

Chance Constrained Optimization and their Distributionally Robust Counterpart using Maximum Mean Discrepancy

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FOR INTELLIGENT SYSTEMS



Challenges in Stochastic Optimization

Chance constraints

Decision-making under uncertainty

$$\min_{x \in \mathcal{X}} c^T x \quad \text{s.t. } f(x, \xi) \leq 0, \quad \xi \in \Xi, \quad \xi \sim P$$



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→ Scenario optimization (data-driven)

Enforce constraint at every sample: $f(x, \xi_i) \leq 0 \quad i = 1, \dots, N$

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- ▶ Chance constraint to handle very unlikely events:

$$\min_{x \in \mathcal{X}} c^T x \quad \text{s.t. } P(f(x, \xi) \leq 0) \geq 1 - \alpha \quad \forall \xi \in \Xi$$

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- ▶ Distributionally robust chance constraint

- ▶ Assume distributional ambiguity in chance constraint
- ▶ Enforce constraint for worst-case distribution within set of distributions

Convex approximation

Conditional Value-at-Risk

$$P[f(x, \xi) \leq 0] \geq 1 - \alpha \iff \text{VaR}_{1-\alpha}^P[f(x, \xi)] \leq 0$$

$$\text{VaR}_{1-\alpha}^P[X] = F_X^{-1}(1 - \alpha)$$

$$\text{CVaR}_{1-\alpha}^P[X] = \mathbb{E}[X | X > \text{VaR}_{1-\alpha}^P(X)]$$

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$$\min_{x \in \mathcal{X}} c^T x$$

$$\text{s.t. } \text{VaR}_{1-\alpha}^P[f(x, \xi)] \leq 0$$

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Chance constraint

$$\begin{aligned} \min_{x \in \mathcal{X}} \quad & c^T x \\ \text{s.t.} \quad & \text{VaR}_{1-\alpha}^P[f(x, \xi)] \leq 0 \end{aligned}$$

CVaR constraint

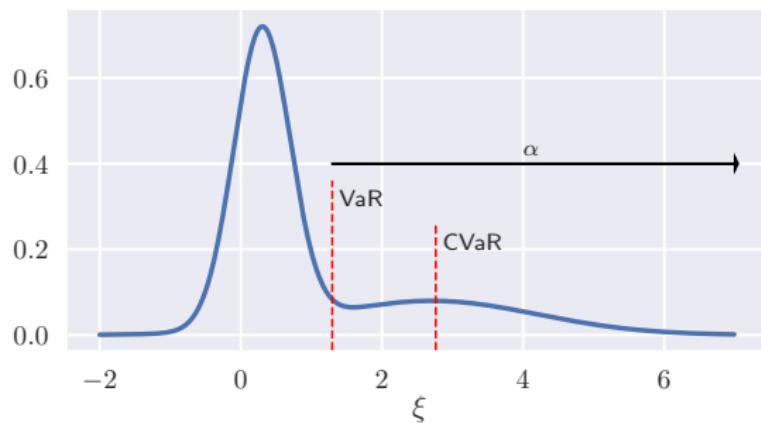
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Chance constraints

How to solve in practice

$$VaR_{1-\alpha}^P := \inf_{t \in \mathbb{R}} P[f(x, \xi) \leq t] \geq 1 - \alpha$$

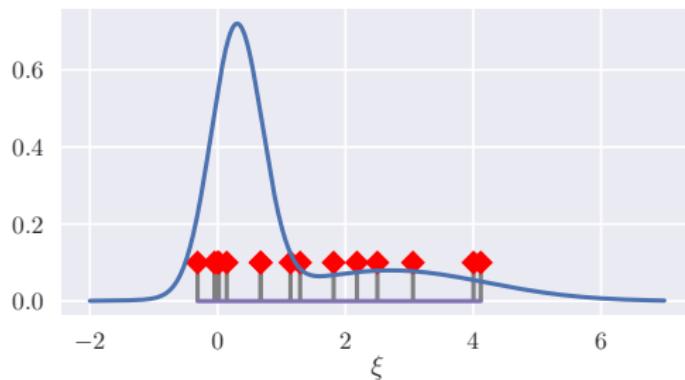
$$CVaR_{1-\alpha}^P := \inf_{t \in \mathbb{R}} \mathbb{E}_P[[f(x, \xi) + t]_+] - t\alpha$$



Distributionally Robust Chance Constraints

DRO

Distributional ambiguity since we only have samples available

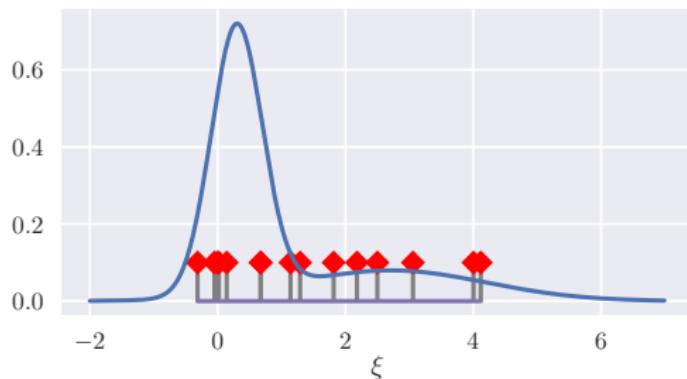


- ▶ $\hat{P} = \sum_{i=1}^N \frac{1}{N} \delta_{\xi_i}$
- ▶ \hat{P} is only a approximation of P_{true}

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Ambiguity set: Metric ball around \hat{P} for worst-case distribution

$$\mathcal{P} := \{P : \|P - \hat{P}\| \leq \epsilon\}$$

$$P(f(x, \xi) \leq 0) \geq 1 - \alpha \quad \rightarrow \quad \inf_{P \in \mathcal{P}} P(f(x, \xi) \leq 0) \geq 1 - \alpha$$

- ▶ If ϵ large enough $P_{true} \in \mathcal{P}$

Ambiguity set

Definition

$$\mathcal{P} := \left\{ P : \|P - \hat{P}\| \leq \epsilon \right\}$$

Wasserstein distance

$$\|P - \hat{P}\| = W_p(P, \hat{P}) = \left(\inf_{\pi \in \Pi(P, \hat{P})} \int \|\xi - \hat{\xi}\|^p \pi(d\xi, d\hat{\xi}) \right)^{\frac{1}{p}}$$

- ▶ Cross-validation: Very costly for large problems (Chen u. a. 2022; Weijun 2018)
- ▶ Empirical likelihood: Limitation w.r.t. constraint function (Blanchet u. a. 2019)

Ambiguity set

Definition

$$\mathcal{P} := \left\{ P : \|P - \hat{P}\| \leq \epsilon \right\}$$

Maximum Mean Discrepancy (MMD)

$$\|P - \hat{P}\| = \text{MMD}(P, Q) := \|\mu_P - \mu_Q\|_{\mathcal{H}}$$

Kernel Mean Embedding: $\mu_P(\cdot) = \int_{\mathcal{X}} k(x, \cdot) dP(x)$

Ambiguity set construction

$$\mathcal{P} := \{P : \text{MMD}(P, \hat{P}) \leq \epsilon\}$$

with

$$\text{MMD}(P, Q) = \sqrt{\mathbb{E}_P k(x, x') + \mathbb{E}_Q k(y, y') - 2\mathbb{E}_{x \sim P, y \sim Q} k(x, y)}$$

- ▶ Closed-form estimator through above definition
- ▶ Concentration rates

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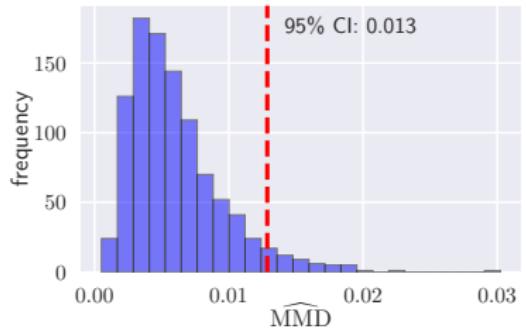
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Bootstrap estimation of MMD

Let $\{\tilde{\xi}_i\}_{i=1}^N$ be a bootstrap sample from \hat{P} with distribution \tilde{P}

$$\text{MMD}(\tilde{P}, \hat{P}) \xrightarrow{P} \text{MMD}(P_{True}, \hat{P})$$

→ Not possible with Wasserstein distances



Distributionally Robust Chance Constraints

Exact reformulation

Primal formulation of feasible set:

$$\begin{aligned} Z &:= \{x \in \mathcal{X} : \inf_{P \in \mathcal{P}} P(f(x, \xi) \leq 0) \geq 1 - \alpha\} \\ &= \{x \in \mathcal{X} : \sup_{P \in \mathcal{P}} \mathbb{E}_P[\mathbb{1}(f(x, \xi) \geq 0)] \leq \alpha\} \end{aligned}$$



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Assumption: Constraint function $f(x, \xi)$ is semi-continuous

Dual formulation of feasible set (Zhu u. a. 2020):

$$Z := \left\{ x \in \mathcal{X} : \begin{array}{l} g_0 + \frac{1}{N} \sum_{i=0}^N g(\xi_i) + \varepsilon \|g\|_{\mathcal{H}} \leq \alpha \\ \mathbb{1}(f(x, \xi) > 0) \leq g(\xi) + g_0 \quad \forall \xi \in \Xi \\ g \in \mathcal{H}, \quad g_0 \in \mathbb{R} \end{array} \right\}$$

Distributionally Robust Chance Constraints

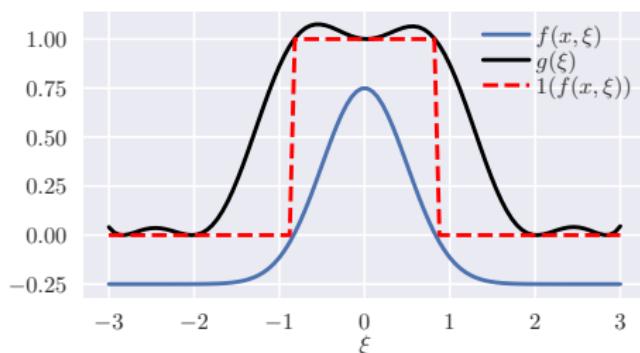
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$$\mathbb{1}(f(x, \xi) > 0) \leq g(\xi) + g_0 \quad \forall \xi \in \Xi$$

- ▶ Non-convex
- ▶ semi-inf constraint

Convex conservative approximation

Using CVaR

$$\sup_{P \in \mathcal{P}} \text{VaR}_{1-\alpha}^P(f(x, \xi)) \leq 0 \quad \rightarrow \quad \sup_{P \in \mathcal{P}} \text{CVaR}_{1-\alpha}^P(f(x, \xi)) \leq 0$$

$$Z_{\text{CVaR}} := \left\{ x \in \mathcal{X} : \begin{array}{l} g_0 + \frac{1}{N} \sum_{i=1}^N g(\xi_i) + \varepsilon \|g\|_{\mathcal{H}} \leq t\alpha \\ [f(x, \xi) + t]_+ \leq g_0 + g(\xi) \quad \forall \xi \in \Xi \\ g \in \mathcal{H}, \quad g_0, t \in \mathbb{R} \end{array} \right\}$$

$$g(\xi) = \sum_{i=1}^N \gamma_i k(\xi_i, \xi) \quad \rightarrow \quad \|g\|_{\mathcal{H}} = \sqrt{\gamma K \gamma} \quad K_{ij} = k(\xi_i, \xi_j)$$

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Constraint relaxation

$$[f(x, \xi_i) + t]_+ \leq g_0 + (K\gamma)_i \quad \forall i = 1, \dots, N$$

- ▶ Avoid ad-hoc reformulation limiting constraint function
- ▶ Statistical guarantee for constraint satisfaction

Numerical experiments

Chance constrained portfolio optimization

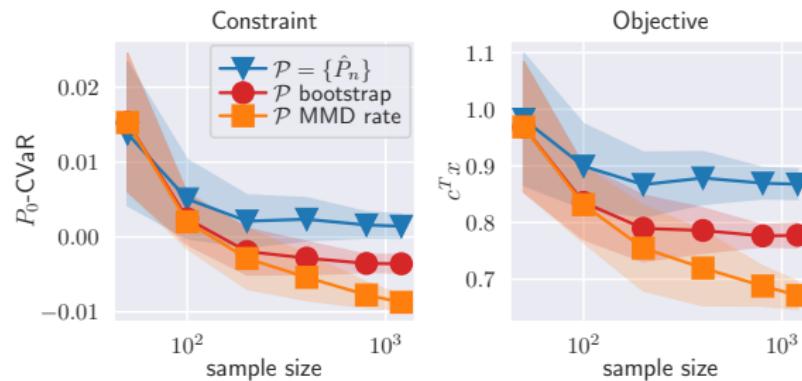
$$\max_{x \in \mathcal{X}} \quad c^T x$$

$$\text{s.t.} \quad P[(x^T \xi)^2 - 1 \leq 0] \geq 1 - \alpha$$

↓

$$\sup_{P \in \mathcal{P}} \text{CVaR}_{1-\alpha}^P[(x^T \xi)^2 - 1] \leq 0$$

$$\mathcal{X} = \{x \in \mathbb{R}^3 : \sum_{i=1}^3 x_i \leq 1, \\ x_i \geq 0 \quad \forall i = 1, 2, 3\}$$



-  Blanchet, Jose, Yang Kang und Karthyek Murthy (Sep. 2019). „Robust Wasserstein Profile Inference and Applications to Machine Learning“. In: *Journal of Applied Probability* 56.3, S. 830–857.
-  Chen, Zhi, Daniel Kuhn und Wolfram Wiesemann (Mai 2022). *Data-Driven Chance Constrained Programs over Wasserstein Balls*.
-  Hota, Ashish R., Ashish Cherukuri und John Lygeros (Okt. 2018). „Data-Driven Chance Constrained Optimization under Wasserstein Ambiguity Sets“. In: *arXiv:1805.06729 [cs, math]*.
-  Weijun, Xie (Juni 2018). „On Distributionally Robust Chance Constrained Programs With Wasserstein Distance“. In: *arXiv*.
-  Zhu, Jia-Jie u. a. (Dez. 2020). „Kernel Distributionally Robust Optimization“. In: *arXiv:2006.06981 [cs, math, stat]*.

CVaR reformulations

Tractable reformulation of semi-inf constraint

Ad-hoc reformulations of CVaR relaxation

- ▶ Wasserstein DR-CC: e.g., piece-wise affine constraint, quadratic constraints (Hota u. a. 2018; Weijun 2018)
 - ▶ Assumptions on support of ξ
 - ▶ Limit constraint functions
- ▶ MMD DR-CC:
 - ▶ Limit support
 - ▶ Adjust kernel choice to constraint function: e.g. linear kernel for piecewise-affine $f(x, \xi)$
 - Non-characteristic kernel limits MMD: Finite moment comparison of distributions

Reproducing Kernel Hilbert Space

Kernel DRO

Consider a positive definite kernel $k : \mathcal{X} \times \mathcal{X} \rightarrow \mathbb{R}$
→ similarity measure for $x \in \mathcal{X}$

Let \mathcal{H} be a Hilbert space of functions $\mathcal{X} \rightarrow \mathbb{R}$ with associated inner product $\langle \cdot, \cdot \rangle_{\mathcal{H}}$

k is a reproducing kernel of \mathcal{H} $k(x, x') = \langle \phi(x), \phi(x') \rangle_{\mathcal{H}}$

- ▶ $k(x, \cdot) \in \mathcal{H} \quad \forall x \in \mathcal{X}$
- ▶ $f(x) = \langle f, k(\cdot, x) \rangle_{\mathcal{H}} \quad \forall f \in \mathcal{H}, x \in \mathcal{X}$

Kernel Mean Embedding:

$$\mu_P(\cdot) = \int_{\mathcal{X}} k(\cdot, x) dP(x) \quad \mathbb{E}[f(x)] = \int_{\mathcal{X}} f(x) dP(x) = \langle f, \mu_P \rangle_{\mathcal{H}}$$

$$\text{MMD}(P, Q) := \|\mu_P - \mu_Q\|_{\mathcal{H}}$$

Kernel DRO(Zhu u. a. 2020)

An introduction

► Primal:

$$\min_{\theta} \sup_{P \in K} \int \ell(\theta, \xi) dP(\xi)$$

► Dual:

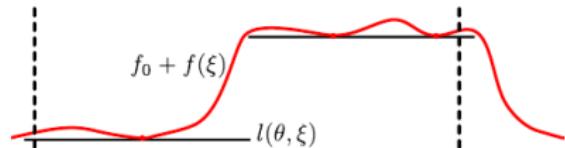
$$\min_{\theta, f_0, \alpha} f_0 + \delta_K(f)$$

subject to $\ell(\theta, \xi) \leq f_0 + f(\xi), \forall \xi \in \mathcal{X}$

with

$$f(\xi) = \sum_i \alpha_i \cdot k(\xi_i, \xi),$$

$$f(\xi) \in \mathcal{H}, f_0 \in \mathbb{R}.$$



RKHS-function f such that it
majorizes ℓ

Finite-sample guarantee

Concentration rate of MMD:

$$\text{MMD}(P_{true}, \hat{P}) \leq \sqrt{\frac{C}{N}} + \sqrt{\frac{2C \log(1/\delta)}{N}},$$

with probability $1 - \delta$ and $C \geq \sup_x k(x, x)$

$$\text{CVaR}_{1-\alpha}^P[f(x, \xi)] \leq M \sqrt{\frac{2 \log(1/\delta)}{N}}$$

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Chance constraint guarantee

$$P(f(x, \xi) \leq M \sqrt{\frac{2 \log(1/\delta)}{N}}) \geq 1 - \alpha,$$

with probability $1 - \delta$.

Numerical experiments

MPC with nonlinear constraint

Linear tube-based MPC

- ▶ Nonlinear SVM constraint
- ▶ Linear dynamics

