Linear Contextual Bandits

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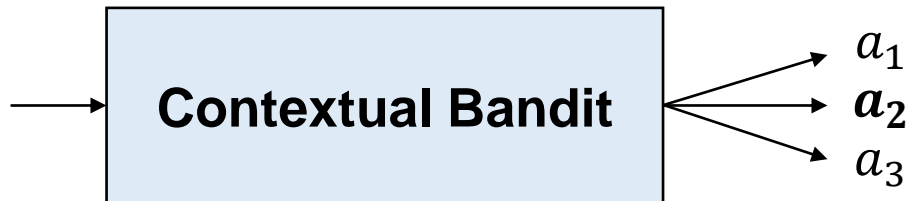
Contextual Bandits

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

all-user recommendation system

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

personalized recommendation system

Context

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

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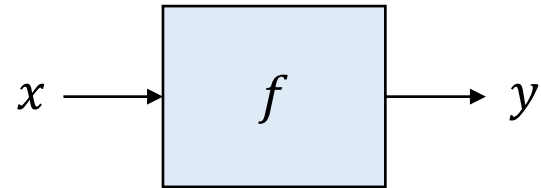
$$\text{Regret} = {\color{red}\max_{\pi}} \sum_{t=1}^{T} R(x_t, {\color{red}\pi(x_t)}) - \sum_{t=1}^{T} R(x_t, a_t)$$

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
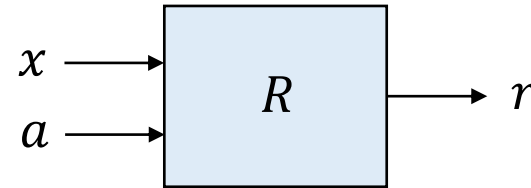
Function Approximation in Contextual Bandits

x: context, a: action, r: reward
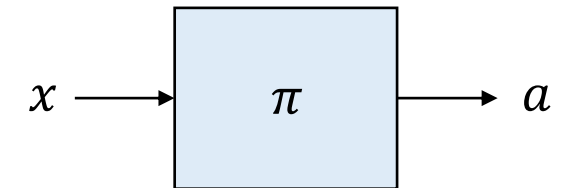

$x \longrightarrow \boxed{f} \longrightarrow y$

🐱	C
🐈	C
🐕	D
⋮	⋮
🐶	?

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

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

Linear Contextual Bandits

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 $\phi: \mathcal{X} \times \mathcal{A} \to \mathbb{R}^d$

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

$$\phi(x,a) = e_a$$

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

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

$$\uparrow$$

a-th entry

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

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

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

How to Estimate the Reward Function $R(x, a)$?

- 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 $\phi_i = \phi(x_i, a_i)$)

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

$\Rightarrow \hat{R}_t(x, a) = \phi(x, a)^\top \hat{\theta}_t$ (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 <u>lecture</u>)

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

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

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

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 $\hat{\theta} - \theta^\star$?

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

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

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

$$\downarrow$$
$$a \overset{\downarrow}{M} a = \|a\|_M^2$$

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

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

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

$$= \Lambda$$

Let's check the covariance matrix of

$$\boxed{\Lambda^{1/2}(\hat{\theta} - \theta^*)}$$

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

$$\underbrace{\Lambda^{-1} z z^\top \Lambda^{-1}}$$

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

$$\Rightarrow \mathbb{E}\left[\|\hat{\theta} - \theta^*\|_\Lambda^2 \right] = d$$

Geometric Intuition

$$\| \hat{\theta} - \theta^* \|_\Lambda^2 = (\hat{\theta} - \theta^*) \begin{bmatrix} \Lambda_{11} & & O \\ & \Lambda_{22} & \\ & & \ddots \\ O & & \Lambda_{dd} \end{bmatrix} (\hat{\theta} - \theta^*) \leq d$$
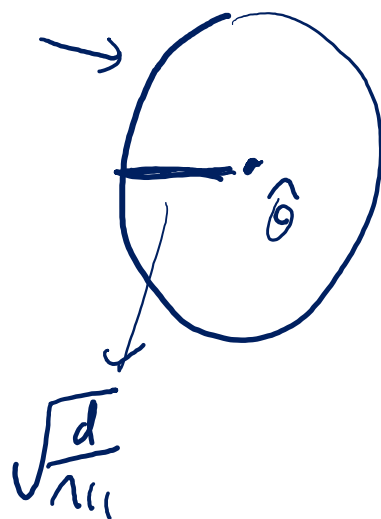
$$\sum_i \left(\hat{\theta}_i - \theta_i^* \right)^2 \Lambda_{ii} \leq d$$

$$\boxed{\left(\hat{\theta}_1 - \theta_1^* \right)^2 \Lambda_{11} = d} \Rightarrow radius_1 = \sqrt{\frac{d}{\Lambda_{11}}}$$

$\hat{\theta}$

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

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

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

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

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

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

$$= \underbrace{\sum_{i=1}^{t-1} \left(\phi_i^\top \theta^\star - \phi_i^\top \hat{\theta}_t \right)^2} + \left\| \theta^\star - \hat{\theta}_t \right\|^2 = O(d \log(T/\delta))$$

The difference between the predictions of $\theta^\star$ and $\hat{\theta}_t$ over the past samples

LinUCB

LinUCB

In round t, receive x_t, draw

$$a_t = \text{argmax}_{a \in \mathcal{A}}$$
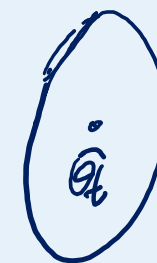
Observe $r_t = \phi(x_t, a_t)^\top \theta^\star + w_t.$

LinUCB

$$\max_\theta \quad \phi(x_t, a)^\top \theta = \underbrace{\phi(x_t, a)^\top \hat{\theta_t}} + \underbrace{\phi(x_t, a)^\top (\theta - \hat{\theta_t})}$$

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

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

LinUCB

In round t, receive x_t, draw

$$a_t = \text{argmax}_{a \in \mathcal{A}} \quad \max_{\theta : \| \theta - \hat{\theta}_t \|_{\Lambda_t}^2 \leq \beta} \quad \phi(x_t, a)^\top \theta$$

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

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

Regret Analysis for LinUCB

Regret Bound of LinUCB

With probability at least $1 - \delta$,

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

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

$$= \sum_{t=1}^{T}\left[\max_{a} \phi(x_t, a)^\top \theta^*\right] - \phi(x_t, a_t)^\top \theta^*$$

$$\square \leq \phi(x_t, a_t)^\top \hat{\theta}_t + \sqrt{\beta}\,\|\phi(x_t, a_t)\|_{\Lambda_t^{-1}}$$

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

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

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

Elliptical Potential Lemma

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

Then

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

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

when $0 \leq a_t \leq 1$

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

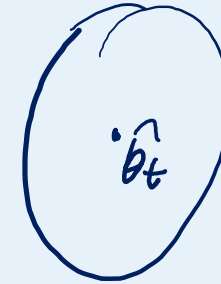$$\approx O\left(d\sqrt{T} \log(\cdots)\right)$$

Thompson Sampling

Thompson Sampling for Linear Contextual Bandits

In round t, receive x_t, draw

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

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

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?