Distributional Robust Bayesian Optimization with ϕ -divergences



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D = MMD

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Summary: (i) A theoretical result showing DRO-BO breaks down into a finite dimensional optimization problem (ii) A practical algorithm to solve DRO-BO (iii) A regret analysis that holds for most choices of φ .

Distributional Robust Bayesian Optimization

$$\mathcal{U}_D = \left\{ Q : D(P, Q) \le \varepsilon \right\}$$

$$\max_{x} \min_{Q \in \mathcal{U}_{D}} \mathbb{E}_{Q(c)} \left[f(x, c) \right]$$

Kernel Distributional Robust Bayesian Optimization

Computationally expensive: Requires solving the minimax directly
 Limited to the setting when contexts are finite.

Can we solve the DRO-BO more efficiently with another choice of D?

(φ -)Distributional Robust Bayesian Optimization

$$\operatorname{Pick} \mathsf{D}_{\varphi}(P,Q) = \int_{\mathscr{C}} \varphi\left(\frac{dP}{dQ}\right) dQ$$

- Total Variation
- Kullback-Leibler Divergence
- χ^2 -divergence

$$B_{\phi}^{t}(p) := \left\{ q \in \Delta(\mathscr{C}) : \mathsf{D}_{\phi}(q, p_{t}) \leq \varepsilon_{t} \right\}$$

$$\chi^{2}\text{-divergence}$$

$$\sup_{t \to \infty} \left(\mathbb{E}_{p_{t}(c)}[f(x,c)] - \sqrt{\varepsilon_{t} \cdot \operatorname{Var}_{p_{t}(c)}[f(x,c)]} \right)$$

 $=\chi^2$

$$\max_{x \in \mathcal{X}} \inf_{q \in B_{\phi}^{t}(p)} \mathbb{E}_{c \sim q}[f(x, c)] = \max_{x \in \mathcal{X}, \lambda \geq 0, b \in \mathbb{R}} \left(b - \lambda e_{t} - \lambda \mathbb{E}_{p_{t}(c)} \left[\varphi^{\star} \left(\frac{b - f(x, c)}{\lambda} \right) \right] \right)$$

D = TV

Total Variation Distance

$$\sup_{x \in \mathcal{X}} \left(\mathbb{E}_{p_t(c)}[f(x,c)] - \frac{\varepsilon_t}{2} \left(\sup_{c \in \mathscr{C}} f(x,c) - \inf_{c \in \mathscr{C}} f(x,c) \right) \right)$$

Regret Analysis

$$R_T(\varphi) \leq \frac{\sqrt{8T\beta_T\gamma_T}}{\log(1+\sigma_f^{-2})} + M \sum_{t=1}^T \Gamma_{\varphi}(\varepsilon_t)$$

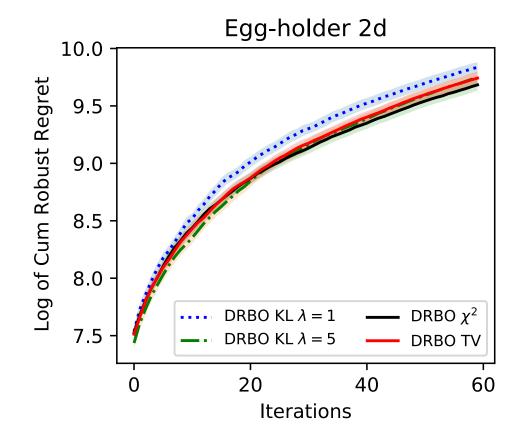
$$M = \sup_{(x,c) \in \mathcal{X} \times \mathcal{C}} |f(x,c)| < \infty$$

$$f \in \text{RKHS}$$

$$\varphi : \mathbb{R} \to (-\infty, \infty]$$

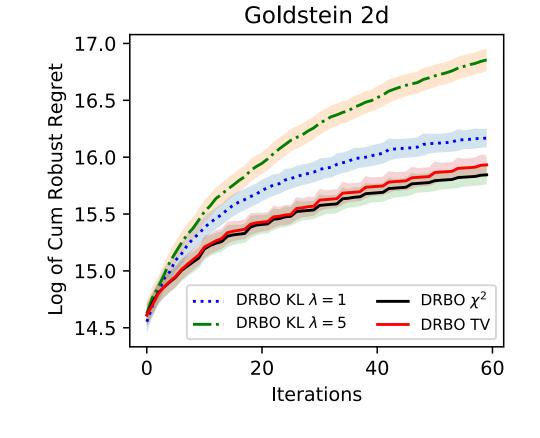
$$\Gamma_{\varphi} : [0,\infty) \to \mathbb{R}$$

$$\mathsf{TV}(p,q) \leq \Gamma_{\varphi}(\mathsf{D}_{\varphi}(p,q))$$



Cosines 2d

Iterations



Rosenbrock f(x, c)

input x

0.0 -

-1.5

- DR Optimum

Stochastic Optimum

-1000

-1500

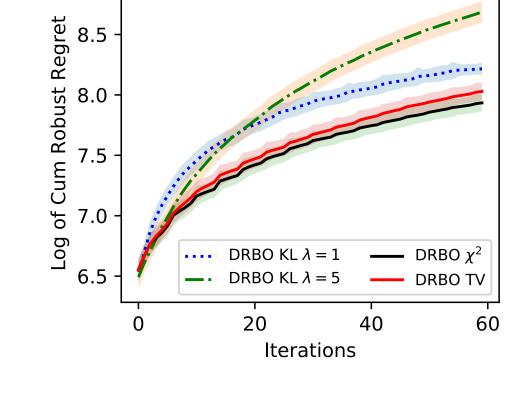
-2000

-2500

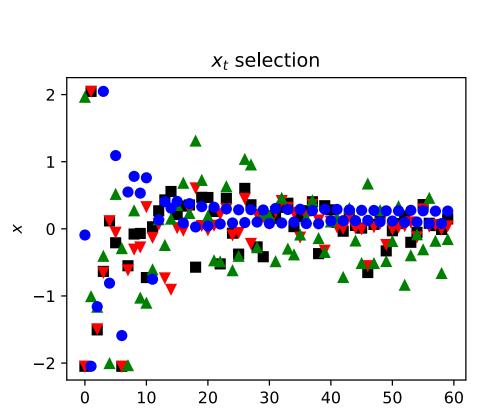
- 3000

- 3500

□ _4000



Branin 2d



 \blacksquare χ^2 \blacktriangledown TV \blacktriangle MMD \bullet BO

