Linear Contextual Bandits

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Contextual Bandits

Multi-armed Bandit $\rightarrow a_1, \boldsymbol{a_2}, a_3$

all-user recommendation system

Context

e.g. the user’s historical purchase record, location, social network activity, …

$\rightarrow$ **Contextual Bandit** $\rightarrow a_1, \boldsymbol{a_2}, a_3$

personalized recommendation system

This example is from Chicheng Zhang’s lecture notes

Contextual Bandits

For time $t = 1, 2, \ldots, T$:

Environment generates a context $x_t \in \mathcal{X}$

Learner chooses an action $a_t \in \mathcal{A}$

Learner observes $r_t = R(x_t, a_t) + w_t$

$$\text{Regret} = \max_{\pi} \sum_{t=1}^{T} R(x_t, \pi(x_t)) - \sum_{t=1}^{T} R(x_t, a_t)$$

Optimal policy: $\pi(x) = \operatorname*{argmax}_{a \in \mathcal{A}} R(x, a)$

$$= \sum_{t=1}^{T} \max_{a \in \mathcal{A}} R(x_t, a) - \sum_{t=1}^{T} R(x_t, a_t)$$

View Each Context as a Separate MAB

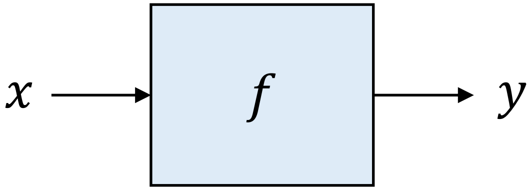
$$\text{Regret} = \sum_{t=1}^{T} \max_{a \in \mathcal{A}} R(x_t, a) \; - \sum_{t=1}^{T} R(x_t, a_t)$$

$$= \sum_{x \in \mathcal{X}} \left(\sum_{t: x_t = x} \max_{a \in \mathcal{A}} R(x, a) \; - \sum_{t: x_t = x} R(x, a_t) \right)$$

Not scalable and not generalizable

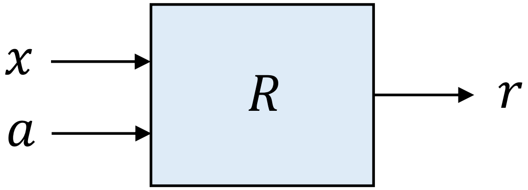
Function Approximation in Contextual Bandits

x: context, a: action, r: reward

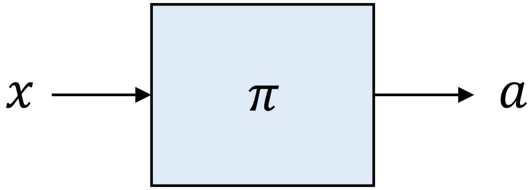


Find an f so that $f(x) \approx y$ for **seen** (x, y) pairs

Hoping that $f(x') \approx y'$ also holds for **unseen** x'



value-based approach



policy-based approach

If a good approximation $\hat{R}$ is found, a good policy can be derived as

$$\pi(x) = \underset{a}{\operatorname{argmax}}\, \hat{R}(x, a)$$

Linear Contextual Bandits

This is a linear **assumption**, not just linear **function approximation**. The former is stronger.

Linear Reward Assumption: $R(x, a) = \phi(x, a)^\top \theta^\star$

$\phi(x, a) \in \mathbb{R}^d$ is a **feature vector** for the context-action pair (known to learner)

$\theta^\star \in \mathbb{R}^d$ is the ground-truth **weight vector** (hidden from learner)

Given: feature mapping $\phi: \mathcal{X} \times \mathcal{A} \rightarrow \mathbb{R}^d$

For time $t = 1, 2, \dots, T$:

Environment generates a context $x_t \in \mathcal{X}$

Learner chooses an action $a_t \in \mathcal{A}$

Learner observes $r_t = \phi(x_t, a_t)^\top \theta^\star + w_t$ (w_t is zero-mean)

$$\text{Regret} = \sum_{t=1}^{T} \max_{a \in \mathcal{A}} R(x_t, a) - \sum_{t=1}^{T} R(x_t, a_t) = \sum_{t=1}^{T} \max_{a \in \mathcal{A}} \phi(x_t, a)^\top \theta^\star - \sum_{t=1}^{T} \phi(x_t, a_t)^\top \theta^\star$$

Linear CB is a Generalization of MAB

$\phi(x, a) = e_a$

$e_a: (0, 0, \cdots, 1, 0, \cdots, 0)$

a-th entry

$\theta^* = \begin{bmatrix} R(1) \\ \vdots \\ R(A) \end{bmatrix}$

Key Questions in Linear Contextual Bandits

- How to obtain an estimated reward function $\hat{R}(x, a)$?
  - Was easy in multi-armed bandits – today we'll see how to do this in linear CB
- How to explore?
  - ϵ-greedy

$$a_t = \begin{cases} \text{uniform}(\mathcal{A}) & \text{with prob. } \epsilon \\ \text{argmax}_a \, \hat{R}_t(x_t, a) & \text{with prob. } 1-\epsilon \end{cases}$$

  - Boltzmann exploration

$$p_t(a) \propto \exp\left(\lambda_t \, \hat{R}_t(x_t, a)\right)$$

  - Optimism in the face of uncertainty (LinUCB)
  - Thompson Sampling

How to Estimate the Reward Function $\boldsymbol{R(x, a)}$?

- Recall $R(x, a) = \phi(s, a)^\top \theta^\star$. We only need to estimate $\theta^\star$.
- At time t, we already gathered

$$r_1 = \phi(x_1, a_1)^\top \theta^\star + w_1$$
$$r_2 = \phi(x_2, a_2)^\top \theta^\star + w_2$$
$$\vdots$$
$$r_{t-1} = \phi(x_{t-1}, a_{t-1})^\top \theta^\star + w_{t-1}$$

How to estimate $\theta^\star$?

Linear Regression

Linear Regression

At time t, we have collected $(x_1, a_1, r_1), (x_2, a_2, r_2), \ldots, (x_{t-1}, a_{t-1}, r_{t-1})$.

We want to generate an estimation $\hat{\theta}_t$ such that $\phi(x_i, a_i)^\top \hat{\theta}_t \approx r_i$

Linear Regression / Ridge Regression (define $\phi_i = \phi(x_i, a_i)$)

$$\hat{\theta}_t = \min_{\theta} \sum_{i=1}^{t-1} \left(\phi_i^\top \theta - r_i\right)^2 + \lambda \|\theta\|^2 \quad \Leftrightarrow \quad \hat{\theta}_t = \left(\lambda I + \sum_{i=1}^{t-1} \phi_i \phi_i^\top\right)^{-1} \left(\sum_{i=1}^{t-1} \phi_i r_i\right)$$

$\Rightarrow \hat{R}_t(x, a) = \phi(x, a)^\top \hat{\theta}_t$ (Use this directly in ϵ-greedy or Boltzmann exploration!)

To design a UCB algorithm, we have to quantify the estimation error $\hat{\theta}_t - \theta^\star$

What can we say about $\hat{\theta}_t - \theta^\star$?

Let's develop some intuition first.. (This intuition comes from Haipeng Luo's lecture)

Let $r_i = \phi_i^\top \theta^\star + w_i$ for $i = 1, \dots, N$

Assume $w_i \sim \mathcal{N}(0, \cancel{\sigma^2} 1)$, and

Assume $\{\phi_1, \dots, \phi_N\}$ are fixed vectors independent from $\{w_1, \dots, w_N\}$

Let

$$\hat{\theta} = \left(\sum_{i=1}^N \phi_i \phi_i^\top\right)^{-1} \left(\sum_{i=1}^N \phi_i r_i\right)$$

Question: What can we say about $\hat{\theta} - \theta^\star$?

$$\hat{\theta} - \theta^* = \left(\sum_{i=1}^N \phi_i \phi_i^T\right)^{-1}\left(\sum_{i=1}^N \phi_i r_i\right) - \left(\sum_{i=1}^N \phi_i \phi_i^T\right)^{-1}\left(\sum_{i=1}^N \phi_i \phi_i^T \theta^*\right)$$

$$= \left(\sum_{i=1}^N \phi_i \phi_i^T\right)^{-1}\left(\sum_{i=1}^N \phi_i \underbrace{(r_i - \phi_i^T \theta^*)}_{w_i}\right)$$

$$= \Lambda^{-1} \underbrace{\left(\sum_{i=1}^N \phi_i w_i\right)}_{z}$$

$$\Lambda = \sum_{i=1}^N \phi_i \phi_i^T$$

$$\mathbb{E}[z z^T] = \mathbb{E}\left[\left(\sum_{i=1}^N \phi_i w_i\right)\left(\sum_{i=1}^N \phi_i w_i\right)^T\right]$$

$$= \mathbb{E}\left[\sum_{i=1}^N w_i^2 \phi_i \phi_i^T\right]$$

$$= \Lambda$$

Let's check the covariance matrix of $\boxed{\Lambda^{1/2}(\hat{\theta} - \theta^*)}$

$$\mathbb{E}\left[\underbrace{\Lambda^{1/2}(\hat{\theta}-\theta^*)(\hat{\theta}-\theta^*)^T\Lambda^{1/2}}_{\Lambda^{-1} z z^T \Lambda^{-1}}\right] = I$$

$$\mathbb{E}\left[(\hat{\theta}-\theta^*)^T \Lambda^{1/2} \Lambda^{1/2} (\hat{\theta}-\theta^*)\right] = d$$

$$a^T M a = \|a\|_M$$

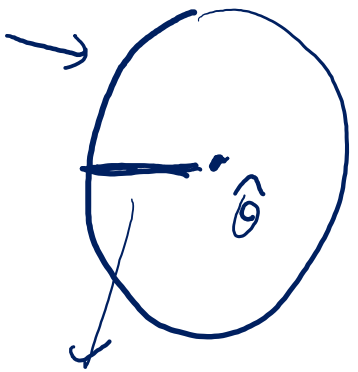
$$\Rightarrow \mathbb{E}\left[\|\hat{\theta}-\theta^*\|_\Lambda\right] = d$$

Geometric Intuition

$$\|\hat{\theta}-\theta^*\|_\Lambda^2 = (\hat{\theta}-\theta^*)\begin{bmatrix}\Lambda_{11} & & 0 \\ & \Lambda_{22} & \\ 0 & & \ddots \ \Lambda_{dd}\end{bmatrix}(\hat{\theta}-\theta^*) \le d$$

$$\sum_i (\hat{\theta}_1-\theta_1^*)^2 \Lambda_{11} \le d$$

$$\boxed{(\hat{\theta}_1-\theta_1^*)^2 \Lambda_{11} = d} \Rightarrow \text{radius}_1 = \sqrt{\frac{d}{\Lambda_{11}}}$$



$$\sqrt{\frac{d}{\Lambda_{11}}}$$

$$\Lambda = \sum_{i=1}^{t-1} \phi_i \phi_i^T + I$$

Concentration Inequality for Linear Regression

Theorem.

In linear contextual bandits, assume w_t is zero-mean and 1-sub-Gaussian.
$\|\phi(x,a)\|_2 \leq 1, \quad \|\theta^\star\|_2 \leq 1.$

Let

$$\hat{\theta}_t = \Lambda_t^{-1}\left(\sum_{i=1}^{t-1} \phi_i r_i\right), \qquad \text{where } \Lambda_t = I + \sum_{i=1}^{t-1} \phi_i \phi_i^\top .$$

Then with probability at least $1-\delta$, for all $t = 1, \ldots, T$,

$$\left\|\theta^\star - \hat{\theta}_t\right\|_{\Lambda_t}^2 \leq \beta \triangleq d \log\left(1 + \frac{T}{d}\right) + 3\log\frac{1}{\delta}$$

Abbasi-Yadkori, Pal, Szepesvari. **Improved algorithms for linear stochastic bandits.** 2011.

Another Viewpoint on the Concentration Inequality

$$\left\|\theta^\star - \hat{\theta}_t\right\|_{\Lambda_t}^2 = \left(\theta^\star - \hat{\theta}_t\right)^\top \left(I + \sum_{i=1}^{t-1} \phi_i \phi_i^\top\right) \left(\theta^\star - \hat{\theta}_t\right)$$

$$= \underbrace{\sum_{i=1}^{t-1} \left(\phi_i^\top \theta^\star - \phi_i^\top \hat{\theta}_t\right)^2}_{\text{The difference between the predictions of } \theta^\star \text{ and } \hat{\theta}_t \text{ over the past samples}} + \left\|\theta^\star - \hat{\theta}_t\right\|^2 = O(d \log(T/\delta))$$

LinUCB

Most “optimistic” estimation for the reward of a

LinUCB

In round t, receive x_t, draw

$$a_t = \text{argmax}_{a \in \mathcal{A}} \boxed{}$$

Observe $r_t = \phi(x_t, a_t)^\top \theta^\star + w_t$.

LinUCB

$$\max_{\theta} \phi(x_t,a)^\top\theta = \underline{\phi(x_t,a)^\top\hat{\theta}_t} + \underline{\phi(x_t,a)^\top(\theta-\hat{\theta}_t)}$$

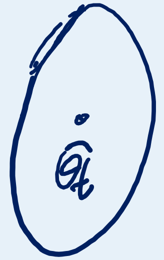
$$\leq \quad '' \quad \|\phi(x_t,a)\|_{\Lambda_t^{-1}} \underbrace{\|\theta-\hat{\theta}_t\|_{\Lambda_t}}_{\sqrt{\beta}}$$

$$= \underline{\phi(x_t,a)^\top\hat{\theta}_t + \sqrt{\beta}\,\|\phi(x_t,a)\|_{\Lambda_t^{-1}}}$$

LinUCB

In round t, receive x_t, draw

$$a_t = \operatorname{argmax}_{a\in\mathcal{A}} \max_{\theta:\|\theta-\hat{\theta}_t\|_{\Lambda_t}\leq\beta} \phi(x_t,a)^\top\theta$$



where

$$\hat{\theta}_t = \Lambda_t^{-1}\left(\sum_{i=1}^{t-1}\phi_i r_i\right), \qquad \Lambda_t = I + \sum_{i=1}^{t-1}\phi_i\phi_i^\top.$$

Observe $r_t = \phi(x_t,a_t)^\top\theta^\star + w_t$.

LinUCB

LinUCB

In round t, receive x_t, draw

$$a_t = \mathrm{argmax}_{a \in \mathcal{A}} \quad \phi(x_t, a)^\top \hat{\theta}_t + \sqrt{\beta} \|\phi(x_t, a)\|_{\Lambda_t^{-1}}$$

where

$$\hat{\theta}_t = \Lambda_t^{-1} \left(\sum_{i=1}^{t-1} \phi_i r_i \right), \qquad \Lambda_t = I + \sum_{i=1}^{t-1} \phi_i \phi_i^\top .$$

Observe $r_t = \phi(x_t, a_t)^\top \theta^\star + w_t$.

$$R(x,a) = \phi(x,a)^T \theta^*$$

Regret Analysis for LinUCB

Regret Bound of LinUCB

With probability at least $1-\delta$,

$$\text{Regret} \ \le O\big(d\sqrt{T}\log(T/\delta)\big) = \tilde{O}(d\sqrt{T}) \ .$$

$$\text{Regret} = \sum_{t=1}^{T} \left(\max_a R(x_t,a) - R(x_t,a_t) \right)$$

$$= \sum_{t=1}^{T} \boxed{\max_a \phi(x_t,a)^T \theta^*} - \phi(x_t,a_t)^T \theta^*$$

$$\boxed{} \le \phi(x_t,a_t)^T \hat{\theta}_t + \sqrt{\beta}\, \|\phi(x_t,a_t)\|_{\Lambda_t^{-1}}$$

$$\text{Regret} \le \sum_t \phi(x_t,a_t)^T(\hat{\theta}_t - \theta^*) + \sqrt{\beta}\, \|\phi(x_t,a_t)\|_{\Lambda_t^{-1}}$$

$$\le \sum_t \|\phi(x_t,a_t)\|_{\Lambda_t^{-1}} \underbrace{\|\hat{\theta}_t - \theta^*\|_{\Lambda_t}}_{\sqrt{\beta}} + \quad ''$$

$$\le 2 \sum_t \|\phi(x_t,a_t)\|_{\Lambda_t^{-1}} \sqrt{\beta}$$

Elliptical Potential Lemma

Let $\phi_i \in \mathbb{R}^d$ and $\|\phi_i\|_2 \le 1$. Define $\Lambda_t = I + \sum_{i=1}^{t-1} \phi_i \phi_i^\top$.

Then

$$\sum_{t=1}^{T} \|\phi_t\|^2_{\Lambda_t^{-1}} \le d \log\left(1 + \frac{T}{d}\right).$$

$$\sum_{t=1}^{T} \frac{a_t}{\left(\sum_{s=1}^{t-1} a_s\right) + 1} \le \log T$$

when $0 \le a_t \le 1$

$$2 \sum_{t=1}^{T} \|\phi_t\|_{\Lambda_t^{-1}} \sqrt{\beta} \le 2\sqrt{\left(\sum_{t=1}^{T} \|\phi_t\|^2_{\Lambda_t^{-1}}\right)\left(\sum_{t=1}^{T} 1\right)\beta} \le 2\sqrt{d \log(\cdots) \cdot T\beta}$$

$$\approx O\left(d\sqrt{T} \log(\cdots)\right)$$

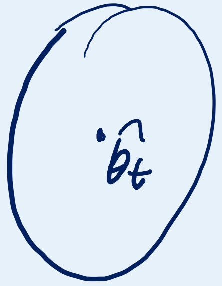
Thompson Sampling

Thompson Sampling for Linear Contextual Bandits

In round t, receive x_t, draw

$$\theta_t \sim \mathcal{N}\left(\hat{\theta}_t, \Lambda_t^{-1}\right)$$

$$a_t = \operatorname{argmax}_{a \in \mathcal{A}} \quad \phi(x_t, a)^\top \theta_t$$



where

$$\hat{\theta}_t = \Lambda_t^{-1}\left(\sum_{i=1}^{t-1} \phi_i r_i\right), \qquad \Lambda_t = I + \sum_{i=1}^{t-1} \phi_i \phi_i^\top .$$

Observe $r_t = \phi(x_t, a_t)^\top \theta^\star + w_t$.

There is no assumption on the distribution of x_t

- How is this possible?