

$$\mathcal{X} = \{x_1, \dots, x_n\} \subset \mathbb{R}^d$$

Assume $\exists \theta_* \in \mathbb{R}^d$: pulling arm x_t @ time $t \in N$

results in a reward $y_t = \underline{x}_t^\top \theta_* + \underline{\xi}_t$

where $\mathbb{E}[\underline{\xi}_t] = 0$, $\mathbb{E}[\exp(\lambda \underline{\xi}_t)] \leq e^{\lambda^2/2}$.

$$\text{Regret} = \max_{x \in \mathcal{X}} \sum_{t=1}^T x^\top \theta_* - x_t^\top \theta_*$$

Suppose we choose $x_1, \dots, x_T \in \mathcal{X}$ and measure

corresponding rewards y_1, \dots, y_T where $y_t = \underline{x}_t^\top \theta_* + \underline{\xi}_t$

$$\hat{\theta} = \underset{\theta \in \mathbb{R}^d}{\operatorname{argmin}} \sum_{t=1}^T (y_t - x_t^\top \theta)^2 \quad \underline{\xi}_t \text{ IID}$$

Recommend $\hat{x} = \underset{x \in \mathcal{X}}{\operatorname{argmax}} x^\top \hat{\theta}$.

What is $\mathbb{E}[(x_* - \hat{x})^\top \theta_*]$ where $x_* = \underset{x \in \mathcal{X}}{\operatorname{argmax}} x^\top \theta_*$

$$\hat{\theta} = \underset{\theta \in \mathbb{R}^d}{\operatorname{argmin}} \sum_{t=1}^T (y_t - x_t^\top \theta)^2$$

$$0 = -\sum_t 2(y_t - x_t^\top \theta) x_t \Rightarrow (\sum_t x_t x_t^\top) \theta = \sum_t x_t y_t$$

$$\hat{\theta} = (\sum_t x_t x_t^\top)^{-1} \sum_t x_t y_t$$

$$\begin{aligned}
\hat{\theta} &= \arg \min_{\theta \in \mathbb{R}^d} \sum_{t=1}^T (y_t - x_t^\top \theta)^2 \\
&= (\sum x_t x_t^\top)^{-1} \sum x_t y_t \\
&= (\sum x_t x_t^\top)^{-1} \sum_t x_t (x_t^\top \theta_0 + \varepsilon_t) \\
&= \theta_0 + (\sum x_t x_t^\top)^{-1} \sum_t x_t \varepsilon_t \\
&= \theta_0 + (X^\top X)^{-1} X^\top \varepsilon
\end{aligned}$$

$$X = \begin{bmatrix} x_1^\top \\ \vdots \\ x_T^\top \end{bmatrix} \in \mathbb{R}^{T \times d} \quad y = \begin{bmatrix} y_1 \\ \vdots \\ y_T \end{bmatrix} \in \mathbb{R}^T \quad \varepsilon = \begin{bmatrix} \varepsilon_1 \\ \vdots \\ \varepsilon_T \end{bmatrix} \in \mathbb{R}^T$$

Fix some $x \in \mathcal{X}$.

$$\mathbb{E}[(\hat{\theta} - \theta_0)(\hat{\theta} - \theta_0)^\top] = X^\top X$$

$$\begin{aligned}
x^\top (\hat{\theta} - \theta_0) &= \underbrace{x^\top (X^\top X)^{-1} X^\top \varepsilon}_{:= w^\top} \\
&= w^\top \varepsilon \\
&= \sum_{t=1}^T w_t \varepsilon_t
\end{aligned}$$

$$\begin{aligned}
\mathbb{E}[\exp(\lambda x^\top (\hat{\theta} - \theta_0))] &= \mathbb{E}[\exp(\lambda \sum_{t=1}^T w_t \varepsilon_t)] \\
&= \mathbb{E}\left[\prod_{t=1}^T \exp(\lambda w_t \varepsilon_t)\right] \\
&= \prod_{t=1}^T \mathbb{E}[\exp(\lambda w_t \varepsilon_t)]
\end{aligned}$$

$$\leq \sum_{t=1}^T \exp(\lambda^2 \omega_t^2 / 2)$$

$$= \exp(\lambda^2 \|\omega\|_2^2 / 2)$$

$$\|\omega\|_2^2 = x^T (x^T x)^{-1} x$$

$$\Rightarrow \Pr((\hat{\theta} - \theta^*)^T x > \varepsilon) \leq \exp\left(-\frac{\varepsilon^2}{2x^T (x^T x)^{-1} x}\right) = \delta$$

$$\Rightarrow (\hat{\theta} - \theta^*)^T x \leq \sqrt{2x^T (x^T x)^{-1} x} \text{ by (18)}, \text{ w.p. } \geq 1 - \delta.$$

$$(x_* - \hat{x})^T \theta_* = \underbrace{(x_* - \hat{x})^T \hat{\theta}}_{\leq 0} + (x_* - \hat{x})^T (\theta^* - \hat{\theta})$$

$$\leq x_*^T (\theta^* - \hat{\theta}) - \hat{x}^T (\theta^* - \hat{\theta})$$

$$\leq 2 \cdot \sqrt{\max_x x^T (x^T x)^{-1} x} \cdot 2 \log(2n/\delta)$$

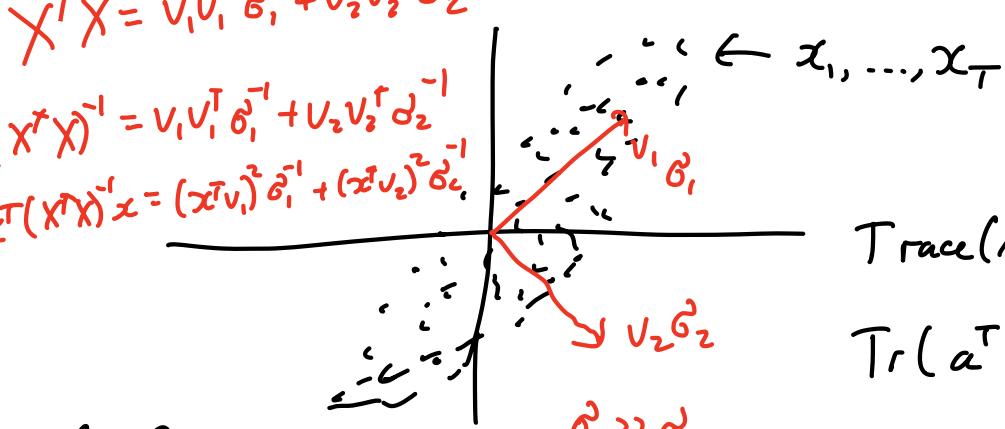
$$\approx 2 \cdot \sqrt{\max_x x^T A(\lambda)^{-1} x} \cdot \frac{2 \log(2n/\delta)}{\lambda} = d \text{ if } \lambda \text{ is } \delta\text{-optimal}$$

$$x^T x = v_1 v_1^T \sigma_1^2 + v_2 v_2^T \sigma_2^2$$

$$(x^T x)^{-1} = v_1 v_1^T \sigma_1^{-2} + v_2 v_2^T \sigma_2^{-2}$$

$$x^T (x^T x)^{-1} x = (x^T v_1)^2 \sigma_1^{-2} + (x^T v_2)^2 \sigma_2^{-2}$$

$$\hat{\theta} = \theta^* + (x^T x)^{-1} x^T z$$



$$\text{Trace}(ABC) = \text{Trace}(BCA) = \text{Tr}(CAB)$$

$$\text{Tr}(a^T B a) = \text{Tr}(B a a^T)$$

$$\mathbb{E}[\|\hat{\theta} - \theta_0\|_2^2] = \mathbb{E}[\|(X^T X)^{-1} X^T z\|_2^2]$$

$$= \mathbb{E}[z^T X (X^T X)^{-1} (X^T X)^{-1} X^T z]$$

$$\begin{aligned}\mathbb{E}[z_i z_j] &= \mathbb{E}[\text{Trace}((X^T X)^{-1} (X^T X)^{-1} X^T z z^T X)] \\&= \mathbb{E}[z_i^2] \mathbb{I}\{i=j\} \\&\leq \mathbb{I}\{i=j\} \\&= \text{Trace}((X^T X)^{-1})\end{aligned}$$

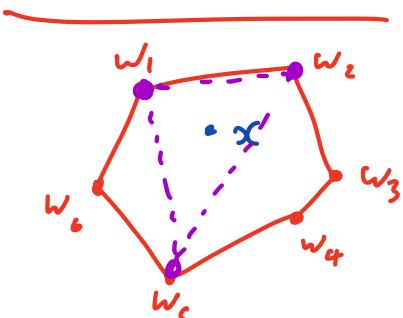
$$\Delta_X = \left\{ \lambda_x \in \mathbb{R}_+^{|X|} : \sum_{x \in X} \lambda_x = 1 \right\}$$

$$X^T X = \sum_{t=1}^T x_t x_t^T$$

$$= T \cdot \underbrace{\sum_{x \in X} \lambda_x x x^T}_{A(\lambda)}$$

$$=: T \cdot \underline{A(\lambda)}$$

where $\lambda_x = \sum_{t=1}^T \mathbb{I}\{x_t = x\}$



$$x = \sum_{i=1}^6 p_i w_i \quad \text{for some } p \in \Delta_6$$

$= p'_1 w_1 + p'_2 w_2 + p'_3 w_3$ *Caratheodory*
Any $x \in \text{conv-hull}(w_1, \dots, w_n) \subset \mathbb{R}^d$
can be represented as convex

$$A(\lambda) = \sum_{x \in \mathcal{X}} \lambda_x x x^T$$

- **A-optimality:** minimize $f_A(\lambda) = \text{Tr}(A_\lambda^{-1})$ minimizes $\mathbb{E}[\|\hat{\theta} - \theta\|_2^2]$

- **E-optimality:** minimize $f_E(\lambda) = \max_{u: \|u\| \leq 1} u^\top A_\lambda^{-1} u$ minimizes $\max_{u: \|u\| \leq 1} \mathbb{E}[(\langle u, \hat{\theta} - \theta \rangle)^2]$

- **D-optimality:** maximize $g_D(\lambda) = \log(|A_\lambda|)$ maximizes the entropy of distribution. Also, if $\mathcal{E}_\lambda = \{x : x^\top A_\lambda^{-1} x \leq d\}$ then D-optimality is the minimum volume ellipsoid that contains \mathcal{X} .

- **G-optimality:** minimize $f_G(\lambda) = \max_{x \in \mathcal{X}} x^\top A_\lambda^{-1} x$ minimizes $\max_{x \in \mathcal{X}} \mathbb{E}[(\langle x, \hat{\theta} - \theta^* \rangle)^2]$

Lemma 10 (Kiefer-Wolfowitz (1960)). For any \mathcal{X} with $d = \dim(\text{span}(\mathcal{X}))$, there exists a $\lambda^* \in \Delta_{\mathcal{X}}$ that

- $\max_{\lambda} g_D(\lambda) = g_D(\lambda^*)$

- $\min_{\lambda} f_G(\lambda) = f_G(\lambda^*)$

- $f_G(\lambda^*) = d$

- $\text{support}(\lambda^*) = (d+1)d/2$

$$\begin{aligned} \frac{\partial}{\partial \lambda} \log |A(\lambda)| \\ = x^T \bar{A}^{-1}(\lambda) x \end{aligned}$$

$$\|x\|_A^2 = x^T A x \quad \text{so} \quad \|x\|_2^2 \equiv \|x\|_I^2$$

Proposition 2. If λ^* is the G-optimal design for \mathcal{X} then if we pull arm $x \in \mathcal{X}$ exactly $\lceil \tau \lambda_x^* \rceil$ times for some $\tau > 0$ and compute the least squares estimator $\hat{\theta}$. Then for each $x \in \mathcal{X}$ we have with probability at least $1 - \delta$

$$x^T x = A(\lceil \tau \lambda_x^* \rceil)$$

$$\begin{aligned} \langle x, \hat{\theta} - \theta^* \rangle &\leq \|x\|_{(\sum_{x \in \mathcal{X}} \lceil \tau \lambda_x^* \rceil x x^T)^{-1}} \sqrt{2 \log(1/\delta)} \\ &\leq \frac{1}{\sqrt{\tau}} \|x\|_{(\sum_{x \in \mathcal{X}} \lambda_x^* x x^T)^{-1}} \sqrt{2 \log(1/\delta)} \\ &\leq \sqrt{\frac{2d \log(1/\delta)}{\tau}} \end{aligned}$$

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and we have taken at most $\tau + \frac{d(d+1)}{2}$ pulls. Thus, for any $\delta' \in (0, 1)$ we have $\mathbb{P}(\bigcup_{x \in \mathcal{X}} \{|\langle x, \hat{\theta} - \theta^* \rangle| > \sqrt{\frac{2d \log(2|\mathcal{X}|/\delta')}{\tau}}\}) \leq \delta'$.

$$\vartheta(z) = \frac{e^z}{e^z + 1} = \frac{1}{1 + e^{-z}}$$

In general for likelihood model $\ell_x(y)$ define

Fisher Info matrix as $\mathbb{E}_{Y} \left[\sum_x \nabla_{\theta} \log \ell_x(Y) \nabla_{\theta} \log \ell_x(Y)^T \right] = I(\theta)$

For linear regression $y \sim N(\langle x, \theta \rangle, 1)$

$$I(\theta) = \sum_x x x^T$$

For logistic regression $y \sim \text{Bernoulli}(\sigma(\langle x, \theta \rangle))$

$$I(\theta) = \sum_x x x^T \sigma(\langle x, \theta \rangle) (1 - \sigma(\langle x, \theta \rangle))$$

$$\begin{aligned}
\|x'\|_{\left(\sum_{x \in X} x x^T \Gamma_{\lambda_x} s\right)^{-1}}^2 &= x'^T \left(\sum_{x \in X} x x^T \Gamma_{\lambda_x} s \right)^{-1} x' \\
&\leq x'^T \left(\sum_{x \in X} x x^T \lambda_x s \right)^{-1} x' \\
&= \frac{1}{3} x'^T \left(\sum_{x \in X} x x^T \lambda_x \right)^{-1} x' \\
&= \frac{1}{3} x'^T A(\lambda)^{-1} x' \\
&= \frac{1}{3} \|x'\|_{A(\lambda)^{-1}}^2
\end{aligned}$$

$$P(A) = \sum_b P(A \cap b)$$

$$\sum_{k=1}^{\infty} \frac{1}{k^2} = \frac{\pi^2}{6} \leq 2$$

Input: Finite set $\mathcal{X} \subset \mathbb{R}^d$, confidence level $\delta \in (0, 1)$.

Let $\mathcal{X}_1 \leftarrow \mathcal{X}, \ell \leftarrow 1$

while $|\mathcal{X}_\ell| > 1$ **do**

Let $\hat{\lambda}_\ell \in \Delta_{\mathcal{X}_\ell}$ be a $\frac{d(d+1)}{2}$ -sparse minimizer of $f(\lambda) = \max_{x \in \mathcal{X}_\ell} \|x\|_{(\sum_{x \in \mathcal{X}_\ell} \lambda_x x x^\top)^{-1}}^2$

$$\epsilon_\ell = 2^{-\ell}, \tau_\ell = 2d\epsilon_\ell^{-2} \log(4\ell^2 |\mathcal{X}| / \delta)$$

Pull arm $x \in \mathcal{X}$ exactly $\lceil \hat{\lambda}_{\ell,x} \tau_\ell \rceil$ times and construct the least squares estimator $\hat{\theta}_\ell$ using only the observations of this round

$$\mathcal{X}_{\ell+1} \leftarrow \mathcal{X}_\ell \setminus \{x \in \mathcal{X}_\ell : \max_{x' \in \mathcal{X}_\ell} \langle x' - x, \hat{\theta}_\ell \rangle > 2\epsilon_\ell\}$$

$$\ell \leftarrow \ell + 1$$

Output: \mathcal{X}_ℓ

On $\mathcal{V} = \mathcal{X}_\ell$

$$\mathcal{E}_{x,\ell}(\mathcal{V}) = \{|\langle x, \hat{\theta}_\ell(\mathcal{V}) - \theta^* \rangle| \leq \epsilon_\ell\}$$

$$\mathbb{P}\left(\bigcap_{x \in \mathcal{X}_\ell} \mathcal{E}_{x,\ell}(\mathcal{V})\right) \geq 1 - \delta$$

$$\begin{aligned} \mathbb{P}\left(\bigcup_{\ell=1}^{\infty} \bigcup_{x \in \mathcal{X}_\ell} \{\mathcal{E}_{x,\ell}^c(\mathcal{X}_\ell)\}\right) &\leq \sum_{\ell=1}^{\infty} \mathbb{P}\left(\bigcup_{x \in \mathcal{X}_\ell} \{\mathcal{E}_{x,\ell}^c(\mathcal{X}_\ell)\}\right) \\ &= \sum_{\ell=1}^{\infty} \sum_{\mathcal{V} \subseteq \mathcal{X}} \mathbb{P}\left(\bigcup_{x \in \mathcal{V}} \{\mathcal{E}_{x,\ell}^c(\mathcal{V})\}, \mathcal{X}_\ell = \mathcal{V}\right) \\ &= \sum_{\ell=1}^{\infty} \sum_{\mathcal{V} \subseteq \mathcal{X}} \underbrace{\mathbb{P}\left(\bigcup_{x \in \mathcal{V}} \{\mathcal{E}_{x,\ell}^c(\mathcal{V})\}\right)}_{\leq \sum_{x \in \mathcal{V}} \mathbb{P}(\mathcal{E}_{x,\ell}^c(\mathcal{V}))} \mathbb{P}(\mathcal{X}_\ell = \mathcal{V}) \\ &\leq \sum_{\ell=1}^{\infty} \sum_{\mathcal{V} \subseteq \mathcal{X}} \frac{\delta |\mathcal{V}|}{2\ell^2 |\mathcal{X}|} \mathbb{P}(\mathcal{X}_\ell = \mathcal{V}) \leq \sum_{\ell=1}^{\infty} \frac{\delta}{2\ell^2} \leq \frac{\delta}{2} \end{aligned}$$

$\mathcal{X}_\ell = \arg \max_{\mathcal{X}} \langle x, \hat{\theta}_\ell \rangle$ then WTS $x \in \mathcal{X}_\ell$ for all ℓ

$$\Rightarrow \max_{x' \in \mathcal{X}_\ell} \langle x' - x_\ell, \hat{\theta}_\ell \rangle = \max_{x' \in \mathcal{X}_\ell} \underbrace{\langle x' - x_\ell, \hat{\theta}_\ell \rangle}_{\leq 0} + \underbrace{\langle x' - x_\ell, \hat{\theta}_\ell - \theta^* \rangle}_{\leq 2\epsilon_\ell} \leq 2\epsilon_\ell$$

$$\max_{x \in \mathcal{X}_\ell} \langle x - x_\ell, \hat{\theta}_\ell \rangle \leq 8\epsilon_\ell \quad \text{by same argument as MAB case.}$$

$$R_T = \sum_{t=1}^T \langle x_t - \bar{x}_t, \theta_t \rangle \quad \Delta_x = \langle \bar{x}_t - \bar{x}, \theta_t \rangle$$

$$= \gamma T + \sum_e \sum_{\substack{x \in X_e \\ \Delta_x > \nu}} \underbrace{\langle x_t - \bar{x}, \theta_t \rangle}_{\leq 8\varepsilon_e} \Gamma_{\lambda_{e,x}} S$$

$$\leq \gamma T + \sum_e \sum_{\substack{x \in X_e \\ \Delta_x > \nu}} 8\varepsilon_e \Gamma_{\lambda_{e,x}} S$$

$$\leq \gamma T + \sum_e \left(8\varepsilon_e d^2 + \sum_{\substack{x \in X_e \\ \Delta_x > \nu}} 8\varepsilon_e \lambda_{e,x} S \right)$$

$$= \gamma T + \sum_e 8\varepsilon_e d^2 + \sum_{\substack{x \in X_e \\ \Delta_x > \nu}} \sum_{\ell=1}^{\log_2(\Delta_x \vee \varepsilon_e)^{-1}} 8\varepsilon_e \lambda_{e,x} S$$

$$\leq \gamma T + d^2 \log(1/\delta) + d (\Delta \vee \nu)^{-1} \log(1/\delta)$$

$$\nu = 0 \quad R_T \leq d^2 \log(1/\delta) + \frac{d}{\Delta} \log(1/\delta)$$

$$\min \text{ wrt } \nu \Rightarrow R_T \leq d^2 \log(1/\delta) + \sqrt{d T \log(1/\delta)}.$$

Linear Bandits - Pure exploration / Best-arm identification

Motivation: If we choose x_1, \dots, x_3 according to λ

(i.e. after rounding via Caratheodory) and

$$y_t = \langle x_t, \theta^* \rangle + \varepsilon_t \quad \text{w/} \quad \varepsilon_t \sim N(0, 1) \quad \text{then}$$

$$\hat{\theta} = \theta^* + \left(\sum_t x_t x_t^\top \right)^{-1} \sum_t x_t \varepsilon_t.$$

If $x_a = \arg\max_{x \in X} \langle x, \theta^* \rangle$ and $\hat{x} = \arg\max_{x \in X} \langle x, \hat{\theta} \rangle$

we have that $\hat{x} = x_a$ if $\langle x_a - x, \hat{\theta} \rangle > 0 \quad \forall x \in X \setminus x_a$.

$$\langle x_a - x, \hat{\theta} \rangle = \langle x_a - x, \theta^* \rangle + \underbrace{\langle x_a - x, \hat{\theta} - \theta^* \rangle}_{\leftarrow}$$

for any $v \in \mathbb{R}^d$ $|v^\top (\hat{\theta} - \theta^*)| \leq \|v\|_{(\sum_t x_t x_t^\top)^{-1}} \sqrt{2 \omega_j(z/\delta)}$

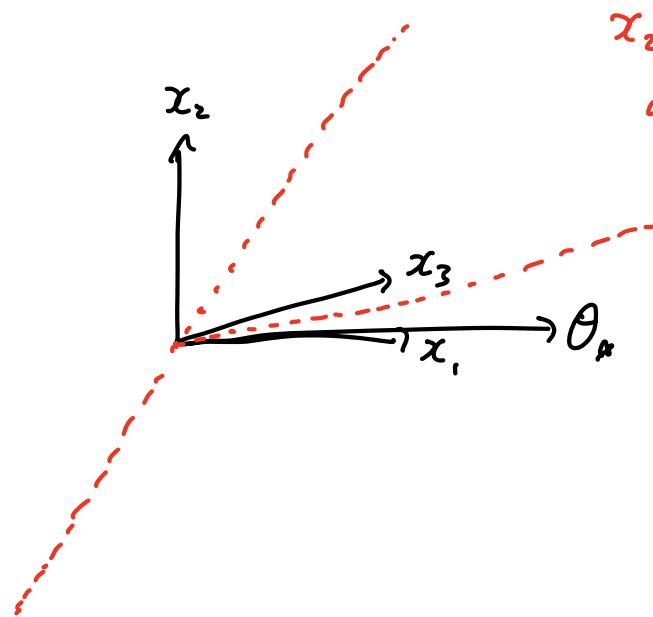
$$\sum_{t=1}^3 x_t x_t^\top \approx 3 \cdot A(\lambda)$$

$$\geq -\|x_a - x\|_{(\sum_t x_t x_t^\top)^{-1}} \sqrt{2 \log |X|/\delta}$$

$$\Rightarrow \frac{\|x_a - x\|_{(\sum_t x_t x_t^\top)^{-1}}}{\langle x_a - x, \theta^* \rangle} \leq \frac{1}{c \log |X|/\delta} \quad \forall x$$

$$\min_{\lambda \in \Delta_x} \max_{x \in \mathcal{X} \setminus x_*} \underbrace{\frac{\|x_* - x\|_{A(\lambda)}^2}{\langle x_* - x, \theta_* \rangle^2} \cdot c \log(1/\delta)}_{=: P_*} \leq 5$$

We need to estimate
 $\langle x_1 - x_3, \theta_* \rangle$ accurately.



x_2 is most aligned w/ $x_1 - x_3$
 and is thus optimally
 reduces # meas
 to identify x_1
 as best.

Input: Finite set $\mathcal{X} \subset \mathbb{R}^d$, confidence level $\delta \in (0, 1)$.

Let $\mathcal{X}_1 \leftarrow \mathcal{X}, t \leftarrow 1$

while $|\mathcal{X}_\ell| > 1$ **do**

Let $\hat{\lambda}_\ell \in \Delta_{\mathcal{X}}$ be a $\frac{d(d+1)}{2}$ -sparse minimizer of $f(\lambda; \mathcal{X}_\ell)$ where

$$f(\mathcal{V}) = \inf_{\lambda \in \mathcal{X}} f(\lambda; \mathcal{V}) = \inf_{\lambda \in \mathcal{X}} \max_{x, x' \in \mathcal{V}} \|x - x'\|_{(\sum_{x \in \mathcal{X}} \lambda_x x x^\top)^{-1}}^2$$

Set $\epsilon_\ell = 2^{-\ell}$, $\tau_\ell = 2\epsilon_\ell^{-2} f(\mathcal{X}_\ell) \log(4\ell^2 |\mathcal{X}| / \delta)$

Pull arm $x \in \mathcal{X}$ exactly $\lceil \tau_\ell \hat{\lambda}_{\ell,x} \rceil$ times and construct $\hat{\theta}_\ell$

$$\mathcal{X}_{\ell+1} \leftarrow \mathcal{X}_\ell \setminus \{x \in \mathcal{X}_\ell : \max_{x' \in \mathcal{X}_\ell} \langle x' - x, \hat{\theta}_\ell \rangle > \epsilon_\ell\}$$

$t \leftarrow t + 1$

Output: \mathcal{X}_{t+1}

$$\Delta_x = \langle x_a - x, \theta_x \rangle$$

$$\Delta = \min_{x \neq x_a} \Delta_x$$

$$P_x^* = \min_{\lambda \in \Delta_x} \max_{x \in \mathcal{X} \setminus \{x_a\}} \frac{\|x - x_a\|_{A(\lambda)}^2}{\Delta_x^2}$$

Theorem 5. Assume that $\max_{x \in \mathcal{X}} \langle x^* - x, \theta^* \rangle \leq 2$. Then with probability at least $1 - \delta$, x^* is returned from the algorithm at a time τ that satisfies

$$\tau \leq c\rho^* \log(\Delta^{-1}) [\log(1/\delta) + \log(\log(\Delta^{-1})) + \log(|\mathcal{X}|)].$$

Furthermore, any algorithm requires $\mathbb{E}[\tau] \geq p_x \log(1/\delta)$.

Thompson Sampling / linear UCB

Define prior $P_t = \mathcal{N}(0, I_d)$, P_t prior over \mathcal{F}

for $t=1, 2, \dots$

$$\theta_t \sim P_t(\cdot) \quad f_t \sim P_t$$

$$x_t := \underset{x \in X}{\operatorname{argmax}} \langle x, \theta_t \rangle \quad x_t = \underset{x \in X}{\operatorname{argmax}} f_t(x)$$

$$\text{Observe } y_t = \langle x_t, \theta_t \rangle + \eta_t$$

$$\text{Model } \eta_t \text{ as } \mathcal{N}(\langle x_t, \theta_t \rangle, 1)$$

$$\text{Update posterior } \underbrace{P_{t+1}(\theta | \{\langle x_s, y_s \rangle\}_{s=1}^t)}_{\sim \mathcal{N}(\hat{\theta}, (I + \sum_t x_t x_t^\top)^{-1})} \quad \text{Update } P_t \mapsto P_{t+1}$$

$$\sim \mathcal{N}(\hat{\theta}, (I + \sum_t x_t x_t^\top)^{-1})$$

$$\hat{\theta} = (\sum_t x_t x_t^\top)^{-1} \sum_t x_t y_t$$