate Gaussian distribution, e.g.

$$\tilde{\theta}_t = \hat{\theta}_t^\lambda + \sigma \left(B_t^\lambda\right)^{-1/2} X$$

where X is a vector with d independent $\mathcal{N}(0,1)$ entries.

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Regret guarantees : [Agrawal and Goyal, 2013] prove that (a variant of) Thompson Sampling attains sub-linear regret :

$$\mathcal{R}_T(\mathrm{TS}) = \mathcal{O}\left(d^{3/2}\sqrt{T}\right) \quad \text{with high probability}$$

Outline

Regret minimization

For simplicity, we will define regret for **episodic MDPs**, in which

$$V^\pi(s) = V_1^\pi(s) = \mathbb{E}^\pi\left[\sum_{h=1}^{H} r(s_t, a_t) \middle| s_1 = s\right].$$

For each episode $t \in \{1, \dots, T\}$, an episodic RL algorithm

- starts in some initial state $s_1^t \sim \rho$
- selects a policy π^t (based on observations from past episodes)
- uses this policy to generate an episode of length H :

$$s_1^t, a_1^t, r_1^t, s_2^t, \dots, s_H^t, a_H^t, r_H^t$$

where $a_h^t = \pi_h^t(s_h^t)$ and $(r_h^t, s_{h+1}^t) = \mathrm{step}(s_h^t, a_h^t)$

Definition

The (pseudo)-regret of an episodic RL algorithm $\pi = (\pi^t)_{t\in\mathbb{N}}$ in T episodes is

$$\mathcal{R}_T(\pi) = \sum_{t=1}^{T}\left[V^\star(s_1^t) - V^{\pi^t}(s_1^t)\right].$$

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Definition

The (pseudo)-regret of an episodic RL algorithm $\pi = (\pi^t)_{t\in\mathbb{N}}$ in T episodes is

$$\mathcal{R}_T(\pi) = \sum_{t=1}^{T}\left[\max_a r(s_1, a) - r(s_1, a_1^t)\right] \quad H = 1, \text{single state } s_1.$$

Regret minimization

For simplicity, we will define regret for **episodic MDPs**, in which

$$V^\pi(s) = V_1^\pi(s) = \mathbb{E}^\pi\left[\sum_{h=1}^{H} r(s_t, a_t) \,\middle|\, s_1 = s\right].$$

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Definition

The (pseudo)-regret of an episodic RL algorithm $\pi = (\pi^t)_{t\in\mathbb{N}}$ in T episodes is

$$\mathcal{R}_T(\pi) = \sum_{t=1}^{T}\left[\mu^\star - \mu_{a_1^t}\right] \quad H = 1, \text{single state } s_1.$$

Reminder : Minimizing regret in bandits

Small regret requires to introduce the right amount of exploration, which can be done with

- ϵ-greedy

explore uniformly with probability ϵ, otherwise trust the estimated model

- Upper Confidence Bounds algorithms

act as if the optimistic model were the true model

- Thompson Sampling

act as if a model sampled from the posterior distribution were the true model

What is wrong with ε-greedy in RL ?

Example : Q-Learning with ε-greedy

- ➜ ε-greedy exploration

$$a_t = \begin{cases} \operatorname{argmax}_{a \in \mathcal{A}} \hat{Q}_t(s_t, a) & \text{with probability } 1 - \varepsilon_t \\ \sim \mathcal{U}(\mathcal{A}) & \text{with probability } \epsilon_t \end{cases}$$

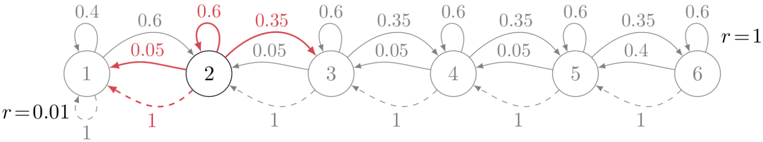
- ➜ Q-Learning update

$$\hat{Q}_t(s_t, a_t) = \hat{Q}_{t-1}(s_t, a_t) + \alpha_t \left(r_t + \gamma \max_b \hat{Q}_{t-1}(s_t, b) - \hat{Q}_{t-1}(s_t, a_t) \right)$$

⚠ $\hat{Q}_t(s, a)$ is *not* an unbiased estimate of $Q^\star(s, a)$...
(except in the bandit case)

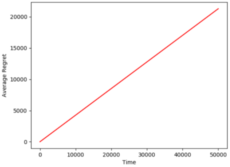
What is wrong with ε-greedy ?

The RiverSwim MDP :

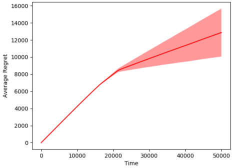


⚠ ε can be hard to tune...

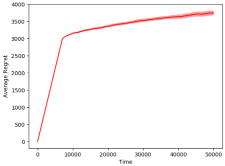
What is wrong with ε-greedy ?



$$\epsilon_t = 0.5$$



$$\epsilon_t = \frac{\epsilon_0}{(N(s_t) - 1000)^{2/3}}$$



$$\epsilon_t = \begin{cases} 1 & \text{if } t < 7000 \\ \frac{\epsilon_0}{\sqrt{N(s_t)}} & \text{otherwise} \end{cases}$$

credit : Alessandro Lazaric

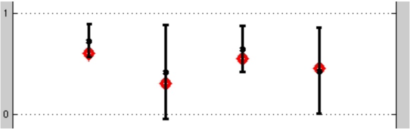
⚠ ε-greedy performs undirected exploration

- alternative : model-based methods in which exploration is targeted towards *uncertain regions* of the state/action space

Outline

Towards an optimistic learning algorithm

- **Reminder** : Optimistic Bandit model



set of possible bandit models $\boldsymbol{\mu} = (\mu_1, \mu_2, \mu_3, \mu_4)$:

$$\mathcal{M}_t = \mathcal{I}_1(t) \times \mathcal{I}_2(t) \times \mathcal{I}_3(t) \times \mathcal{I}_4(t)$$

An optimistic bandit model is

$$\boldsymbol{\mu}_t^+ \in \underset{\boldsymbol{\mu} \in \mathcal{M}_t}{\mathrm{argmax}} \ \mu^\star$$

➜ the best arm in $\boldsymbol{\mu}_t^+$ is $A_t = \underset{a \in \mathcal{A}}{\text{argmax}} \ \mathrm{UCB}_a(t)$

(arm selected by UCB)

Towards an optimistic learning algorithm

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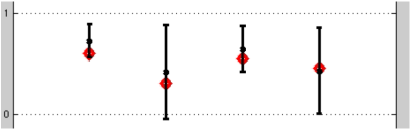

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(arm selected by UCB)

Towards an optimistic learning algorithm

- **Extension** : Optimistic Markov Decision Process

  set of possible MDPs $\boldsymbol{M} = \langle \mathcal{S}, \mathcal{A}, r, p \rangle$:

$$\mathcal{M}_t = \{\langle \mathcal{S}, \mathcal{A}, r, p \rangle : r, p \in \mathcal{B}_t^r \times \mathcal{B}_t^p\}$$

An optimistic Markov Decision Process is

$$\boldsymbol{M}_t^+ \in \operatorname*{argmax}_{\boldsymbol{M} \in \mathcal{M}_t} V_{\boldsymbol{M}}^\star(s_1)$$

→ an optimal policy in $\boldsymbol{M}_t^+$ is such that

$$\pi_t^+ \in \operatorname*{argmax}_{\pi} \max_{\boldsymbol{M} \in \mathcal{M}_t} V_{\boldsymbol{M}}^\pi(s_1)$$

Challenges

1. How to construct the set $\mathcal{M}_t$ of possible MDPs ?
2. How to numerically compute π_t^+ ?

Towards an optimistic learning algorithm

- **Extension** : Optimistic Markov Decision Process

$$\text{set of possible MDPs} \quad \boldsymbol{M} = \langle \mathcal{S}, \mathcal{A}, r, p \rangle :$$

$$\mathcal{M}_t = \{\langle \mathcal{S}, \mathcal{A}, r, p \rangle : r, p \in \mathcal{B}_t^r \times \mathcal{B}_t^p\}$$

An optimistic Markov Decision Process is

$$\boldsymbol{M}_t^+ \in \operatorname*{argmax}_{\boldsymbol{M} \in \mathcal{M}_t} \max_{\pi} V_{\boldsymbol{M}}^{\pi}(s_1)$$

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Challenges

1. How to construct the set $\mathcal{M}_t$ of possible MDPs ?
2. How to numerically compute π_t^+ ?

Step 1 : Constructing $\mathcal{M}_t$

$$\mathcal{M}_t = \Big\{ \langle \mathcal{S}, \mathcal{A}, r, p \rangle : \forall (s,a) \in \mathcal{S} \times \mathcal{A}, r(s,a) \in \mathcal{B}_t^r(s,a), p(\cdot|s,a) \in \mathcal{B}_t^p(s,a) \Big\}$$

Idea : build individual confidence regions

- on the average reward $r(s,a)$: $\mathcal{B}_t^r(s,a) \subseteq \mathbb{R}$
- on the transition probability vector $p(\cdot|s,a)$: $\mathcal{B}_t^p(s,a) \subseteq \Delta(\mathcal{S})$

that rely on the empirical estimates

$$\hat{r}_t(s,a) = \frac{1}{n_t(s,a)} \sum_{i=1}^{n_t(s,a)} r[i] \quad \text{and} \quad \hat{p}_t(s'|s,a) = \frac{n_t(s,a,s')}{n_t(s,a)}$$

$n_t(s,a)$: number of visits of (s,a) until episode t
$n_t(s,a,s')$: number of times s' was the next state when the transition (s,a) was performed until episode t

Goal : $\mathbb{P}_{\boldsymbol{M}} \left(\boldsymbol{M} \in \mathcal{M}_t \right)$ is close to 1

Step 1 : Constructing $\mathcal{M}_t$

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Assuming bounded rewards,

$$\mathcal{B}_t^r(s,a) = \left[\hat{r}_t(s,a) - \sqrt{\frac{\ln(4(n_t(s,a))^2/\delta)}{2n_t(s,a)}} ; \hat{r}_t(s,a) + \sqrt{\frac{\ln(4(n_t(s,a))^2/\delta)}{2n_t(s,a)}} \right]$$

satisfies

$$\mathbb{P}\Big(\exists t \in \mathbb{N} : r(s,a) \notin \mathcal{B}_t^r(s,a) \Big) \leq \delta.$$

(Hoeffding inequality + union bound)

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Assuming bounded rewards,

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Idea : build individual confidence regions

- on the transition probability vector $p(\cdot|s,a)$: $\mathcal{B}_t^p(s,a) \subseteq \Delta(\mathcal{S})$

$$\mathcal{B}_t^p(s,a) = \left\{ p(\cdot|s,a) \in \Delta(\mathcal{S}) : \|p(\cdot|s,a) - \hat{p}_t(\cdot|s,a)\|_1 \leq C \sqrt{\frac{S \ln(n_t(s,a)/\delta)}{n_t(s,a)}} \right\}$$

satisfies

$$\mathbb{P}\Big(\exists t \in \mathbb{N} : p(\cdot|s,a) \notin \mathcal{B}_t^p(s,a) \Big) \leq \delta.$$

(Freedman inequality + union bound)
[Auer et al., 2008]

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Idea : build individual confidence regions

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$$\mathcal{B}_t^p(s,a) = \left\{ p(\cdot|s,a) \in \Delta(\mathcal{S}) : \left\| p(\cdot|s,a) - \hat{p}_t(\cdot|s,a) \right\|_1 \leq \beta_t^p(s,a) \right\}$$

satisfies

$$\mathbb{P}\Big(\exists t \in \mathbb{N} : p(\cdot|s,a) \notin \mathcal{B}_t^p(s,a) \Big) \leq \delta.$$

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$$\begin{aligned} \mathcal{B}_t^r(s,a) &= \left[\hat{r}_t(s,a) - \beta_t^r(s,a); \hat{r}_t(s,a) + \beta_t^r(s,a) \right] \\ \mathcal{B}_t^p(s,a) &= \left\{ p(\cdot|s,a) \in \Delta(\mathcal{S}) : \|p(\cdot|s,a) - \hat{p}_t(\cdot|s,a)\|_1 \leq \beta_t^p(s,a) \right\} \end{aligned}$$

with exploration bonuses :

$$\begin{aligned} \beta_t^r(s,a) &\propto \sqrt{\frac{\ln(n_t(s,a)/\delta)}{n_t(s,a)}} \\ \beta_t^p(s,a) &\propto \sqrt{\frac{S \ln(n_t(s,a)/\delta)}{n_t(s,a)}} \end{aligned}$$

Step 2 : Optimistic Value Iteration

Goal : Approximate $\pi^+ \in \operatorname{argmax}_{\pi} \max_{\boldsymbol{M} \in \mathcal{M}} V^{\pi}_{\boldsymbol{M}}$ for a set of MDPs

$$\mathcal{M} = \left\{ \langle \mathcal{S}, \mathcal{A}, r, p \rangle : \forall (s,a) \in \mathcal{S} \times \mathcal{A}, r(s,a) \in \mathcal{B}^r(s,a), p(\cdot|s,a) \in \mathcal{B}^p(s,a) \right\}$$

Recall the optimal solution for a fixed MDP : $\pi^\star_h = \text{greedy}(Q^\star_h)$ where

$$Q^\star_h(s,a) = r(s,a) + \sum_{s'} p(s'|s,a) \max_b Q^\star_{h+1}(s',b)$$

➜ $\pi^+_h = \text{greedy}(Q^+_h)$ where

$$Q^+_h(s,a) = \max_{(r,p) \in \mathcal{M}} \left[r(s,a) + \sum_{s'} p(s'|s,a) \max_b Q^+_{h+1}(s',b) \right]$$

Step 2 : Optimistic Value Iteration

$$Q_h^+(s,a) = \max_{(r,p)\in\mathcal{B}^r(s,a)\times\mathcal{B}^p(s,a)} \left[r(s,a) + p(\cdot|s,a)^\top \underbrace{\left(\max_b Q_{h+1}^+(s',b)\right)_{s'\in\mathcal{S}}}_{V_{h+1}^+} \right]$$

$$= \max_{r\in\mathcal{B}^r(s,a)} r + \max_{p\in\mathcal{B}^p(s,a)} p^\top V_{h+1}^+$$

$$= \hat{r}_t(s,a) + \beta_t^r(s,a) + \max_{p\in\mathcal{B}^p(s,a)} p^\top V_{h+1}^+$$

$$= \hat{r}_t(s,a) + \beta_t^r(s,a) + \hat{p}_t(\cdot|s,a)^\top V_{h+1}^+ + \max_{p\in\mathcal{B}^p(s,a)} (p - \hat{p}_t(\cdot|s,a))^\top V_{h+1}^+$$

$$\leq \hat{r}_t(s,a) + \beta_t^r(s,a) + \hat{p}_t(\cdot|s,a)^\top V_{h+1}^+ + \max_{p\in\mathcal{B}^p(s,a)} \|p - \hat{p}_t(\cdot|s,a)\|_1 \|V_{h+1}^+\|_\infty$$

$$= \hat{r}_t(s,a) + \beta_t^r(s,a) + \hat{p}_t(\cdot|s,a)^\top V_{h+1}^+ + \beta_t^p(s,a)(H-h)r_{\max}$$

$$= \hat{r}_t(s,a) + \underbrace{[\beta_t^r(s,a) + \beta_t^p(s,a)(H-h)r_{\max}]}_{\text{exploration bonus}} + \hat{p}_t(\cdot|s,a)^\top V_{h+1}^+$$

Optimistic algorithm

A family of algorithms

An **optimistic algorithm** uses in episode $t+1$ the exporation policy $\pi_h^{t+1} = \text{greedy}\left(\overline{Q}_h\right)$ where $\overline{Q}_h(s,a)$ is an optimistic Q-value function

$$\overline{Q}_h(s,a) = \hat{r}_t(s,a) + \beta_t(s,a) + \sum_{s' \in \mathcal{S}} \hat{p}_t(s'|s,a) \max_b \overline{Q}_{h+1}(s',b)$$

where $\beta_t(s,a)$ is some exploration bonus.

From the previous calculation, one can propose

$$\beta_t(s,a) = \beta_t^r(s,a) + C\beta_t^p(s,a) \simeq \sqrt{\frac{\ln(n_t(s,a))}{n_t(s,a)}} + C\sqrt{\frac{S\ln(n_t(s,a))}{n_t(s,a)}}$$

➜ $\beta_t(s,a)$ scales in $1/\sqrt{n_t(s,a)}$ where $n_t(s,a)$ is the number of previous visits to (s,a).

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where $\beta_t(s,a)$ is some exploration bonus.

- An example of optimistic algorithm in the episodic setting : UCB-VI [Azar et al., 2017]
- Optimistic algorithms were first proposed in the more complex average-reward MDPs : UCRL [Auer et al., 2008]

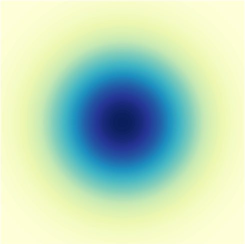
Regret

UCB-VI achieves $R_T = \mathcal{O}(\sqrt{H^2 SAT})$ w.h.p.

Outline

Posterior Sampling for RL

Bayesian assumption : $\boldsymbol{M}$ is drawn from some prior distribution ν_0.



$$\nu_t \in \Delta(\mathcal{M}) : \quad \text{posterior distribution over the set of MDPs}$$

Optimism	**Posterior Sampling**
Set of possible MDPs	Posterior distribution over MDPs
Compute the optimistic MDP	Sample from the posterior distribution

Posterior Sampling for Episodic RL

Algorithm 1: PSRL

Input : Prior distribution ν_0

for $t = 1, 2, \dots$ **do**

  $s_1 \sim \rho$ \\\\ get the starting state of episode t

  Sample $\widetilde{M}_t \sim \nu_{t-1}$ \\\\ sample an MDP from the current posterior distribution

  Compute $\tilde{\pi}^t$ an optimal policy for $\widetilde{M}_t$

  for $h = 1, \dots, H$ **do**

    $a_h = \tilde{\pi}^t_h(s_h)$ \\\\ choose next action according to $\tilde{\pi}^t$

    $r_h, s_{h+1} = \mathrm{step}(s_h, a_h)$

  end

  Compute ν_t based on ν_{t-1} and $\{(s_h, a_h, r_h, s_{h+1})\}_{h=1}^H$

end

[Strens, 2000, Osband et al., 2013]

Outline

Limitations of optimistic approaches

An important message from optimistic approaches :

➜ Do not only trust the estimated MDP $\hat{M}_t$, but take into account the uncertainty in the underlying estimate

$$
\begin{aligned}
\mathcal{B}_t^r(s,a) &= \left[\hat{r}_t(s,a) - \beta_t^r(s,a); \hat{r}_t(s,a) + \beta_t^r(s,a)\right] \\
\mathcal{B}_t^p(s,a) &= \left\{p(\cdot|s,a) \in \Delta(\mathcal{S}) : \|p(\cdot|s,a) - \hat{p}_t(\cdot|s,a)\|_1 \leq \beta_t^p(s,a)\right\}
\end{aligned}
$$

expressed by exploration bonuses scaling in $\sqrt{\frac{1}{n_t(s,a)}}$ where $n_t(s,a)$ is the count (=number of visits) of (s,a).

Scaling for large state action spaces ?

- each state action pair may be visited only very little...
- UCB-VI is quite inefficient in practice for large state-spaces (efficient, continuous variants is an active research direction)

A heuristic : count-based exploration

General principle

1. Estimate a "proxi" for the number of visits of a state $\tilde{n}_t(s)$
2. Add an exploration bonus directly to the collected rewards :

$$r_t^+ = r_t + c\sqrt{\frac{1}{\tilde{n}_t(s_t)}}$$

3. Run any DeepRL algorithm on

$$\mathcal{D} = \bigcup_t \left\{ \left(s_t, a_t, r_t^+, s_{t+1} \right) \right\}$$

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Example of pseudo-counts :

- use a hash function, e.g. $\phi : \mathcal{S} \to \{-1, 1\}^k$
  $n(\phi(s_t)) \leftarrow n(\phi(s_t)) + 1$
  (possibly learn a good hash function)

[Tang et al., 2017]

Limitations of Posterior Sampling

An important message from posterior sampling :

➜ Adding some noise to the estimated MDP $\hat{M}_t$ is helpful !

$$\begin{aligned} \tilde{r}_t(s,a) &= \hat{r}_t(s,a) + \epsilon_t(s,a) \\ \tilde{p}_t(s'|s,a) &= \hat{p}_t(\cdot|s,a) + \epsilon'_t(s,a). \end{aligned}$$

Scaling for large state action spaces ?

- maintaining independent posterior over all state action rewards and transitions can be costly
- more sophisticated prior distributions encoding some structure and the associated posteriors can be hard to sample from

➜ use other type of (non-Bayesian) randomized exploration ?
Noisy Networks [Fortunato et al., 2017]
Bootstrap DQN [Osband et al., 2016] ...

Outline

Monte-Carlo Tree Search

MCTS is a family of methods that use possibly random exploration to explore the tree of possible next states.

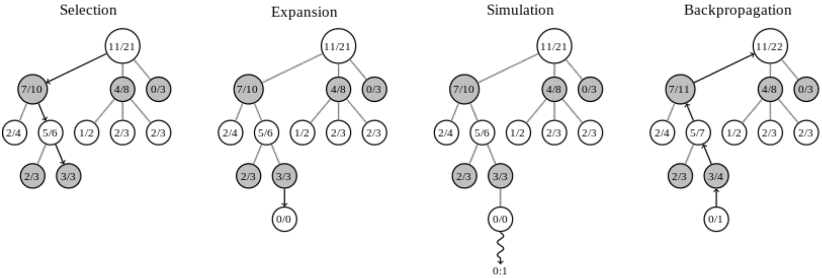


FIGURE – An generic MCTS algorithm illustrated for a game

The UCT algorithm

Bandit-Based Monte-Carlo planning : to select a path in the tree, run a bandit algorithm each time a children (next action) needs to be selected

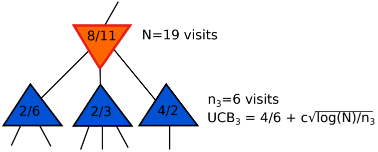
UCT = UCB for Trees [Kocsis and Szepesvári, 2006]

UCT in a Game Tree

In a MAX node s (= root player move), select an action

$$\underset{a \in \mathcal{C}(s)}{\operatorname{argmax}} \ \frac{S(s,a)}{N(s,a)} + c\sqrt{\frac{\ln\left(\sum_b N(s,b)\right)}{N(s,a)}}$$

$N(s,a)$: number of visits of (s,a)
$S(s,a)$: number of visits of (s,a) ending with the root player winning



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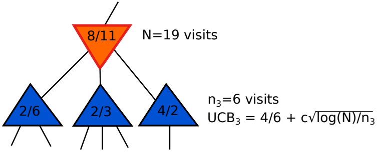
UCT = UCB for Trees [Kocsis and Szepesvári, 2006]

UCT in a Game Tree

In a MIN node s (= adversary move), select an action

$$\underset{a \in \mathcal{C}(s)}{\operatorname{argmin}} \ \frac{S(s,a)}{N(s,a)} - c\sqrt{\frac{\ln\left(\sum_b N(s,b)\right)}{N(s,a)}}$$

$N(s,a)$: number of visits of (s,a)
$S(s,a)$: number of visits of (s,a) ending with the root player winning



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$N(s,a)$: number of visits of (s,a)
$S(s,a)$: number of visits of (s,a) ending with the root player winning

When a leaf (or some maximal depth) is reached :

- a playout is performed (play the game until the end with a simple heuristic, or produce a random evaluation of the leaf position)
- the outcome of the playout (typically 1/0) is stored in all the nodes visited in the previous trajectory

The UCT algorithm

- first good AIs for Go where based on variants on UCT
- it remains a heuristic (no sample complexity guarantees, parameter c fined-tuned for each application)
- many variants have been proposed

[Browne et al., 2012]

Alpha Zero

AlphaZero learns a good policy by using a MCTS algorithm guided by a neural network
$\neq$ pure play-out based MCTS

Input

A neural network predicting a policy $\boldsymbol{p} \in \Delta(\mathcal{A})$ and a value $v \in \mathbb{R}$ from the current state s : $(\boldsymbol{p}, v) = f_\theta(s)$.

The MCTS algorithm maintains for each visited state/action the counts and cumulated values + a vector of prior action probabilities :

$$\{N(s,a), S(s,a), P(s,a)\}$$

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$$\{N(s,a), S(s,a), P(s,a)\}$$

Selection step : in some state s, choose the next action to be

$$\underset{a \in \mathcal{C}(s)}{\operatorname{argmax}} \left[\frac{S(s,a)}{N(s,a)} + c \times P(s,a) \frac{\sqrt{N(s)}}{1 + N(s,a)} \right]$$

for some (fine-tuned) constant c.

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The MCTS algorithm maintains for each visited state/action the counts and cumulated values + a vector of prior action probabilities :

$$\{N(s,a), S(s,a), P(s,a)\}$$

Expansion step : once a leaf s_L is reached, compute $(\boldsymbol{p}, v) = f_\theta(s_L)$.

- Set v to be the value of the leaf
- For all possible next actions b :
  - ➜ initialize the count $N(s_L, b) = 0$
  - ➜ initialize the prior probability $P(s_L, b) = \boldsymbol{p}_b$ (possibly add some noise)

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The MCTS algorithm maintains for each visited state/action the counts and cumulated values + a vector of prior action probabilities :

$$\{N(s,a), S(s,a), P(s,a)\}$$

Back-up step : for all ancestor s_t, a_t in the trajectory that end in leaf s_L,

$$\begin{aligned} N(s_t, a_t) &\leftarrow N(s_t, a_t) + 1 \\ S(s_t, a_t) &\leftarrow S(s_t, a_t) + v \end{aligned}$$

Alpha Zero

AlphaZero learns a good policy by using a MCTS algorithm guided by a neural network

$\neq$ pure play-out based MCTS

Input

A neural network predicting a policy $\boldsymbol{p} \in \Delta(\mathcal{A})$ and a value $v \in \mathbb{R}$ from the current state s : $(\boldsymbol{p}, v) = f_\theta(s)$.

The MCTS algorithm maintains for each visited state/action the counts and cumulated values + a vector of prior action probabilities :

$$\{N(s,a), S(s,a), P(s,a)\}$$

Output of the planning algorithm ? select an action a at random according to

$$\pi(a) = \frac{N(s_0,a)^{1/\tau}}{\sum_b N(s_0,b)^{1/\tau}}$$

for some (fine-tuned) temperature τ.

Training the neural network

- In AlphaGo, f_θ was trained on a database of games played by human
- In AlphaZero, the network is trained using only self-play

[Silver et al., 2016, Silver et al., 2017]

Let θ be the current parameter of the network $(\boldsymbol{p}, v) = f_\theta(s_L)$.

1. generate N games where each player uses MCTS(θ) to select the next action a_t (and output a probability over actions π_t)

$$\mathcal{D} = \bigcup_{i=1}^{\text{Nb games}} \left\{ \left(s_t, \pi_t, \pm r_{T_i}\right) \right\}_{i=1}^{T_i}$$

T_i : length of game i, $r_{T_i} \in \{-1, 0, 1\}$ outcome of game i for one player

2. Based on a sub-sample of $\mathcal{D}$, train the neural network using stochastic gradient descent on the loss function

$$L(s, \boldsymbol{\pi}, z; \boldsymbol{p}, v) = (z - v)^2 - \boldsymbol{\pi}^\top \ln(\boldsymbol{p}) + c\|\theta\|^2$$

A nice actor-critic architecture

AlphaZero alternates between

- **The actor** : MCTS(θ)
  generates trajectories guided by the network f_θ but still exploring

➜ act as a policy improvement
  ($N = 25000$ games played, each call to MCTS uses 1600 simulations)

- **The critic** : neural network f_θ
  updates θ based on trajectories followed by the critic

➜ evaluate the actor's policy

Summary

Bandit tools can be useful in more realistic, contextual models

Bandits tools are useful for Reinforcement Learning :

- UCRL, PSRL : bandit-based exploration for tabular MDPs
- ... that can motivate "deeper" heuristics

Bandit tools lead to big success in Monte-Carlo planning

- ... without proper sample complexity guarantees

➜ Unifying theory and practice is a big challenge in RL !

Perspective : bandit tools are also useful beyond RL (i.e. with no rewards to maximize) : best arm identification, black box optimization...

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