Kernel Embedding for Particle Gibbs-Based Optimal Control

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Motivation

[Xiloyannis, Chiaradia, Frisoli and Masia 2019]

Challenges:

- Unknown dynamics
- Latent states
- Safety

Problem Statement - System

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

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

Assumptions

- Known system structure

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

- 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:

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

Problem: Underlying data distribution is unknown

Related Works

Particle Gibbs based optimal control **[Lefringhausen+ 2024]**

$\Rightarrow$ Guarantees determined retroactively via scenario theory

Alternative approaches:

- Wasserstein ambiguity [Hota+ 2019]
  - $\Rightarrow$ Constraints limited to affine functions
- Kernel embeddings **[Nemmour+ 2022]**
  [Thorpe+ 2022]

Particle Gibbs Scenarios

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

$\Rightarrow$ Scenarios **and** input $\boldsymbol{u}_{0:H}$ define the trajectory

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

Chance Constraints

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

$$\Downarrow$$

Scenario Approach ([Lefringhausen+ 2024])

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

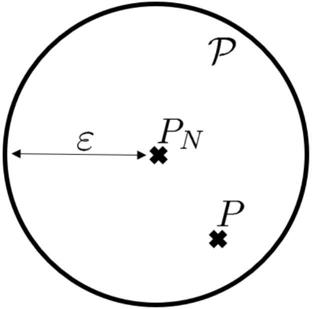
$\Rightarrow$ Risk factor α not considered in optimization

Maximum Mean Discrepancy (MMD) ambiguity sets

Required: Reformulate chance-constraint problem with scenarios $\boldsymbol{\delta}^{[1:N]}$
Approach: Replace distribution P with the ambiguity set $\mathcal{P}$

MMD ambiguity set

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



Radius ε obtained via bootstrap construction

$$\Downarrow$$

Expanded Chance-Constraints

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

Constraint Reformulation

Feasible Region of chance constraint

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

$$\Downarrow$$

Reformulated Feasible Region [Nemmour+ 2022]

$$\hat{Z} := \left\{ \boldsymbol{u}_{0:H} \in \mathcal{U}^{H+1} : \begin{array}{l} g_0 + \frac{1}{N} \sum_{n=1}^{N} (\boldsymbol{K}\boldsymbol{\gamma})_n + \varepsilon \sqrt{\boldsymbol{\gamma}^\top \boldsymbol{K} \boldsymbol{\gamma}} \leq t' \alpha \\ \left[h(\boldsymbol{u}_{0:H}, \boldsymbol{x}_{0:H}^{[n]}, \boldsymbol{y}_{0:H}^{[n]}) + t'\right]_+ \leq g_0 + (\boldsymbol{K}\boldsymbol{\gamma})_n, \ n = 1, \ldots, N \\ g_0 \in \mathbb{R}, \boldsymbol{\gamma} \in \mathbb{R}^N, t' \in \mathbb{R} \end{array} \right\}$$

Hyperparameter Tuning

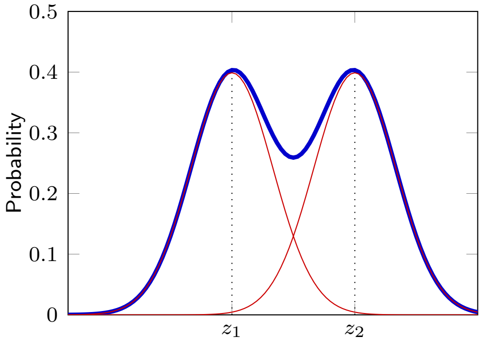
- Gaussian kernels

$$k(z, z') = \exp\left(-\frac{1}{2\sigma^2}(z - z')^2\right)$$

- Split scenarios into training set $\{z_i\}$ and test set $\{z'_j\}$
- Create likelyhood function

$$p(z) = \frac{1}{N_{\text{train}}} \sum_{i=1}^{N_{\text{train}}} \frac{1}{\sqrt{2\pi\sigma^2}} k(z, z_i)$$

- Maximize sum of likelyhoods over test set by selected a good σ



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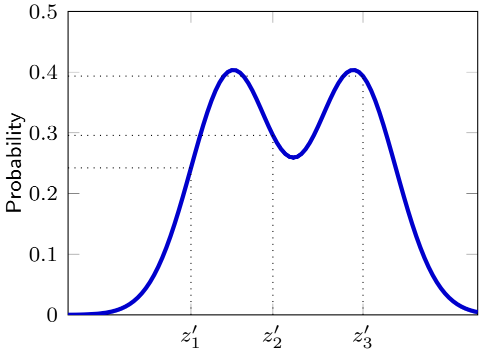


Reformulated Optimal Control Problem

$$\min_{\boldsymbol{u}_{0:H}, g_0, \boldsymbol{\gamma}, t'} J_H(\boldsymbol{u}_{0:H})$$

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

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

$$\left.\boldsymbol{u}_{0:H} \in \hat{Z}(g_0, \boldsymbol{\gamma}, t')\right\} \text{ Reformulated Chance Constraints}$$

Simulation Setup

- Unknown linear 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: $\boldsymbol{f}(\boldsymbol{x},u) = \boldsymbol{A}\,[x_1, x_2, u]^{\mathsf{T}}, \ \boldsymbol{v}_t \sim \mathcal{N}(\boldsymbol{0}, \boldsymbol{Q})$
- Priors: $\boldsymbol{Q} \sim \mathcal{IW}(100\boldsymbol{I}_2, 10)$

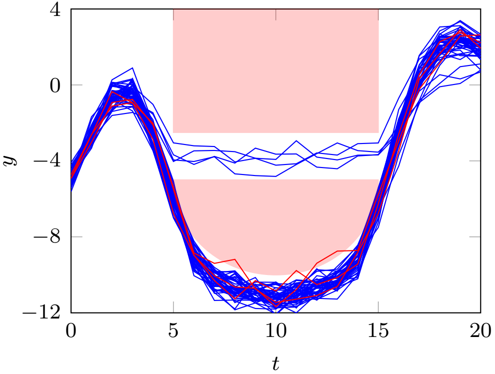
$$\boldsymbol{A} \sim \mathcal{MN}(\boldsymbol{0}, \boldsymbol{Q}, 10\boldsymbol{I}_2)$$ [Svensson+ 2017]

$$\boldsymbol{x}_{\text{-}T} \sim \mathcal{N}([2,2]^{\mathsf{T}}, \boldsymbol{I}_2)$$

- Known measurement model $g(\boldsymbol{x},u) = x_1, \ w_t \sim \mathcal{N}(0, 0.1)$ (w.l.o.g.)
- Cost function $J_H = \sum_{t=0}^{H} u_t^2$
- Input constraints $|u| \leq 10$
- Number of scenarios used for optimization: $N = 100$

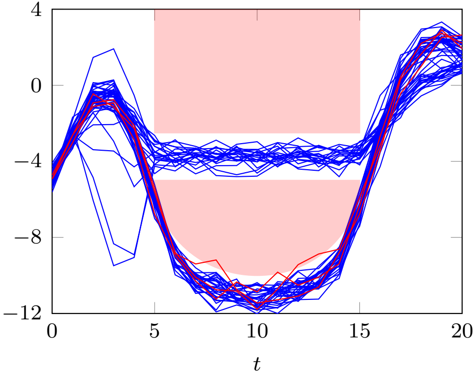
Risk Tuning

Scenario Approach



Average Cost $J_H = 338.4$

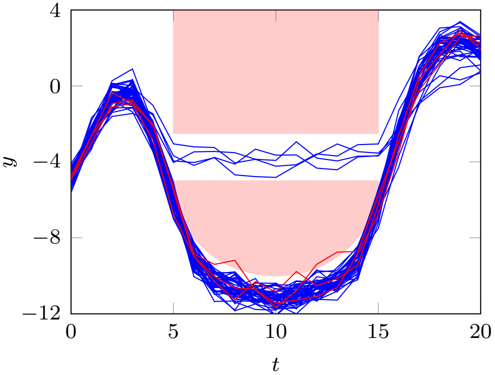
Kernel Approach ($\alpha = 0.1$)



Average Cost $J_H = 255.9$

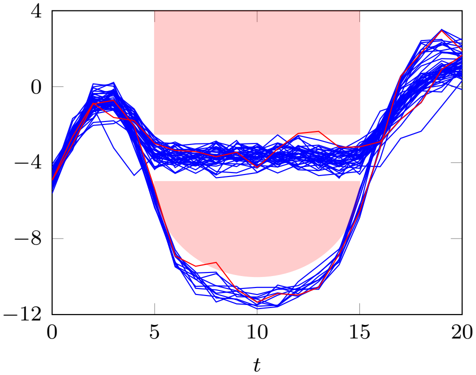
Risk Tuning

Scenario Approach



Average Cost $J_H = 338.4$

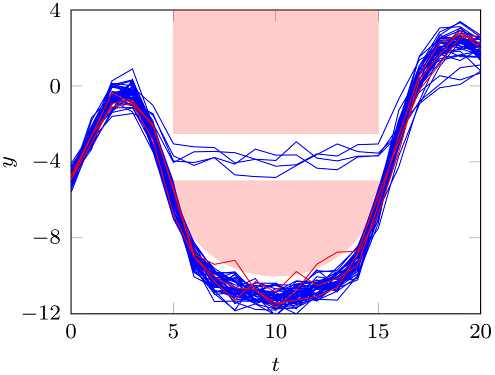
Kernel Approach ($\alpha = 0.2$)



Average Cost $J_H = 129.5$

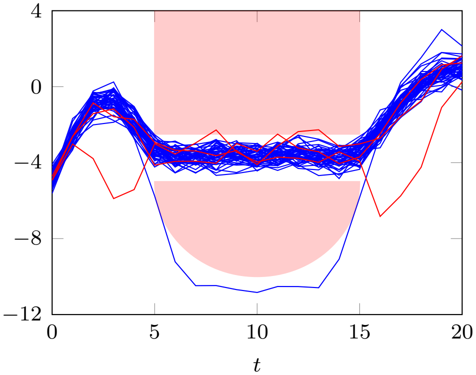
Risk Tuning

Scenario Approach



Average Cost $J_H = 338.4$

Kernel Approach ($\alpha = 0.3$)



Average Cost $J_H = 69.9$

Nonlinear System

Nonlinear System

$$\boldsymbol{f}(\boldsymbol{x}, u) = \begin{bmatrix} 0.8x_1 - 0.5x_2 + 0.1\cos(3x_1)x_2 \\ 0.4x_1 + 0.5x_2 + (1 + 0.3\sin(2x_2))u \end{bmatrix}$$

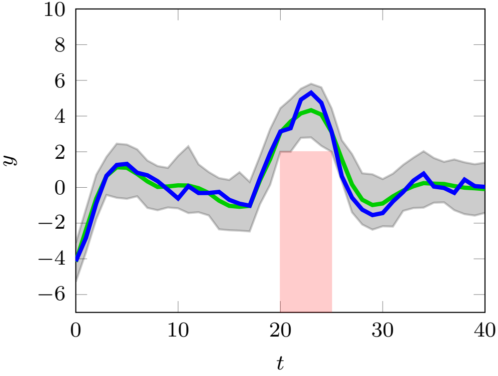
- Known system structure: $\boldsymbol{f}(\boldsymbol{x}, u) = \boldsymbol{A}\left[x_1, x_2, u, \cos(3x_1)x_2, \sin(2x_2)u\right]^\mathsf{T}$
- Input constraints $|u| \leq 5$
- Number of scenarios used for optimization: $N = 200$

Challenge: Numerical issues complicates solving OCPs with

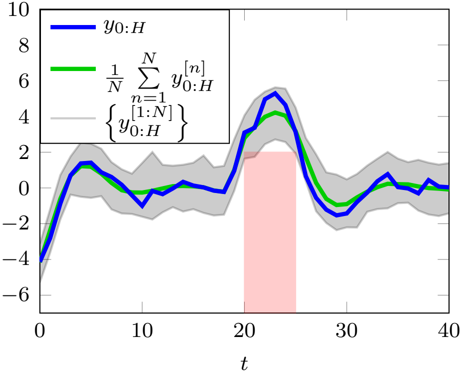
- Low number of samples N
- Low Risk Factor α
- High number of constraints

Optimal Control of Nonlinear Systems

Scenario Approach

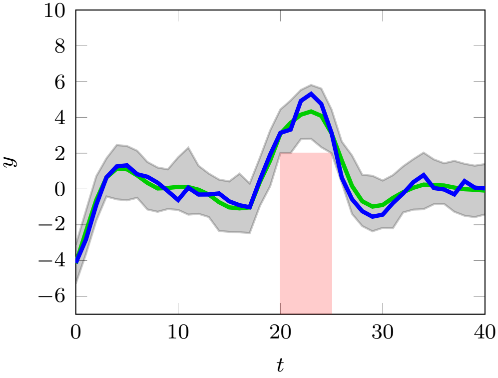


Kernel Approach ($\alpha = 0.2$)

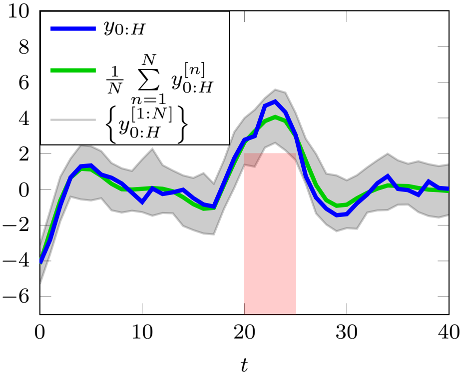


Optimal Control of Nonlinear Systems

Scenario Approach

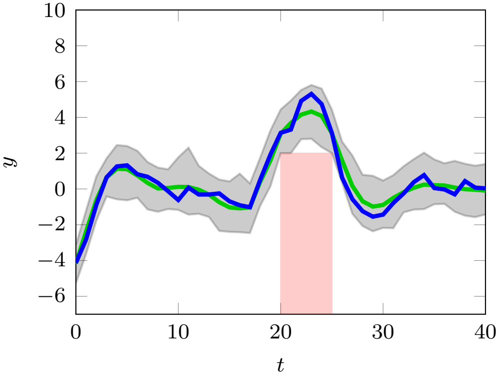


Kernel Approach ($\alpha = 0.4$)

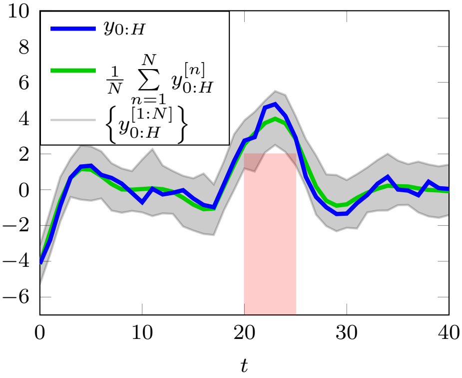


Optimal Control of Nonlinear Systems

Scenario Approach



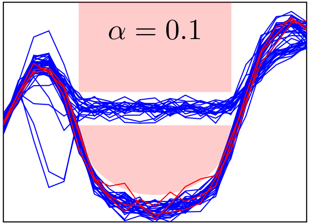
Kernel Approach ($\alpha = 0.6$)



Conclusion

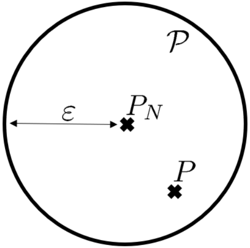
Summary:

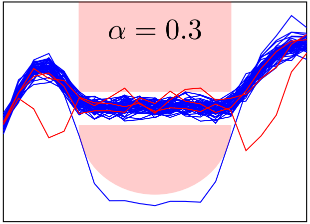
- Sampling from unknown system with particle Gibbs
- Ambiguity set around empirical distribution
- Optimization over ambuiguity set for robust solution



Kernel Embeddings allow for ...

- solving chance-constrained OCPs
- Choosing risk factor α





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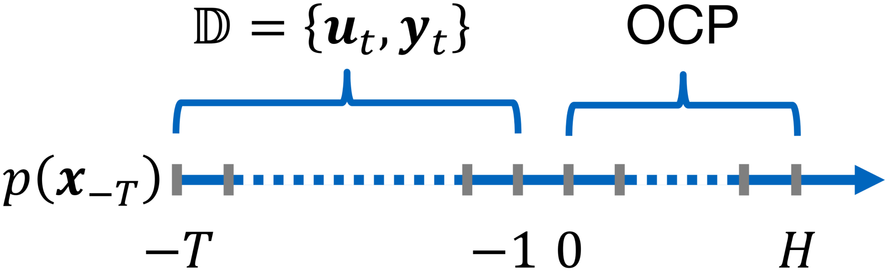
Timeline



$\mathbb{D} = \{\boldsymbol{u}_t, \boldsymbol{y}_t\}$
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 $\{\boldsymbol{\theta}, \boldsymbol{x}_{-T:-1}\}^{[n]}$ from $p\left(\boldsymbol{\theta}, \boldsymbol{x}_{-T:-1} \mid \mathbb{D}\right)$ 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 $t = -1, ..., H$
3. Set $\boldsymbol{x}_0^{[n]} = \boldsymbol{f}_{\boldsymbol{\theta}^{[n]}}\left(\boldsymbol{x}_{-1}^{[n]}, \boldsymbol{u}_{-1}\right) + \boldsymbol{v}_{-1}^{[n]}$

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 $\{1, \ldots N\}$ 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. $\quad \mathrm{MMD}[m] \leftarrow \frac{1}{N^2}\left(K_x + K_y - 2K_{xy}\right)$
6. **End For**
7. MMD $\leftarrow$ *sort*(MMD)
8. $\varepsilon \leftarrow \mathrm{MMD}[$*ceil*$(B\beta)]$

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

$B = 1000, \beta = 0.95$

Maximum Mean Discrepancy (MMD)

Maximum Mean Discrepancy

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

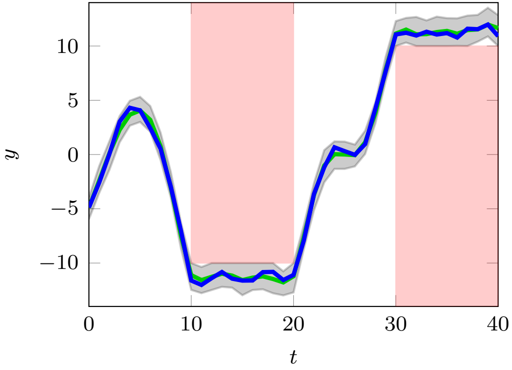
(Biased) MMD estimator

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

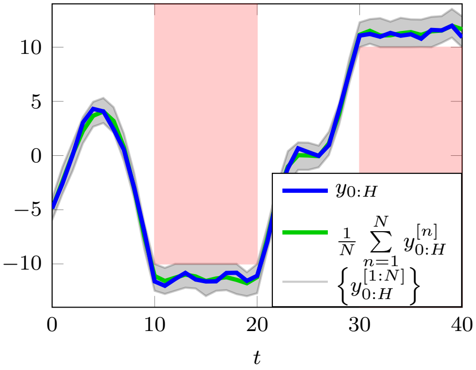
Optimal Control with Constrained Outputs

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

Scenario Approach



Kernel Approach ($\alpha = 0.01$)



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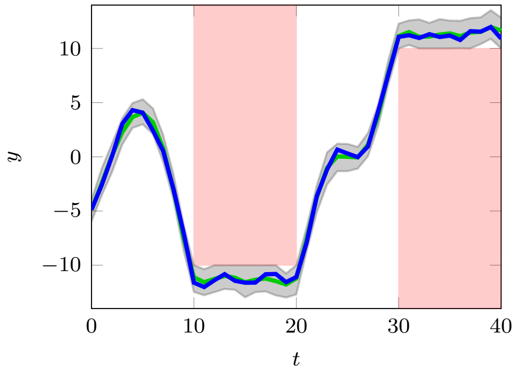
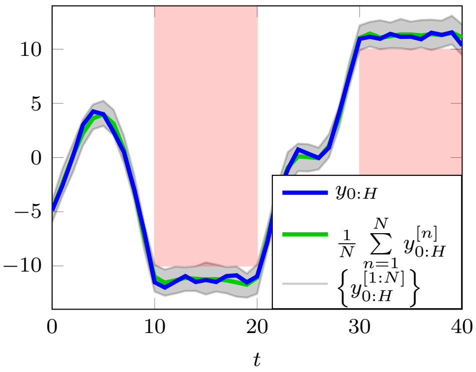


Kernel Approach ($\alpha = 0.2$)



Optimal Control with Constrained Outputs

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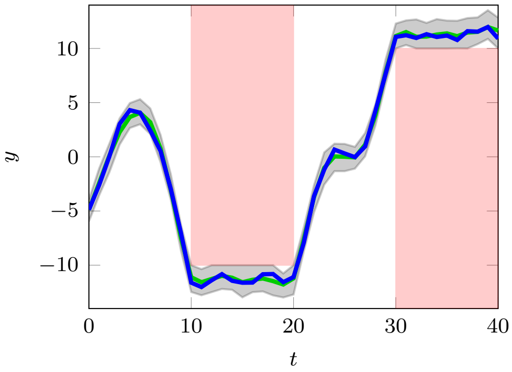
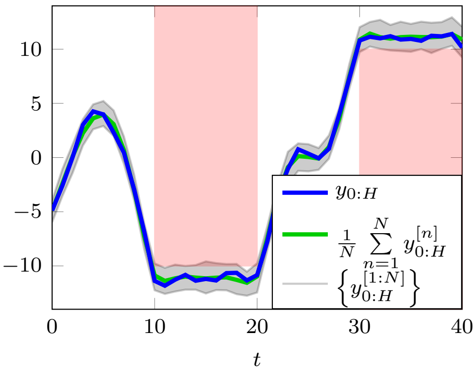
Scenario Approach

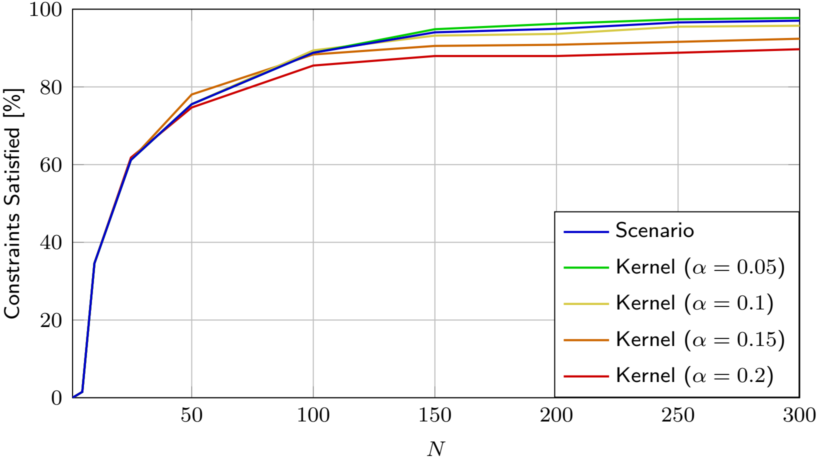


Kernel Approach ($\alpha = 0.5$)



Successrate of Solution

$N' = 2000$ scenarios used to test $u_{0:H}$



Empirical Distribution

Given: Samples $z_i, i = 1, ..., N$

Empirical Distribution

$$P_N(z) = \frac{1}{N}\sum_{i=1}^{N} \mathrm{dirac}(z - z_i)$$