Kernel Embedding for Particle Gibbs-Based Optimal Control

L. Hochschwarzer
Intermediate Report Master's Thesis
Supervisor: R. Lefringhausen

Chair of Information-oriented Control
Technical University of Munich

Motivation

[Xiloyannis, Chiaradia, Frisoli and Masia 2019]

Challenges:

- Unknown Dynamic
- Latent States
- Safety

Problem Statement - System

Given: Dataset $\mathbb{D} = \{\boldsymbol{u}_t, \boldsymbol{y}_t\}_{t=\text{-}T:\text{-}1}$ from unknown system

$$\begin{aligned} \boldsymbol{x}_{t+1} &= \boldsymbol{f}\left(\boldsymbol{x}_t, \boldsymbol{u}_t\right) + \boldsymbol{v}_t, \qquad && \boldsymbol{v}_t \sim \boldsymbol{\mathcal{V}}, \\ \boldsymbol{y}_t &= \boldsymbol{g}\left(\boldsymbol{x}_t, \boldsymbol{u}_t\right) + \boldsymbol{w}_t, \qquad && \boldsymbol{w}_t \sim \boldsymbol{\mathcal{W}} \end{aligned}$$

Assumptions

- Known system structure

$$\begin{aligned} \boldsymbol{x}_{t+1} &= \boldsymbol{f}_{\boldsymbol{\theta}}\left(\boldsymbol{x}_t, \boldsymbol{u}_t\right) + \boldsymbol{v}_t, \qquad && \boldsymbol{v}_t \sim \boldsymbol{\mathcal{V}}_{\boldsymbol{\theta}}, \\ \boldsymbol{y}_t &= \boldsymbol{g}_{\boldsymbol{\theta}}\left(\boldsymbol{x}_t, \boldsymbol{u}_t\right) + \boldsymbol{w}_t, \qquad && \boldsymbol{w}_t \sim \boldsymbol{\mathcal{W}}_{\boldsymbol{\theta}}. \end{aligned}$$

- Known priors $p(\boldsymbol{\theta})$ and $p(\boldsymbol{x}_{\text{-}T})$

Problem Statement - Optimal Control Problem

Goal: Solve optimal control problem (OCP)

Stochastic OCP

$$\min_{\boldsymbol{u}_{0:H}} J_H(\boldsymbol{u}_{0:H})$$

subject to:

$$P\left[h_i(\boldsymbol{u}_{0:H}, \boldsymbol{x}_{0:H}, \boldsymbol{y}_{0:H}) \leq 0\right] \geq 1 - \alpha, \ \forall i = 1, ..., n_c$$

Problem: Underlying data distribution P is unknown

Related Works

Particle Gibbs Based Optimal Control **[Lefringhausen, Srithasan, Lederer and Hirche 2024]**

$\Rightarrow$ Guarantees determined retroactively

Alternative Approaches:

- Wasserstein Ambiguity [Hota, Cherukuri and Lygeros 2019]
  $\Rightarrow$ Constraints limited to affine functions
- Kernel Embeddings **[Nemmour, Kremer, Schoelkopf and Zhu 2022]**
  [Thorpe, Lew, Oishi and Zhu 2022]

Particle Gibbs Scenarios

Particle Gibbs gives us the scenarios $\boldsymbol{\delta}^{[1:N]} = \{\boldsymbol{\theta}, \boldsymbol{x}_0, \boldsymbol{v}_{0:H}, \boldsymbol{w}_{0:H}\}^{[1:N]}$ that characterize the system

Goal: Reformulate chance-constraint problem with scenarios $\boldsymbol{\delta}^{[1:N]}$

Chance Constraints

$$P\left[h_i(\boldsymbol{u}_{0:H}, \boldsymbol{x}_{0:H}, \boldsymbol{y}_{0:H}) \leq 0\right] \geq 1 - \alpha, \ \forall i = 1, ..., n_c$$

$$\Downarrow$$

Scenario Approach (used in [Lefringhausen+ 2024])

$$\boldsymbol{h}(\boldsymbol{u}_{0:H}, \boldsymbol{x}_{0:H}^{[n]}, \boldsymbol{y}_{0:H}^{[n]}) \leq 0, \ \forall n = 1, ..., N$$

$\Rightarrow$ Risk factor α not considered in optimization

Maximum Mean Discrepancy (MMD) ambiguity sets

Goal: Reformulate chance-constraint problem with scenarios $\boldsymbol{\delta}^{[1:N]}$

Idea: Replace distribution P with the ambiguity set $\mathcal{P}$

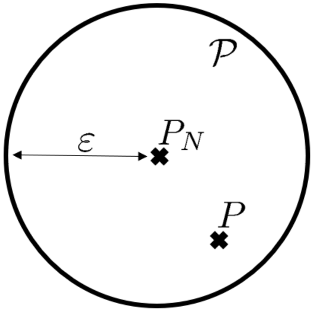
MMD ambiguity set

$$\mathcal{P} = \left\{ \tilde{P} : \mathsf{MMD}(\tilde{P}, P_N) \leq \varepsilon \right\}.$$

$$\Downarrow$$

Expanded Chance-Constraints

$$\inf_{\tilde{P} \in \mathcal{P}} \tilde{P}\left[h_i(\boldsymbol{u}_{0:H}, \boldsymbol{x}_{0:H}, \boldsymbol{y}_{0:H}) \leq 0\right] \geq 1 - \alpha.$$



Constraint Reformulation

Goal: Reformulate chance-constraint problem with scenarios $\boldsymbol{\delta}^{[1:N]}$

Feasible Region of chance constraint

$$Z_i := \left\{ \boldsymbol{u}_{0:H} \in \mathcal{U}^{H+1} : \inf_{\tilde{P} \in \mathcal{P}} \tilde{P}\left[\tilde{h}_i(\boldsymbol{u}_{0:H}, \boldsymbol{\delta}) \leq 0 \right] \geq 1 - \alpha \right\}$$

$$\Downarrow$$

Reformulated Feasible Region [Nemmour+ 2022]

$$Z_i := \left\{ \boldsymbol{u}_{0:H} \in \mathcal{U}^{H+1} : \begin{array}{l} g_0 + \dfrac{1}{N} \displaystyle\sum_{n=1}^{N} (\boldsymbol{K\gamma})_n + \varepsilon \sqrt{\boldsymbol{\gamma}^\mathsf{T} \boldsymbol{K} \boldsymbol{\gamma}} \leq t' \alpha \\ [\tilde{h}_i(\boldsymbol{u}_{0:H}, \boldsymbol{\delta}^{[n]}) + t']_+ \leq g_0 + (\boldsymbol{K\gamma})_n, \ n = 0, \ldots, N \\ g_0 \in \mathbb{R}, \boldsymbol{\gamma} \in \mathbb{R}^N, t' \in \mathbb{R} \end{array} \right\}$$

Problem Formulation

Goal: Reformulate chance-constraint problem with scenarios $\boldsymbol{\delta}^{[1:N]}$

$$\min_{\boldsymbol{u}_{0:H},\{g_0,\boldsymbol{\gamma},t'\}^{[1:n_c]}} J_H(\boldsymbol{u}_{0:H})$$

subject to: $\forall n \in \mathbb{N}_{\leq N},\ \forall t \in \mathbb{N}^0_{\leq H},\ \forall i \in \mathbb{N}_{\leq n_c}$

$$\left.\begin{aligned} \boldsymbol{x}_{t+1}^{[n]} &= \boldsymbol{f}_{\boldsymbol{\theta}^{[n]}}\left(\boldsymbol{x}_t^{[n]}, \boldsymbol{u}_t\right) + \boldsymbol{v}_t^{[n]} \\ \boldsymbol{y}_t^{[n]} &= \boldsymbol{g}_{\boldsymbol{\theta}^{[n]}}\left(\boldsymbol{x}_t^{[n]}, \boldsymbol{u}_t\right) + \boldsymbol{w}_t^{[n]} \end{aligned}\right\} \text{Dynamic Constraints}$$

$$\left.\boldsymbol{u}_{0:H} \in Z_i(g_0^{[i]}, \boldsymbol{\gamma}^{[i]}, t'^{[i]})\right\} \text{Reformulated Chance Constraints}$$

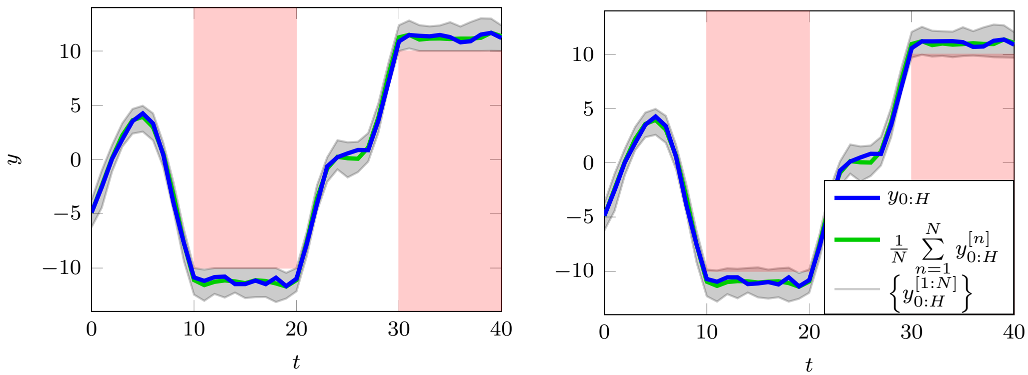
Simulation Setup

- Unknown system: $$\boldsymbol{f}(\boldsymbol{x},u)=\begin{bmatrix}0.8x_1-0.5x_2\\0.4x_1+0.5x_2+u\end{bmatrix}$$ $$\boldsymbol{v}_t\sim\mathcal{N}\left(\boldsymbol{0},\boldsymbol{Q}=\begin{bmatrix}0.03 & \text{-}0.004\\ \text{-}0.004 & 0.01\end{bmatrix}\right).$$
- Known system structure: $\boldsymbol{f}(\boldsymbol{x},u)=\boldsymbol{A}\,[x_1,x_2,u]^\mathsf{T}+\boldsymbol{v}_t,\ \boldsymbol{v}_t\sim\mathcal{N}(\boldsymbol{0},\boldsymbol{Q})$
- Priors: $\boldsymbol{Q}\sim\mathcal{IW}(100\boldsymbol{I}_2,10)$
  $\boldsymbol{A}\sim\mathcal{MN}(\boldsymbol{0},\boldsymbol{Q},10\boldsymbol{I}_2)$ [Andrieu+ 2017]
  $\boldsymbol{x}_{\text{-}T}\sim\mathcal{N}([2,2]^\mathsf{T},\boldsymbol{I}_2)$
- Known measurement model $g(\boldsymbol{x},u)=x_1,\ w_t\sim\mathcal{N}(0,0.1)$
- Cost function $J_H=\sum_{t=0}^{H}u_t^2$
- Input constraints $|u|\leq 10$
- Gaussian kernels with bandwidth σ set via the median heuristic [Garreau+ 2018]
- Ambiguity set radius ε set via bootstrap construction [Nemmour+ 2022].

Optimal Control with Constrained Outputs

Number of scenarios used for optimization: $N = 200$

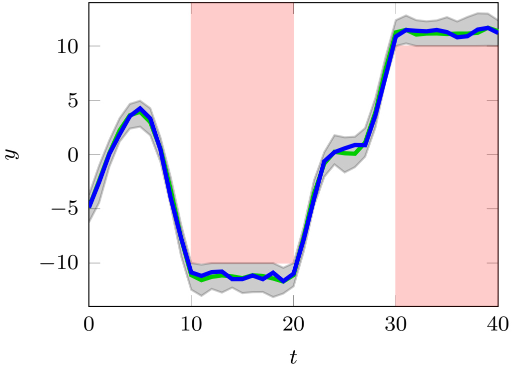
Scenario Approach | Kernel Approach ($\alpha = 0.1$)



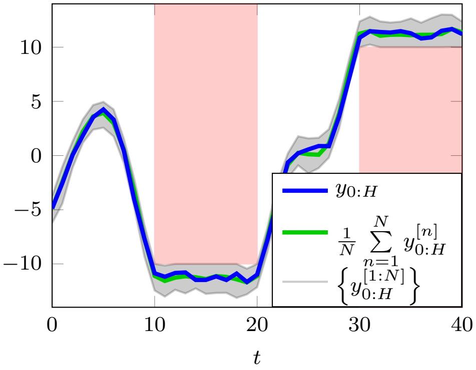
Optimal Control with Constrained Outputs

Number of scenarios used for optimization: $N = 200$

Scenario Approach



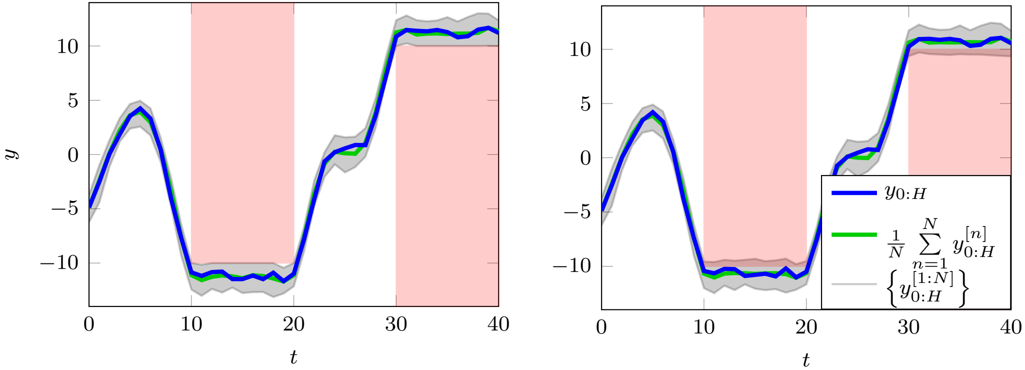
Kernel Approach ($\alpha = 0.01$)



Optimal Control with Constrained Outputs

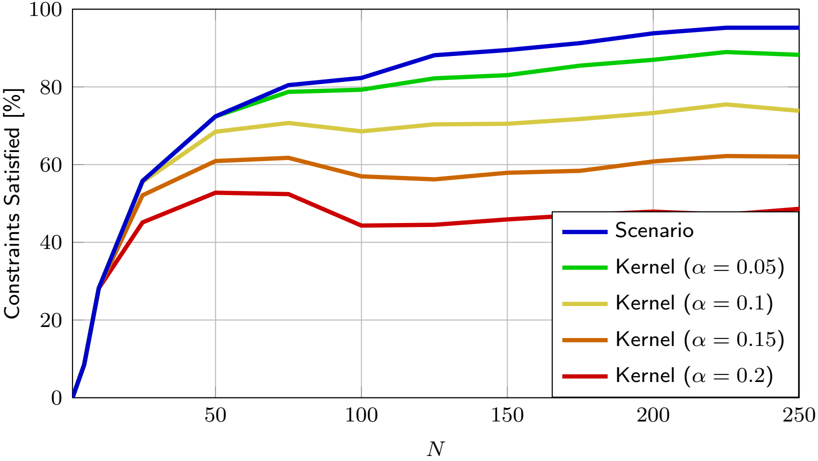
Number of scenarios used for optimization: $N = 200$

Scenario Approach　　　　Kernel Approach ($\alpha = 0.3$)



Successrate of Solution

$N = 2000$: Number of Scenarios used to test $u_{0:H}$



Conclusion

Summary: Kernel Embeddings allow for ...

- Solving of chance-constrained OCPs
- Controlling of risk factor α

Future Plans:

- Use Kernel Embeddings on non-linear systems
- Parameter tuning of σ
- Alternative approach of reformulating chance constraints

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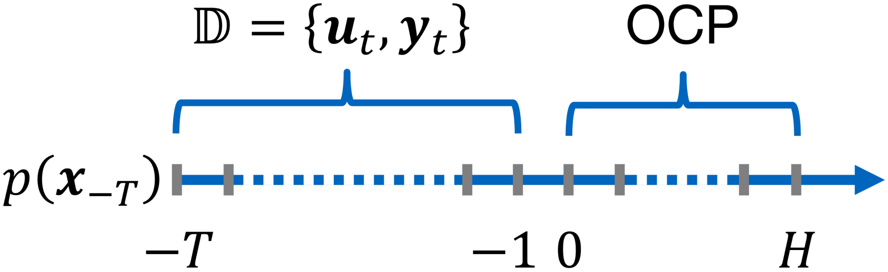
Timeline


$\mathbb{D} = \{\boldsymbol{u}_t, \boldsymbol{y}_t\}$
OCP
$p(\boldsymbol{x}_{-T})$
$-T$
-1
0
H

Scenario Generation

Goal: Generate scenarios $\boldsymbol{\delta}^{[1:N]}$ using the observations $\mathbb{D}$

Algorithm: Scenario Generation

For $n = 1, ..., N$:

1. Sample $\{\boldsymbol{\theta}, \boldsymbol{x}_{\text{-}T:\text{-}1}\}^{[n]}$ from $p\left(\boldsymbol{\theta}, \boldsymbol{x}_{\text{-}T:\text{-}1} \mid \mathbb{D}\right)$ using PMCMC [Lefringhausen+ 2024].
2. Sample $\boldsymbol{v}_t^{[n]}$ from $\boldsymbol{\mathcal{V}}_{\boldsymbol{\theta}^{[n]}}$ and $\boldsymbol{w}_t^{[n]}$ from $\boldsymbol{\mathcal{W}}_{\boldsymbol{\theta}^{[n]}}$ for $t = \text{-}1, ..., H$
3. Set $\boldsymbol{x}_0^{[n]} = \boldsymbol{f}_{\boldsymbol{\theta}^{[n]}}\left(\boldsymbol{x}_{\text{-}1}^{[n]}, \boldsymbol{u}_{\text{-}1}\right) + \boldsymbol{v}_{\text{-}1}^{[n]}$

Output: Scenarios $\boldsymbol{\delta}^{[1:N]} = \{\boldsymbol{\theta}, \boldsymbol{x}_0, \boldsymbol{v}_{0:H}, \boldsymbol{w}_{0:H}\}^{[1:N]}$

Bootstrap Construction

Algorithm: Bootstrap MMD ambiguity set

1. $\boldsymbol{K} \leftarrow$ *kernel*$(\boldsymbol{\delta}, \boldsymbol{\delta})$
2. **For** $m = 1, ..., B$
3. $\quad I \leftarrow N$ numbers from $\{1, \dots N\}$ with replacement
4. $\quad K_x \leftarrow \sum_{i,j=1}^{N} K_{ij},\ K_y \leftarrow \sum_{i,j \in I} K_{ij},\ K_{xy} \leftarrow \sum_{j \in I} \sum_{i=1}^{N} K_{ij}$
5. $\quad \text{MMD}[m] \leftarrow \frac{1}{N^2}\left(K_x + K_y - 2K_{xy}\right)$
6. **End For**
7. MMD $\leftarrow$ *sort*(MMD)
8. $\varepsilon \leftarrow$ MMD[*ceil*$(B\beta)$]

Output: Gram matrix $\boldsymbol{K}$, Radius of MMD ambiguity set ε

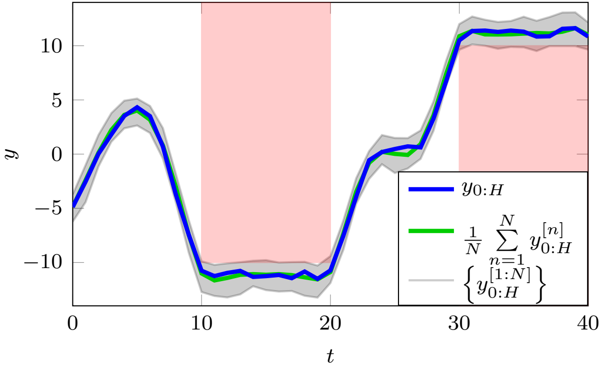
$B = 1000, \beta = 0.95$

Max Constraint

Chance Constraint

$$P\left[\max(\boldsymbol{h}(\boldsymbol{u}_{0:H}, \boldsymbol{x}_{0:H}, \boldsymbol{y}_{0:H})) \leq 0\right] \geq 1 - \alpha$$

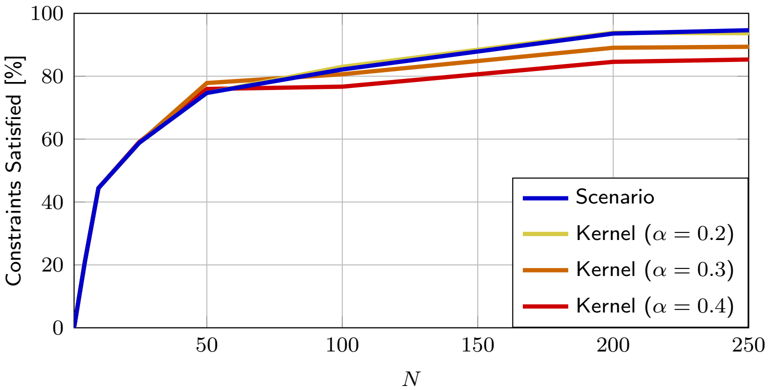
Constrained Output ($\alpha = 0.5$)



Max Constraint

Chance Constraint

$$P\left[\max(\boldsymbol{h}(\boldsymbol{u}_{0:H}, \boldsymbol{x}_{0:H}, \boldsymbol{y}_{0:H})) \leq 0\right] \geq 1 - \alpha$$



Maximum Mean Discrepancy (MMD)

Maximum Mean Discrepancy

$$\begin{aligned}\mathsf{MMD}(\tilde{P}, P_N) &= ||\mu_{\tilde{P}} - \mu_{P_N}||_{\mathcal{H}} \\ &= \mathsf{E}_{x,x'\sim\tilde{P}}[k(x,x')] + \mathsf{E}_{y,y'\sim P_N}[k(y,y')] - 2\mathsf{E}_{x\sim\tilde{P},y\sim P_N}[k(x,y)]\end{aligned}$$

(Biased) MMD estimator

$$\widehat{\mathsf{MMD}}(\tilde{P}, P_N) = \frac{1}{N^2}\sum_{i,j=1}^{N} k(\boldsymbol{\delta}^{[i]}, \boldsymbol{\delta}^{[j]}) + k(\tilde{\boldsymbol{\delta}}^{[i]}, \tilde{\boldsymbol{\delta}}^{[j]}) - 2k(\boldsymbol{\delta}^{[i]}, \tilde{\boldsymbol{\delta}}^{[j]})$$