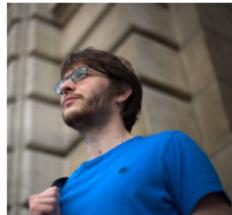


# Gamification of Pure Exploration for Linear Bandits

ICML 2020



Rémy Degenne



Pierre Ménard



Xuedong Shang



Michal Valko



# Linear Bandits

Finite set  $\mathcal{A}$  (size  $A$ ) of vectors in  $\mathbb{R}^d$ .

At time  $t$ : choose  $a_t \in \mathcal{A}$ , observe

$$Y_t = \langle \theta, a_t \rangle + \eta_t \quad \text{where } \eta_t \sim \mathcal{N}(0, 1).$$

$\theta \in \mathbb{R}^d$  **unknown parameter.**

**Goal: sample arms, then answer a query about  $\theta$ .**

# Pure exploration for linear bandits

## Question

- Which arm  $a \in \mathcal{A}$  has highest mean  $\langle \theta, a \rangle$ ?  $\rightarrow$  answer set  $\mathcal{A}$
- Is there  $a \in \mathcal{A}$  with mean  $< 0$ ?  $\rightarrow$  answer set  $\{\text{yes, no}\}$
- In general, finite answer set  $\mathcal{I}$

$$\begin{aligned} i^* : \mathbb{R}^d &\rightarrow \mathcal{I} \\ \theta &\mapsto i^*(\theta) \end{aligned}$$

## Pure exploration

- *sampling rule*  $(a_t)_{t \geq 1}$
- *stopping rule*  $\tau_\delta$ , a stopping time for the filtration  $(\mathcal{F}_t)_{t \geq 1}$
- *decision rule*  $\hat{i} \in \mathcal{I}$  which is  $\mathcal{F}_{\tau_\delta}$ -measurable.

**Objective** **Minimize**  $\mathbb{E}_\theta[\tau_\delta]$  under the constraint  $\mathbb{P}_\theta(\hat{i} \neq i^*(\theta)) \leq \delta$

# Contributions

**Insight on complexities** used in linear bandits

**Saddle-point approach** with a convexified point of view for simpler proofs

**Two algorithms with**

- **asymptotically optimal sample complexity** (as  $\delta \rightarrow 0$ )
- **competitive empirical performance**
- **small computational cost**

## Lower Bound

Alternative  $\neg i := \{\theta \in \mathbb{R}^d : i \neq i^\star(\theta)\}$

Design matrix  $V_w := \sum_{a \in \mathcal{A}} w^a aa^\top$  ( $\|x\|_V := \sqrt{x^\top V x}$ )

## Lower Bound

Alternative  $\neg i := \{\theta \in \mathbb{R}^d : i \neq i^*(\theta)\}$

Design matrix  $V_w := \sum_{a \in \mathcal{A}} w^a a a^\top$  ( $\|x\|_V := \sqrt{x^\top V x}$ )

**Asymptotic lower bound:**

$$\liminf_{\delta \rightarrow 0} \frac{\mathbb{E}_\theta[\tau_\delta]}{\log(1/\delta)} \geq T^*(\theta)$$

where the *characteristic time*  $T^*(\theta)$  is defined by

$$T^*(\theta)^{-1} := \max_{w \in \Sigma_A} \inf_{\lambda \in \neg i^*(\theta)} \frac{1}{2} \|\theta - \lambda\|_{V_w}^2$$

## Lower Bound

Alternative  $\neg i := \{\theta \in \mathbb{R}^d : i \neq i^*(\theta)\}$

Design matrix  $V_w := \sum_{a \in \mathcal{A}} w^a aa^\top$  ( $\|x\|_V := \sqrt{x^\top V x}$ )

**Asymptotic lower bound:**

$$\liminf_{\delta \rightarrow 0} \frac{\mathbb{E}_\theta[\tau_\delta]}{\log(1/\delta)} \geq T^*(\theta)$$

where the *characteristic time*  $T^*(\theta)$  is defined by

$$T^*(\theta)^{-1} := \max_{w \in \Sigma_A} \inf_{\lambda \in \neg i^*(\theta)} \frac{1}{2} \|\theta - \lambda\|_{V_w}^2$$

**Asymptotically optimal algorithm** if

$$\limsup_{\delta \rightarrow 0} \frac{\mathbb{E}_\theta[\tau_\delta]}{\log(1/\delta)} \leq T^*(\theta)$$

# Pure Exploration as a Game

$T^*(\theta)^{-1}$  **value of a zero-sum game** between the **agent** playing action  $a \sim w$  and the **nature** playing alternative  $\lambda$

$$T^*(\theta)^{-1} = \max_{w \in \Sigma_A} \inf_{\lambda \in -i^*(\theta)} \frac{1}{2} \sum_{a \in \mathcal{A}} w^a \|\theta - \lambda\|_{aa^\top}^2$$

## Pure Exploration as a Game

$T^*(\theta)^{-1}$  **value of a zero-sum game** between the **agent** playing action  $a \sim w$  and the **nature** playing alternative  $\lambda$

$$T^*(\theta)^{-1} = \max_{w \in \Sigma_A} \inf_{\lambda \in -i^*(\theta)} \frac{1}{2} \sum_{a \in \mathcal{A}} w^a \|\theta - \lambda\|_{aa^\top}^2$$

Nature plays in  $-i^*(\theta)$  unknown!

## Pure Exploration as a Game

$T^*(\theta)^{-1}$  **value of a zero-sum game** between the **agent** playing action  $a \sim w$  and the **nature** playing alternative  $\lambda$

$$T^*(\theta)^{-1} = \max_{w \in \Sigma_A} \inf_{\lambda \in \neg i^*(\theta)} \frac{1}{2} \sum_{a \in \mathcal{A}} w^a \|\theta - \lambda\|_{aa^\top}^2$$

Nature plays in  $\neg i^*(\theta)$  unknown!

**Convexified Game:** the **agent** plays action and answer  $(a, i) \sim \tilde{w}$  and the **nature** plays vector of alternatives  $\tilde{\lambda}$

$$T^*(\theta)^{-1} = \max_{\tilde{w} \in \Sigma_{AI}} \inf_{\tilde{\lambda} \in \prod_i (\neg i)} \frac{1}{2} \sum_{(a,i) \in \mathcal{A} \times \mathcal{I}} \tilde{w}^{a,i} \|\theta - \tilde{\lambda}^i\|_{aa^\top}^2$$

## Example: Best Arm Identification

**Question:** Which arm  $a \in \mathcal{A}$  has highest mean  $\langle \theta, a \rangle$ ?

## Example: Best Arm Identification

**Question:** Which arm  $a \in \mathcal{A}$  has highest mean  $\langle \theta, a \rangle$ ?

**Estimate uniformly the means of the arms:** Optimal Design

$$\mathcal{A}\mathcal{A} = \min_{w \in \Sigma_A} \max_{a \in \mathcal{A}} \|a\|_{V_w^{-1}}^2$$

## Example: Best Arm Identification

**Question:** Which arm  $a \in \mathcal{A}$  has highest mean  $\langle \theta, a \rangle$ ?

**Estimate uniformly the means of the arms:** Optimal Design

$$\mathcal{A}\mathcal{A} = \min_{w \in \Sigma_A} \max_{a \in \mathcal{A}} \|a\|_{V_w^{-1}}^2$$

**Estimate uniformly the mean of the directions:** Transductive design

$$\mathcal{AB}_{\text{dir}} = \min_{w \in \Sigma_A} \max_{b \in \mathcal{B}_{\text{dir}}} \|b\|_{V_w^{-1}}^2 \quad \mathcal{B}_{\text{dir}} := \{a - a' : (a, a') \in \mathcal{A} \times \mathcal{A}\}$$

## Example: Best Arm Identification

**Question:** Which arm  $a \in \mathcal{A}$  has highest mean  $\langle \theta, a \rangle$ ?

**Estimate uniformly the means of the arms:** Optimal Design

$$\mathcal{AA} = \min_{w \in \Sigma_A} \max_{a \in \mathcal{A}} \|a\|_{V_w^{-1}}^2$$

**Estimate uniformly the mean of the directions:** Transductive design

$$\mathcal{AB}_{\text{dir}} = \min_{w \in \Sigma_A} \max_{b \in \mathcal{B}_{\text{dir}}} \|b\|_{V_w^{-1}}^2 \quad \mathcal{B}_{\text{dir}} := \{a - a' : (a, a') \in \mathcal{A} \times \mathcal{A}\}$$

**Estimate the mean of the gap-weighted directions:** Best Arm Identification

$$\mathcal{AB}^*(\theta) := \min_{w \in \Sigma_A} \max_{b \in \mathcal{B}^*(\theta)} \|b\|_{V_w^{-1}}^2 \quad \mathcal{B}^* := \{(a^*(\theta) - a) / |\langle \theta, a^*(\theta) - a \rangle| : a \in \mathcal{A} / \{a^*(\theta)\}\}$$

## Example: Best Arm Identification

**Question:** Which arm  $a \in \mathcal{A}$  has highest mean  $\langle \theta, a \rangle$ ?

**Estimate uniformly the means of the arms:** Optimal Design

$$\mathcal{A}\mathcal{A} = \min_{w \in \Sigma_A} \max_{a \in \mathcal{A}} \|a\|_{V_w^{-1}}^2$$

**Estimate uniformly the mean of the directions:** Transductive design

$$\mathcal{A}\mathcal{B}_{\text{dir}} = \min_{w \in \Sigma_A} \max_{b \in \mathcal{B}_{\text{dir}}} \|b\|_{V_w^{-1}}^2 \quad \mathcal{B}_{\text{dir}} := \{a - a' : (a, a') \in \mathcal{A} \times \mathcal{A}\}$$

**Estimate the mean of the gap-weighted directions:** Best Arm Identification

$$\mathcal{A}\mathcal{B}^*(\theta) := \min_{w \in \Sigma_A} \max_{b \in \mathcal{B}^*(\theta)} \|b\|_{V_w^{-1}}^2 \quad \mathcal{B}^* := \{(a^*(\theta) - a) / |\langle \theta, a^*(\theta) - a \rangle| : a \in \mathcal{A} / \{a^*(\theta)\}\}$$

## Ordering

$$T^*(\theta) = 2\mathcal{A}\mathcal{B}^*(\theta) \leq 2 \frac{\mathcal{A}\mathcal{B}_{\text{dir}}}{\Delta_{\min}(\theta)^2} \leq 8 \frac{\mathcal{A}\mathcal{A}}{\Delta_{\min}(\theta)^2}$$

# Designing algorithms with a game

## When do we stop?

At  $t$ , each arm  $a$  is played  $N_t^a$  times.  $\hat{\theta}_t$  is our estimate for  $\theta$ .

**Concentration result:** with probability  $1 - \delta$ ,

$$\log \frac{1}{\delta} > \frac{1}{2} \|\hat{\theta}_t - \theta\|_{V_{N_t}}^2$$

**Conclusion:** if we have

$$\log \frac{1}{\delta} \leq \inf_{\lambda \in \neg i^*(\hat{\theta}_t)} \frac{1}{2} \|\hat{\theta}_t - \lambda\|_{V_{N_t}}^2$$

then w.p.  $1 - \delta$ ,  $\theta \notin \neg i^*(\hat{\theta}_t)$ , which means  $i^*(\theta) = i^*(\hat{\theta}_t)$ .

# Designing algorithms with a game

What should we pull?

When not stopped:

$$\begin{aligned}\log \frac{1}{\delta} &> \inf_{\lambda \in -i^*(\hat{\theta}_t)} \frac{1}{2} \|\hat{\theta}_t - \lambda\|_{V_{N_t}}^2 \\ &= \inf_{\lambda \in -i^*(\hat{\theta}_t)} \sum_{s=1}^t \frac{1}{2} \|\hat{\theta}_t - \lambda\|_{V_{w_s}}^2\end{aligned}$$

Goal:

$$\begin{aligned}\inf_{\lambda \in -i^*(\hat{\theta}_t)} \sum_{s=1}^t \frac{1}{2} \|\hat{\theta}_t - \lambda\|_{V_{w_s}}^2 &\geq t \max_{w \in \Sigma_A} \inf_{\lambda \in -i^*(\theta)} \frac{1}{2} \|\theta - \lambda\|_{V_w}^2 - o(t) \\ &= t T^*(\theta)^{-1} - o(t)\end{aligned}$$

→ asymptotic optimality.

# Designing algorithms with a game

## Ingredients

- Algorithm (1) playing **arm proportions**  $w_t$ .
- Algorithm (2) playing **alternatives**  $\lambda_t \in \neg i^*(\hat{\theta}_t)$ .
- **Optimism** for added exploration.
- Optional: (1) plays over both  $w_t$  and answer  $i_t \rightarrow$  simpler proof.

**(1) and (2) ensure saddle point property:**

$$\begin{aligned} \inf_{\lambda \in \neg i^*(\hat{\theta}_t)} \sum_{s=1}^t \frac{1}{2} \|\hat{\theta}_t - \lambda\|_{V_{w_s}}^2 &\approx \sum_{s=1}^t \frac{1}{2} \|\hat{\theta}_t - \lambda_s\|_{V_{w_s}}^2 \approx \max_{w \in \Sigma_K} \sum_{s=1}^t \frac{1}{2} \|\theta - \lambda_s\|_{V_w}^2 \\ &\geq t \max_{w \in \Sigma_A} \inf_{\lambda \in \neg i^*(\theta)} \frac{1}{2} \|\theta - \lambda\|_{V_w}^2 \\ &= t T^*(\theta)^{-1} \end{aligned}$$

## Convexified version: LinGame-C

---

### Algorithm 1 LinGame-C

---

**Input:** Agent learner  $\mathcal{L}_{\tilde{w}}$ , threshold  $\beta(\cdot, \delta)$

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

**if**  $\max_{i \in \mathcal{I}} \inf_{\lambda \in \neg i} \frac{1}{2} \|\hat{\theta}_{t-1} - \lambda\|_{V_{N_{t-1}}}^2 \geq \beta(t-1, \delta)$  **then**

stop and **return**  $\hat{i} = i^*(\hat{\theta}_{t-1})$

**end if**

Get  $\tilde{w}_t$  **from**  $\mathcal{L}_{\tilde{w}}$  and update  $\widetilde{W}_t = \widetilde{W}_{t-1} + \tilde{w}_t$

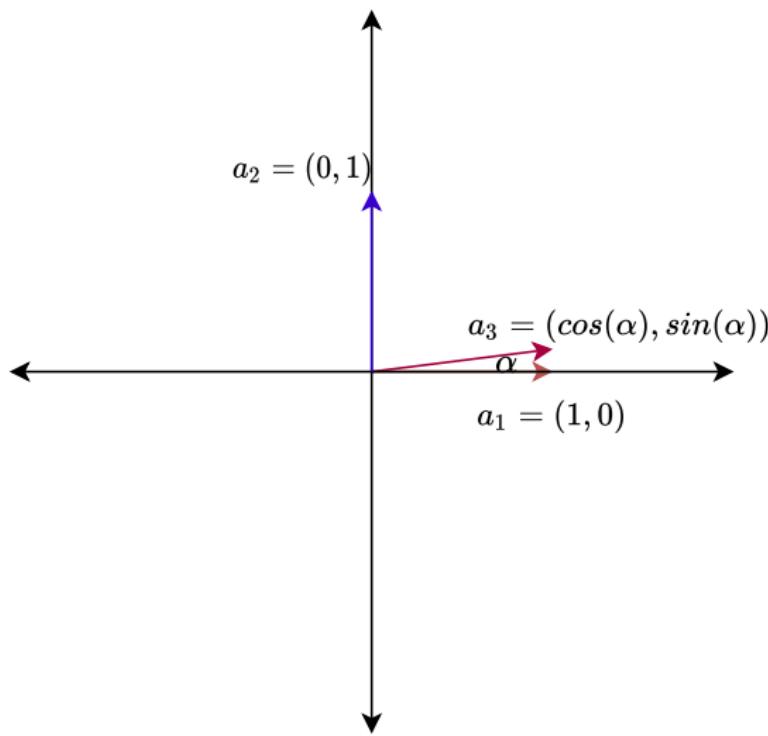
For all  $i \in \mathcal{I}$ ,  $\tilde{\lambda}_t^i \in \arg \min_{\lambda \in \neg i} \|\hat{\theta}_{t-1} - \lambda\|_{V_{\widetilde{w}_t^i}}^2$

Feed learner  $\mathcal{L}_{\tilde{w}}$  with  $g_t(\tilde{w}) = \sum_{(a,i) \in \mathcal{A} \times \mathcal{I}} \tilde{w}^{a,i} U_t^{a,i} / 2$

Pull  $a_t$  such that  $(a_t, i_t) \in \arg \min_{(a,i) \in \mathcal{A} \times \mathcal{I}} N_{t-1}^{a,i} - \widetilde{W}_t^{a,i}$

**end for**

## The usual hard instance

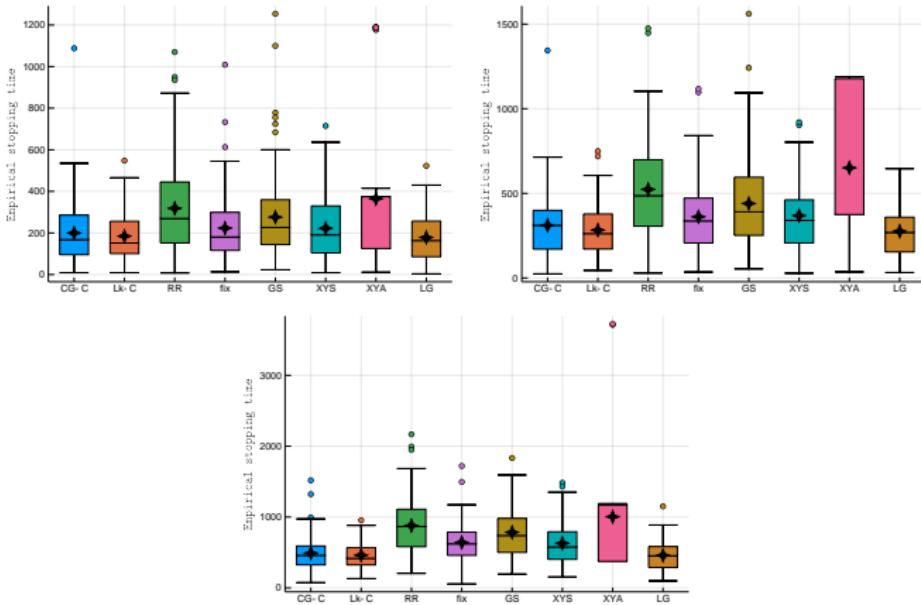


# The usual hard instance

|              | LinGame | LinGame-C   | DKM  |
|--------------|---------|-------------|------|
| $a_1$        | 1912    | 1959        | 1943 |
| $a_2$        | 5119    | 4818        | 4987 |
| $a_3$        | 104     | 77          | 1775 |
| <b>Total</b> | 7135    | <b>6854</b> | 8705 |

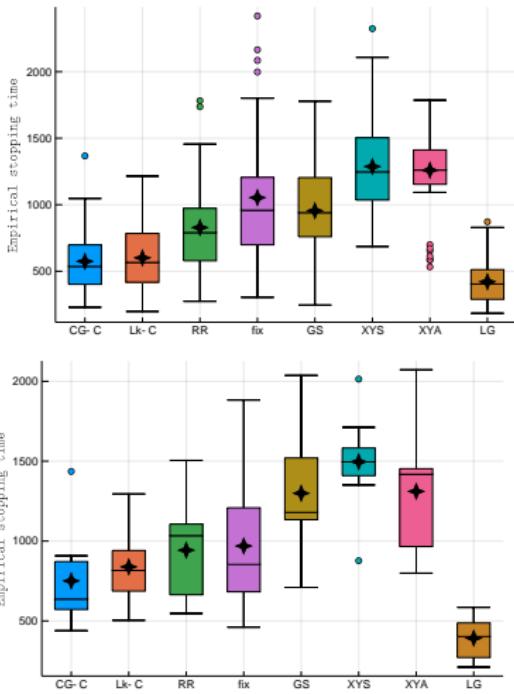
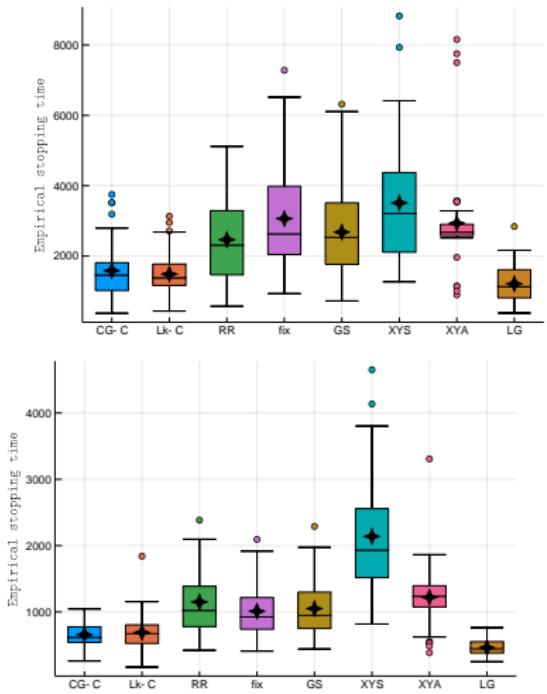
Table: Average number of pulls of each arm.

# Comparison with other algorithms: The usual hard instance ( $\delta = 0.1, 0.01, 0.0001$ )

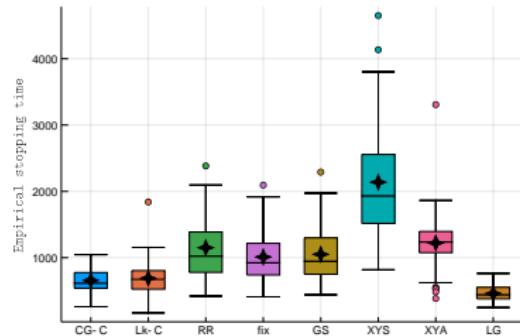
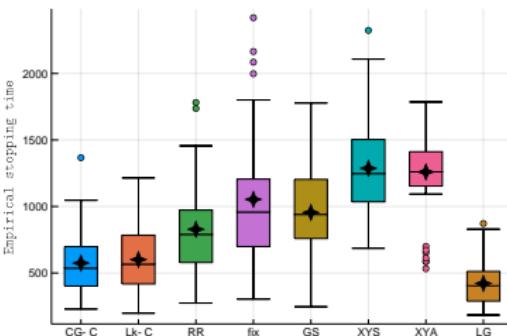
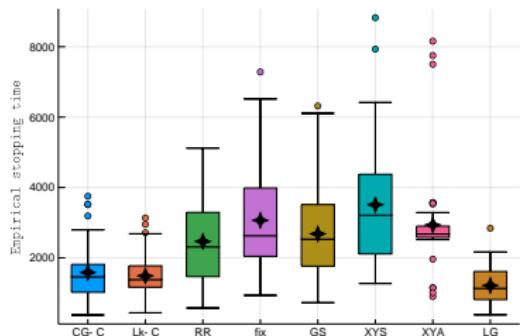


**Figure:** CG = LinGame-C, Lk = LinGame, RR = uniform sampling, fix = tracking the fixed weights, GS =  $\mathcal{XY}$ -Static with  $\mathcal{AA}$ -allocation, XYS =  $\mathcal{XY}$ -Static with  $\mathcal{AB}_{\text{dir}}$ -allocation, LG = LinGapE.

# Comparison with other algorithms: Random unit sphere vectors ( $d = 6, 8, 10, 12$ )



# Comparison with other algorithms: Random unit sphere vectors ( $d = 6, 8, 10, 12$ )



# Thank you!