

where $\|z\|_A^2 := z^T A z$

Lemma 11 (Kiefer-Wolfowitz (1960)). For any $\mathcal{X}$ with $d = \dim(\text{span}(\mathcal{X}))$, there exists a $\lambda^* \in \Delta_{\mathcal{X}}$ that

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

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

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

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

$$g_0(\lambda) = \log |A(\lambda)|$$

$$f_0(\lambda) = \max_{x \in \mathcal{X}} \|x\|_{A(\lambda)}^2$$

$$[\nabla g(\lambda)]_x = \|x\|_{A(\lambda)}^2$$

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 $1 - \delta$

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

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

Frank-Wolfe

Input $K \subset \mathbb{R}^d$, function $f: \mathbb{R}^d \rightarrow \mathbb{R}$
 Init $x_0 \in K$
 for $t=1, 2, \dots$

$$z_t = \argmin_{z \in K} \langle z, \nabla f(x_t) \rangle$$

$$x_{t+1} = (1 - \beta_t) x_t + \beta_t z_t$$

convex

For D-optimal design

Init λ_0 sparsely.

$$x_t = \argmax_{x \in \mathcal{X}} [\nabla g(\lambda)]_x = \argmax_x \|x\|_{A(\lambda)}^2$$

$$\lambda_{t+1} = (1 - \beta_t) \lambda_t + \beta_t x_t$$

- **A-optimality:** minimize $f_A(\lambda) = \text{Tr}(A_\lambda^{-1})$ minimizes $\mathbb{E}[\|\widehat{\theta} - \theta\|_2^2]$
- **E-optimality:** minimize $f_E(\lambda) = \max_{u: \|u\| \leq 1} u^\top A_\lambda^{-1} u$ minimizes $\max_{u: \|u\| \leq 1} \mathbb{E}[(\langle u, \widehat{\theta} - \theta \rangle)^2]$
- **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 $\max_{x \in \mathcal{X}} \mathbb{E}[(\langle x, \widehat{\theta} - \theta^* \rangle)^2]$

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 $f(\lambda) = \max_{x \in \mathcal{X}_\ell} \|x\|^2_{(\sum_{x \in \mathcal{X}_\ell} \lambda_x x x^\top)^{-1}}$

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

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: $\mathcal{X}_\ell$

Lemma 12. Assume that $\max_{x \in \mathcal{X}} \langle x^* - x, \theta^* \rangle \leq 4$. With probability at least $1 - \delta$, we have $x^* \in \mathcal{X}_\ell$ and $\max_{x \in \mathcal{X}_\ell} \langle x^* - x, \theta^* \rangle \leq 8\epsilon_\ell$ for all $\ell \in \mathbb{N}$.

For any $V \subset \mathcal{X}$ let $\hat{\theta}_\ell(V)$ be the least squares solution at stage ℓ if $\mathcal{X}_\ell = V$.

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

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

$$Regret = \sum_{x \in \mathcal{X}} \Delta_x T_x$$

$$\Delta_x = \langle \theta_k, x_k - x \rangle$$

$$x_k = \operatorname{argmax}_{x \in \mathcal{X}} \langle x, \theta_k \rangle$$

$$= \sum_{x: \Delta_x \leq \nu} \Delta_x T_x + \sum_{x: \Delta_x > \nu} \Delta_x T_x$$

$$\leq \nu T + \sum_{x: \Delta_x > \nu} \sum_{\ell=1}^{\infty} \overset{\leq 8\varepsilon_\ell}{\Delta_x \mathbb{1}[\lambda_x \mathcal{I}_\ell]} \mathbb{1}\{x \in \mathcal{X}_\ell\}$$

$$\leq \nu T + \sum_{x: \Delta_x > \nu} \sum_{\ell=1}^{\log_2 \lceil 8(d\nu\nu)^{-1} \rceil} 8\varepsilon_\ell (\lambda_x \mathcal{I}_\ell + \mathbb{1}\{x \in \operatorname{supp}(\lambda_\ell)\})$$

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

$$\searrow = 2d\varepsilon_\ell^{-2} \log(4\ell^2 |\mathcal{X}|/\delta)$$

$$\leq \nu T + 8 \cdot \frac{d(d+1)}{2} + 16d \log(4 \log \lceil 8(d\nu\nu)^{-1} \rceil^2 |\mathcal{X}|/\delta) \sum_{\ell=1}^{\log_2 \lceil 8(d\nu\nu)^{-1} \rceil} \varepsilon_\ell^{-1}$$

$$\ell \leq \log_2 \lceil 8(d\nu\nu)^{-1} \rceil$$

$$\leq \nu T + 4d(d+1) + 128d \log(4 \log \lceil 8(d\nu\nu)^{-1} \rceil^2 |\mathcal{X}|/\delta) \cdot (d\nu\nu)^{-1}$$

$$\text{If } \nu = 0 \quad Regret \leq O(d^2 + \frac{d}{\Delta} \log(\frac{|\mathcal{X}|}{\delta} \log d^{-1}))$$

$$\text{If } \nu > 0 \quad Regret \leq O\left(\sqrt{dT \log(\log(T/\delta) |\mathcal{X}|/\delta)}\right)$$