

Kernel Embedding for Particle Gibbs-Based Optimal Control

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Report Master's Thesis

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Motivation



[Xiloyannis, Chiaradia, Frisoli and Masia 2019]

Challenges:

- Unknown dynamics
- Latent states
- Safety

Problem Statement - System

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

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

Assumptions

- Known system structure

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

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

Problem Statement - Optimal Control Problem

Goal: Solve optimal control problem (OCP)

Stochastic OCP

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

subject to:

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

Problem: Underlying data distribution P is unknown

Related Works

Particle Gibbs based optimal control via scenario theory [Lefringhausen, Srithasan, Lederer and Hirche 2024]

⇒ Guarantees determined retroactively

Alternative Approaches:

- Wasserstein ambiguity [Hota, Cherukuri and Lygeros 2019]

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

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

Chance Constraints

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



Scenario Approach (used in [Lefringhausen+ 2024])

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

⇒ Risk factor α not considered in optimization

Maximum Mean Discrepancy (MMD) ambiguity sets

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

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

MMD ambiguity set

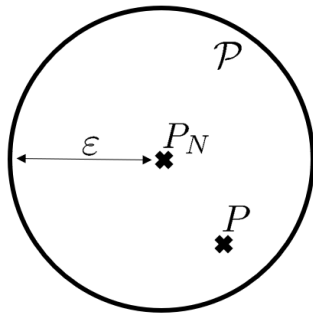
$$\mathcal{P} = \left\{ \tilde{P} : \text{MMD}(\tilde{P}, P_N) \leq \varepsilon \right\}.$$



Expanded Chance-Constraints

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

with $\tilde{h}(\mathbf{u}_{0:H}, \boldsymbol{\delta}) = \max(\mathbf{h}(\mathbf{u}_{0:H}, \mathbf{x}_{0:H}, \mathbf{y}_{0:H}))$.



Constraint Reformulation

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

Feasible Region of chance constraint

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



Reformulated Feasible Region [Nemmour+ 2022]

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

Kernel Approximation

Problem Formulation

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

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

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

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

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

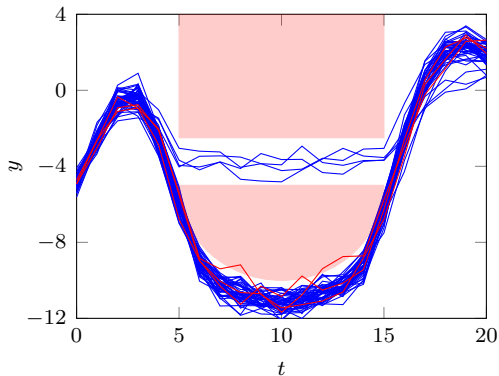
Simulation Setup

- Unknown system:
$$\mathbf{f}(\mathbf{x}, u) = \begin{bmatrix} 0.8x_1 - 0.5x_2 \\ 0.4x_1 + 0.5x_2 + u \end{bmatrix}$$
$$\mathbf{v}_t \sim \mathcal{N}\left(\mathbf{0}, \mathbf{Q} = \begin{bmatrix} 0.03 & -0.004 \\ -0.004 & 0.01 \end{bmatrix}\right).$$
- Known system structure: $\mathbf{f}(\mathbf{x}, u) = \mathbf{A} [x_1, x_2, u]^\top + \mathbf{v}_t, \mathbf{v}_t \sim \mathcal{N}(\mathbf{0}, \mathbf{Q})$
- Priors:
$$\mathbf{Q} \sim \mathcal{IW}(100\mathbf{I}_2, 10)$$
$$\mathbf{A} \sim \mathcal{MN}(\mathbf{0}, \mathbf{Q}, 10\mathbf{I}_2) \quad [\text{Andrieu+ 2017}]$$
$$\mathbf{x}_{-T} \sim \mathcal{N}([2, 2]^\top, \mathbf{I}_2)$$
- Known measurement model $g(\mathbf{x}, u) = x_1, w_t \sim \mathcal{N}(0, 0.1)$
- 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].

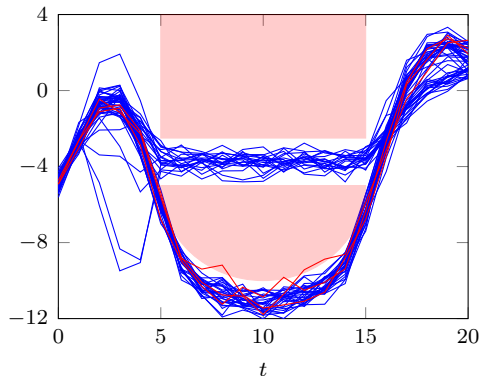
Corridor Test

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

Scenario Approach



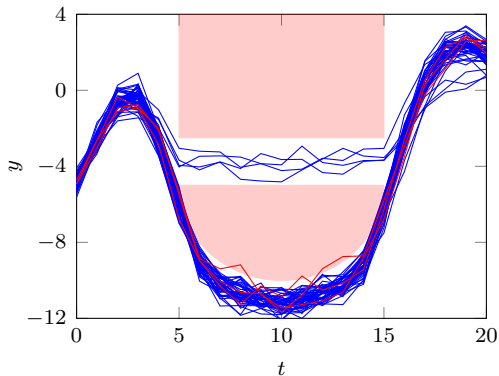
Kernel Approach ($\alpha = 0.1$)



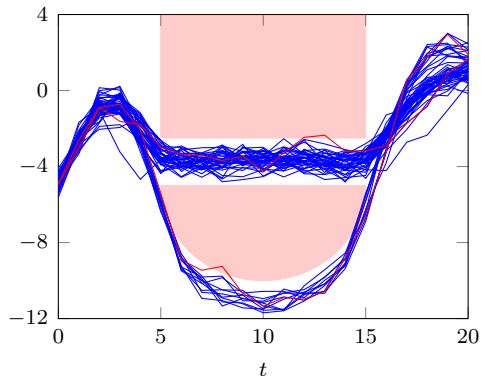
Corridor Test

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Scenario Approach



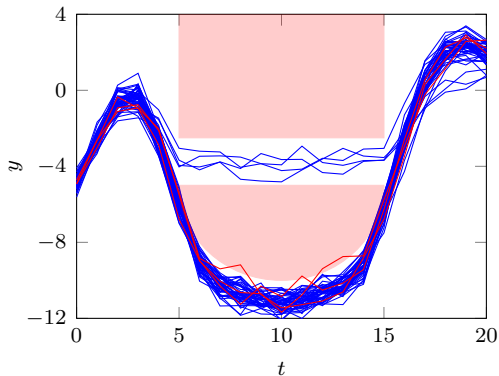
Kernel Approach ($\alpha = 0.2$)



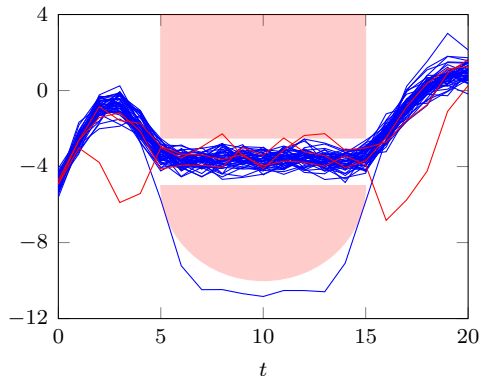
Corridor Test

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

Scenario Approach



Kernel Approach ($\alpha = 0.3$)



Corridor Test

Approach	Scenario	Kernel		
		$\alpha = 10\%$	$\alpha = 20\%$	$\alpha = 30\%$
J_H (mean)	338.4	255.9	129.5	69.9
Risky Runs	8%	40%	78%	98%
Failed Runs	6%	6%	4%	6%

Nonlinear System

Linear System (used in previous simulations)

$$\mathbf{f}(\mathbf{x}, u) = \begin{bmatrix} 0.8x_1 - 0.5x_2 \\ 0.4x_1 + 0.5x_2 + u \end{bmatrix}$$



Nonlinear System

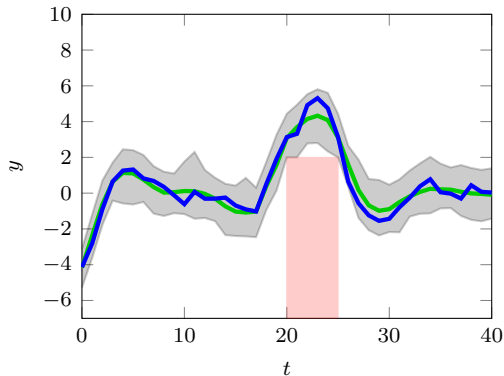
$$\mathbf{f}(\mathbf{x}, u) = \begin{bmatrix} 0.8x_1 - 0.5x_2 + 0.1\cos(3x_1)x_2 \\ 0.4x_1 + 0.5x_2 + (1 + 0.3\sin(2x_2))u \end{bmatrix}$$

- Known system structure: $\mathbf{f}(\mathbf{x}, u) = \mathbf{A} [x_1, x_2, u, \cos(3x_1)x_2, \sin(2x_2)u]^T + \mathbf{v}_t$
- Input constraints $|u| \leq 5$

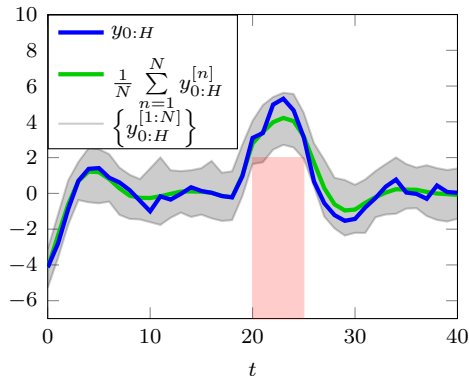
Optimal Control of Nonlinear Systems

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

Scenario Approach



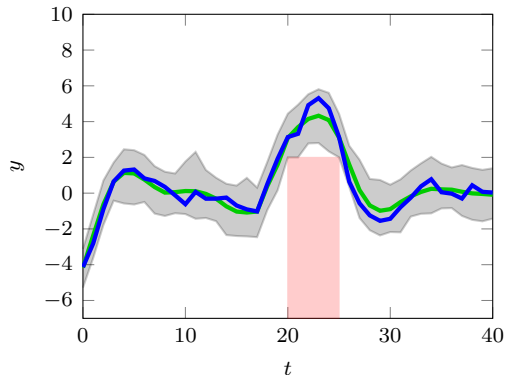
Kernel Approach ($\alpha = 0.2$)



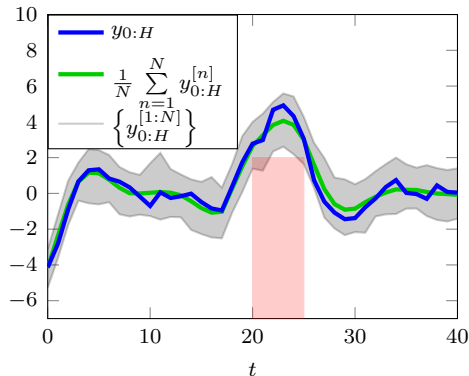
Optimal Control of Nonlinear Systems

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

Scenario Approach



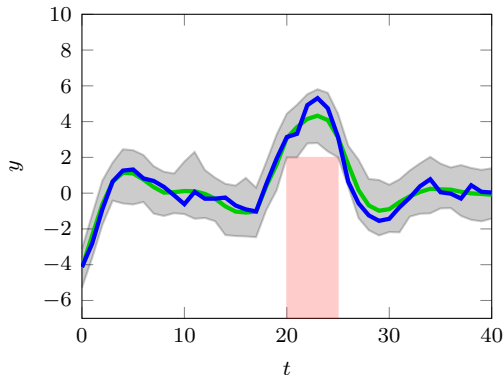
Kernel Approach ($\alpha = 0.4$)



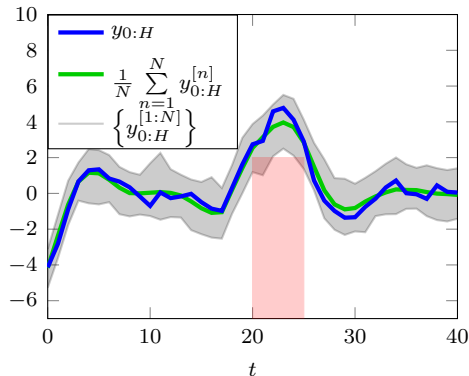
Optimal Control of Nonlinear Systems

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

Scenario Approach



Kernel Approach ($\alpha = 0.6$)



Limitations

Solver unreliable for kernel approach with nonlinear systems

Impossible to solve OCPs with ...

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

Approach	Scenario	Kernel		
		$\alpha = 20\%$	$\alpha = 40\%$	$\alpha = 60\%$
Computation time	32.8s	176.1s	50.9s	41.0s

Conclusion

Summary: Kernel Embeddings allow for ...

- solving chance-constrained OCPs
- Choosing risk factor α

Future Plans:

- Use kernel embeddings on non-linear systems
- Parameter tuning of σ
- Alternative approach of reformulating chance constraints

References



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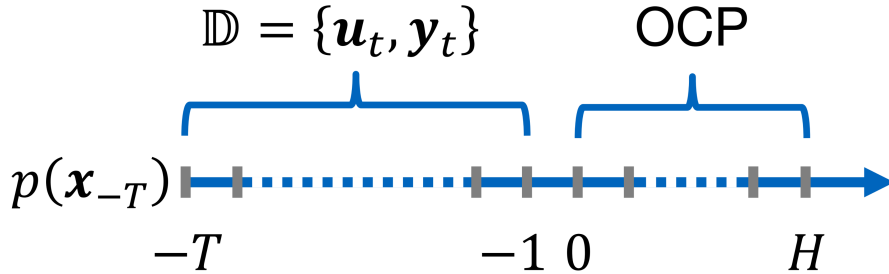


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Timeline



Scenario Generation

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

Algorithm: Scenario Generation

For $n = 1, \dots, N$:

1. Sample $\{\theta, x_{-T:-1}\}^{[n]}$ from $p(\theta, x_{-T:-1} \mid \mathbb{D})$ using PMCMC [Lefringhausen+ 2024].
2. Sample $v_t^{[n]}$ from $\mathcal{V}_{\theta^{[n]}}$ and $w_t^{[n]}$ from $\mathcal{W}_{\theta^{[n]}}$ for $t = -1, \dots, H$
3. Set $x_0^{[n]} = f_{\theta^{[n]}}(x_{-1}^{[n]}, u_{-1}) + v_{-1}^{[n]}$

Output: Scenarios $\delta^{[1:N]} = \{\theta, x_0, v_{0:H}, w_{0:H}\}^{[1:N]}$

Bootstrap Construction

Algorithm: Bootstrap MMD ambiguity set

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

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

$$B = 1000, \beta = 0.95$$

Maximum Mean Discrepancy (MMD)

Maximum Mean Discrepancy

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

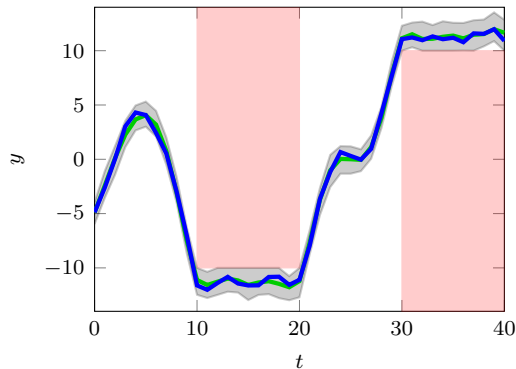
(Biased) MMD estimator

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

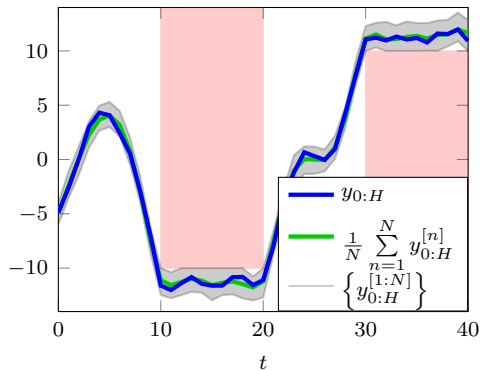
Optimal Control with Constrained Outputs

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

Scenario Approach



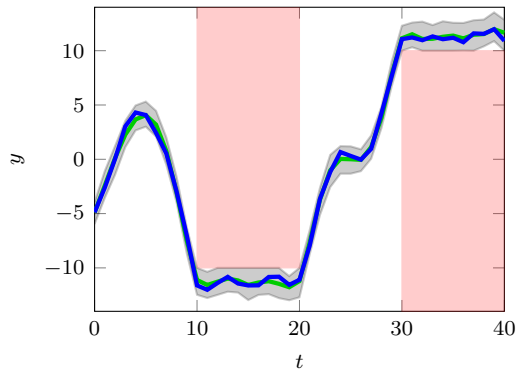
Kernel Approach ($\alpha = 0.01$)



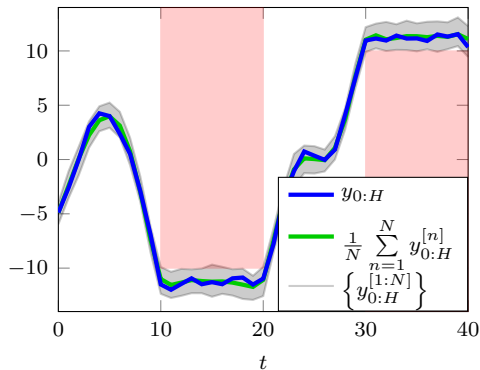
Optimal Control with Constrained Outputs

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

Scenario Approach



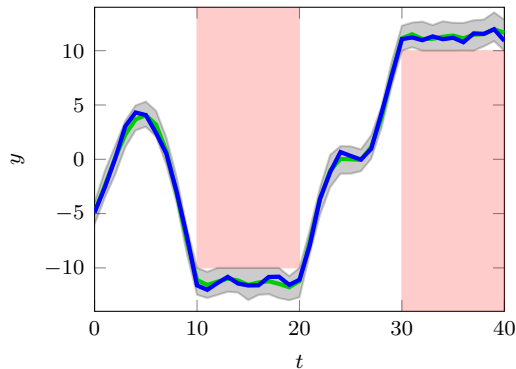
Kernel Approach ($\alpha = 0.2$)



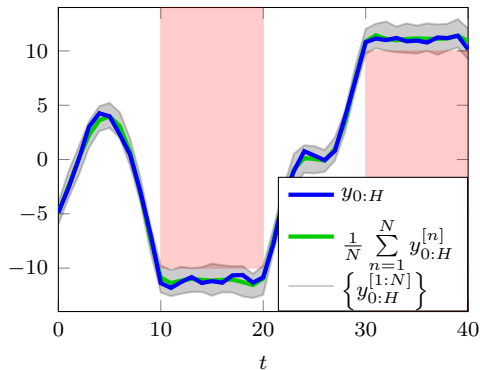
Optimal Control with Constrained Outputs

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

Scenario Approach



Kernel Approach ($\alpha = 0.5$)



Successrate of Solution

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

