On the Use of Nonlinear Moving-Horizon Observers in Batch Terpolymerization Processes with Partially Modelled Dynamics.

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Outline

Observability related definitions

Uncertainty & noise free system

$$\begin{aligned} x(t) &= X(t, t_0, x_0) \\ y(t) &= h(t, x(t)) \end{aligned}$$

Uncertain and noisy system

$$\begin{aligned} x(t) &= X(t, t_0, x_0, w_{t_0}^{t}) \\ y(t) &= h(t, x(t)) + v(t) \end{aligned}$$

Constraints

- $x(t) \in \mathbb{X}(t) \subset \mathbb{R}^n$
- $w(t) \in \mathbb{W}(t) \subset \mathbb{R}^{n_w}$ uncertainties/Disturbances.
- $v(t) \in \mathbb{V}(t) \subset \mathbb{R}^{n_y}$ measurement noise

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Alamir et al. (Nolcos 2007)

Measurements-compatible configurations

Consider

- Time interval $[t - T, t]$
- Measurement profile y_{t-T}^{t}
- $(\xi, \mathbf{w}) \in \mathbb{X}(t - T) \times [\mathbb{R}^{n_w}]^{[t-T,t]}$

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$(\xi,\mathbf{w})$ is (y_{t-T}^{t})-compatible
if for all $\sigma \in [t-T,t]$:

1. $w(\sigma) \in \mathbb{W}(\sigma)$,
2. $X(\sigma,t-T,\xi,\mathbf{w}) \in \mathbb{X}(\sigma)$,
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Notation

$$(\xi, \mathbf{w}) \in \mathbb{C}(t, y_{t-T}^{t})$$

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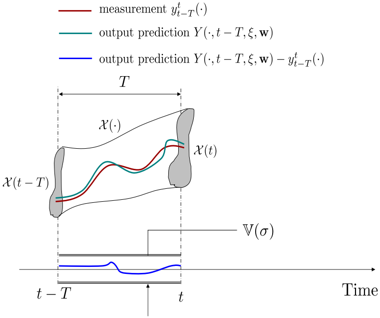

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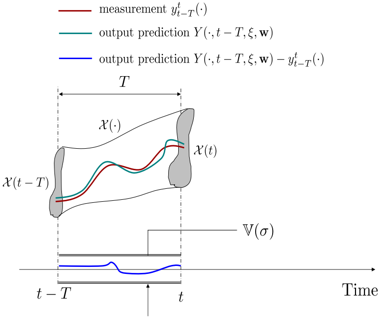

$(\xi, \mathbf{w}) \in \mathbb{C}(t, y_{t-T}^{t})$ if the corresponding trajectory

1. meets the constraints
2. explains the measurements

The finite horizon observation problem

The finite horizon observation problem

Choose $T > 0$ and use at each t, the available information:

1. the system equations
2. the past measurements y_{t-T}^{t},
3. the constraints and
4. *some additional exogenous knowledge*.

in order to produce an estimation $\hat{x}(t)$ of the current state $x(t)$. ♡

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Find $(\xi, \mathbf{w}) \quad \longrightarrow \quad \hat{x}(t) = X(t, t-T, \xi, \mathbf{w})$

The set of candidate estimates $\hat{x}(t)$:

$$\Omega_t = \left\{ X(t, t-T, \xi, \mathbf{w}) \quad | \quad (\xi, \mathbf{w}) \in \mathbb{C}(t, y_{t-T}^{t}) \right\}.$$

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Temporal parametrization

Solve $P(t) \quad : \quad \min_{(\xi,\mathbf{w})\in\mathbb{C}(t)} J(t,\xi,\mathbf{w})$

Use a reduced dimensional parametrization

$$w(t) = \mathcal{W}(t, p_w) \quad ; \quad p_w \in \mathbb{P}.$$

Solve $P(t) \quad : \quad \min_{(\xi,p_w)\in\mathbb{C}(t)} J(t,\xi,\mathcal{W}(\cdot,p_w)) =: J(t,\xi,p_w) \quad \longrightarrow (\hat{\xi}(t), \hat{p}_w(t))$

$$\hat{x}(t) = X(t, t-T, \hat{\xi}(t), \mathcal{W}(\cdot, \hat{p}_w(t)))$$

- $\bar{x} := (x^T, p_w^T)^T \in \mathbb{R}^n \times \mathbb{R}^{n_p}$
- $\dot{p}_w = 0$

New uncertainty-free
extended state estimation problem.

Analytic vs optimization based observer

Analytic observers

$$\text{(System)} \quad \dot{x} = f(x) \ ; \ y = h(x)$$
$$\text{(Observ)} \quad \dot{\hat{x}} = f(\hat{x}) + K(\hat{x}, y)$$

Try to show asymptotic convergence of $e = x - \hat{x}$ governed by

$$\begin{aligned} \dot{x} &= f(x) \\ \dot{e} &= f(x) - f(x-e) - K(x-e, h(x)) \end{aligned}$$

Very Hard Task

- Need for structural properties
- Coordinate transformation
- Constructive assumptions
- Observability $\neq$ Existence of observer

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optimization based observers

Rely on the implication

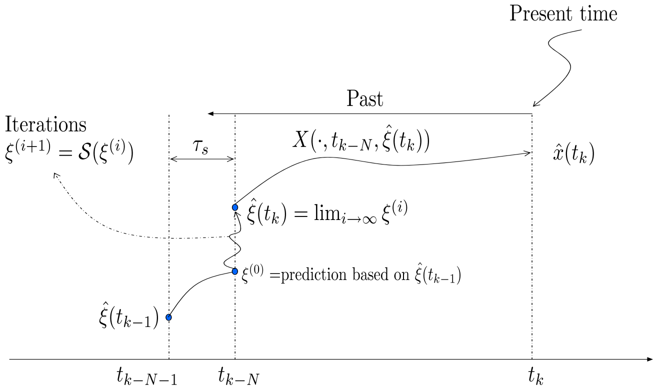
$$\left\{J(t,\xi) \to 0\right\} \Rightarrow \left\{\underbrace{X(t, t-T, \xi)}_{\hat{x}(t)} \to x(t)\right\}$$

+ No need to study e
+ No need for structural assumptions
+ Observability $\Leftrightarrow$ Observer
+ Handling constraints on the state

Potential problems

- Global convergence ?
- Computation time ?

The discrete-time estimation scheme



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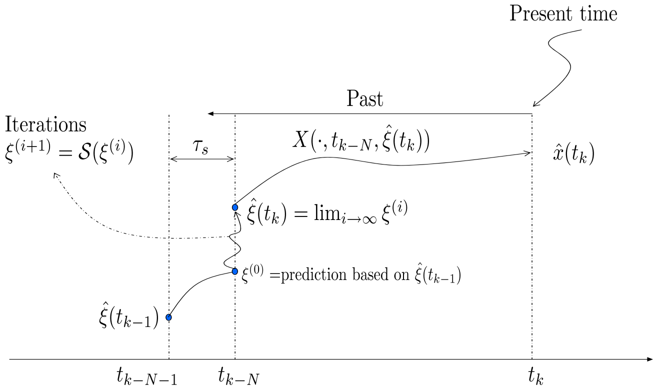

$$\hat{x}(t_k) = X(t_k, t_{k-N}, \hat{\xi}(t_k))$$

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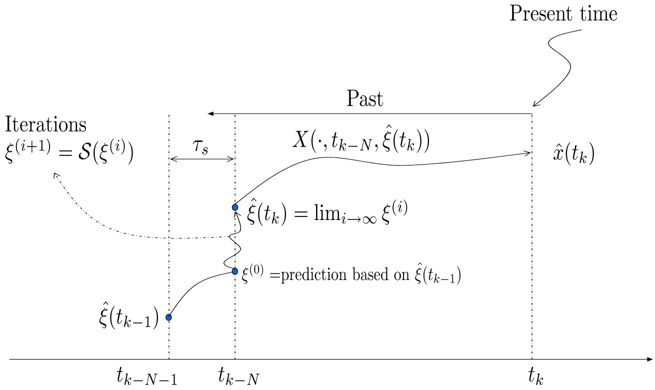

$$\hat{\xi}(t_k) = arg \min_{\xi \in \mathbb{X}(t_{k-N})} \left[J(t_k, \xi) \right] := \sum_{i=k-N}^{k} \| y(t_i) - Y(t_i, t_{k-N}, \xi) \|_{Q_i(k)}^{\;2}$$

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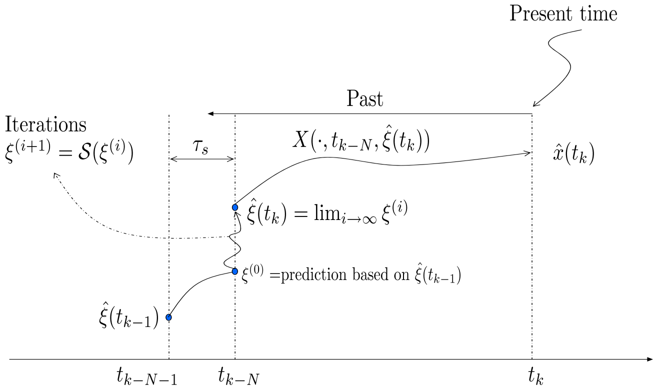

$$\xi^{(0)} = X(t_{k-N}, t_{k-N-1}, \hat{\xi}(t_{k-1}))$$

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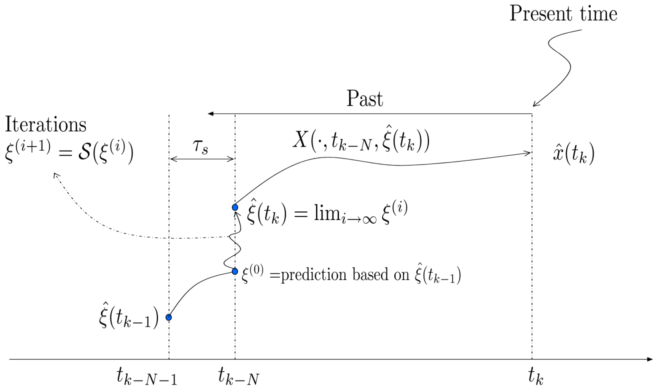

In practice: $\hat{\xi}(t_k) = \xi^{(N_{max})} = \mathcal{S}^{N_{max}}(\xi^{(0)}, t_k, y_{t_{k-N}}^{t_k})$

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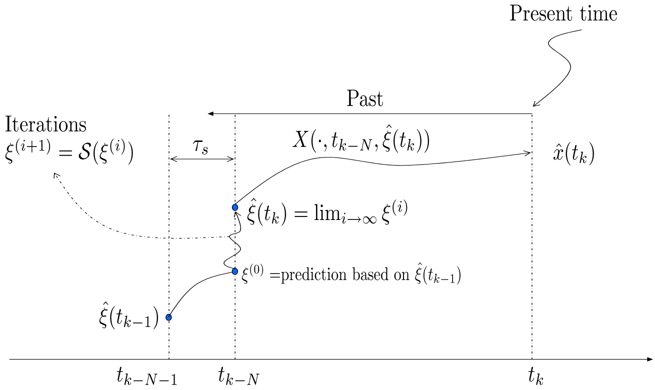

In practice: $\hat{\xi}(t_k) = \xi^{(N_{max})} = \bar{\mathcal{S}}^{N_{max}}(\hat{\xi}(t_{k-1}), t_k, y_{t_{k-N}}^{t_k})$

State estimation is a very particular optimization problem

Particular feature of the state estimation related optimization problem

$x(t_{k-N})$ is the unique global minimum of ALL the optimization problems:

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that may be obtained by changing the positive definite weighting matrices $Q_i(k)$.

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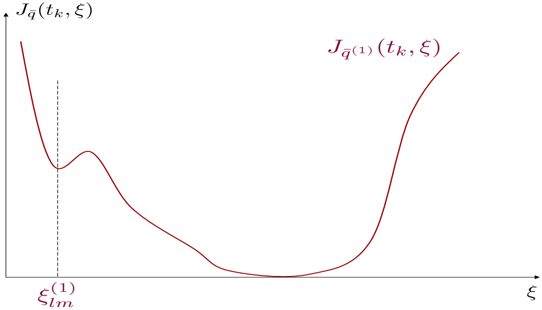
Let us take the following family subset of weighting choices:

$$Q_i(k) = \gamma^{k-i} \cdot q_i \cdot \mathbb{I}_{n_y} \quad \text{s.t} \quad q_i > 0 \quad \text{and} \quad \sum_i q_i = 1 \tag{1}$$

- $\gamma \in]0, 1]$ Forgetting factor
- $\mathbb{I}_{n_y}$ identity matrix in $\mathbb{R}^{n_y \times n_y}$
- Notations: $\bar{q} = \big(q_1, q_2, \ldots, q_N\big)^T$, $J_{\bar{q}}(t_k, \xi)$, $\mathcal{S}_{\bar{q}}^{N_{max}}(\xi^{(0)}, t_k, y_{t_{k-N}}^{t_k})$

Crossing singularity by swapping the weighting vectors



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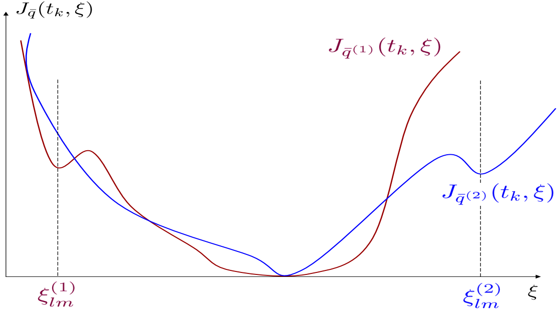

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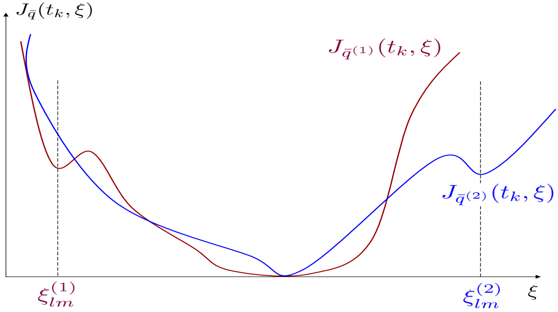

- Generally, $J_{\bar{q}^{(1)}}(t_k, \cdot)$ and $J_{\bar{q}^{(2)}}(t_k, \cdot)$ have *no reasons to share the same* LOCAL *minima*

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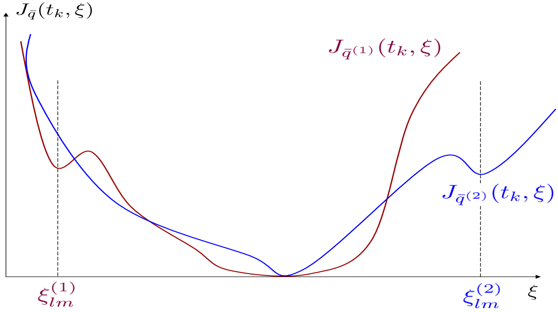

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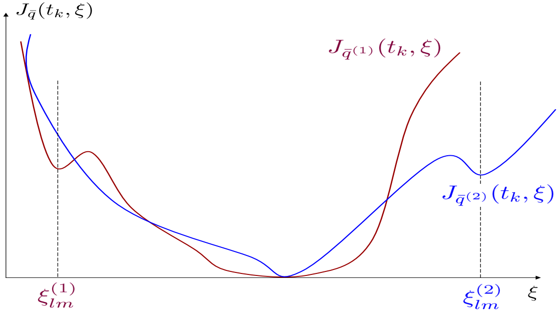

- Generally, $J_{\bar{q}^{(1)}}(t_k, \cdot)$ and $J_{\bar{q}^{(2)}}(t_k, \cdot)$ have *no reasons to share the same* LOCAL *minima*
- They DO share the same global minimum $x(t_{k-N})$
- Think about an infinite number of $J_{\bar{q}}(t_k, \cdot)$ (randomly generated)

This suggests

The crossing singularities heuristic

$$\bar{q} \leftarrow \frac{1}{n_y}\begin{pmatrix}1 & 1 & \dots & 1\end{pmatrix}$$

$$\hat{\xi}(t_k) \leftarrow X(t_{k-N}, t_{k-N-1}, \hat{\xi}(t_{k-1}))$$

for $(i = 1 : N_{\text{trials}})$

$$\hat{\xi}(t_k) \leftarrow \mathcal{S}_{\bar{q}}^{N_{max}}(\hat{\xi}(t_k), t_k, y_{t_{k-N}}^{t_k})$$

Generate randomly new admissible $\bar{q}$

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- This is not a multiple initial guess trials
- Implementation constraint

$$N_{trial} \times N_{max} \times \tau_{iter} \leq \tau_s$$

- The Trade-off is problem dependent

Application: State estimation of terpolymerization reactors

- Produce polymer from multi-monomer
- Controlling the final properties need the state to be estimated
- State: Polymer composition ↔ Monomers concetrations
- Complex equations
- Unknown dynamics
- High gain observers need tremendous simplifications to give rather poor performance

Terpolymerization reactors: The mathematical model

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in which

$$\begin{aligned} \alpha &= [M_1^P](k_{p21}k_{p31}[M_1^P] + k_{p21}k_{p32}[M_2^P] + k_{p31}k_{p23}[M_3^P]) \\ \beta &= [M_2^P](k_{p12}k_{p31}[M_1^P] + k_{p12}k_{p32}[M_2^P] + k_{p13}k_{p32}[M_3^P]) \\ \gamma &= [M_3^P](k_{p13}k_{p21}[M_1^P] + k_{p21}k_{p23}[M_2^P] + k_{p13}k_{p23}[M_3^P]) \end{aligned}$$

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The $[M_i^P]$ depend in the state according to:

$$[M_i^P] = \begin{cases} \dfrac{(1-\phi_p^p)N_i}{\sum_j \dfrac{N_j MW_j}{\rho_j}}, & \text{(Phase II)} \\ \dfrac{N_i}{\sum_j MW_j(\dfrac{N_j^T - N_j}{\rho_{j,h}} + \dfrac{N_j}{\rho_j})} & \text{(Phase III)} \end{cases}$$

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- Measurement

The overall monomer conversion measured by calorimetry:

$$y = \frac{\sum_{i=1}^{3} MW_i(N_i^T - N_i)}{\sum_{j=1}^{3} MW_j N_j^T}$$

Validation Results

1. Simulation results
2. Experimental results

Simulation results

$$\begin{aligned} \dot{N} &= \begin{pmatrix} 1+d_1 & 0 & 0 \\ 0 & 1+d_2 & 0 \\ 0 & 0 & 1+d_3 \end{pmatrix} \cdot f(x,u) \\ \dot{\mu} &= 0 \\ y &= (1+\nu)\cdot h(x) \end{aligned}$$

- The state

$$x := \begin{pmatrix} N_1 & N_2 & N_3 & \mu \end{pmatrix} \in \mathbb{R}_+^4$$

- The uncertainties

$$\begin{aligned} d_i(k) &= d_{max} \cdot r_i(k) \\ \nu(k) &= \nu_{max} \cdot r_\nu(k) \end{aligned}$$

- r_i and ν randomly chosen in $[-1,+1]$

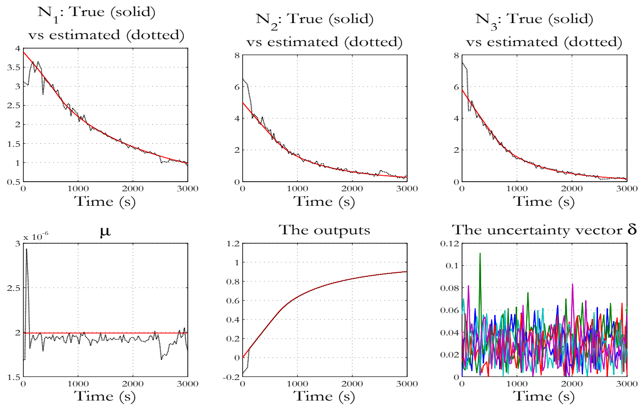


Figure: *Observer behavior under model uncertainty given by (2)-(2) with* $d_{max} = 10\%$ *and no measurement noise* ($\nu_{max} = 0$)*. The observation horizon is* $N = 10$ *and the number of trials for the singularity crossing scheme is* $N_{\text{trials}} = 4$*. Initial state of the observer is* $\hat{x}(0) = diag(0.8, 1.3, 1.3) \cdot x(0)$ *and* $\mu_{obs}(0) = 0.8\mu_{model}$*.*

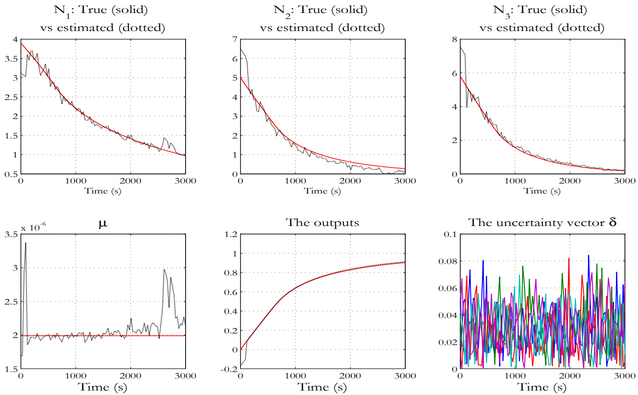


Figure: *Observer behavior under model uncertainty given by (2)-(2) with $d_{max} = 10\%$ and in the presence of measurement noise ($\nu_{max} = 0.01$). The observation horizon is $N = 15$ and the number of trials for the singularity crossing scheme is $N_{\text{trials}} = 4$. $\mu_{obs}(0) = 0.8\mu_{model}$. Note that concerning the output, only the true output and the estimated one are shown, measurement noise is not presented. This scenario uses a tolerance $\varepsilon = 10^{-8}$ for the optimization subroutine.*

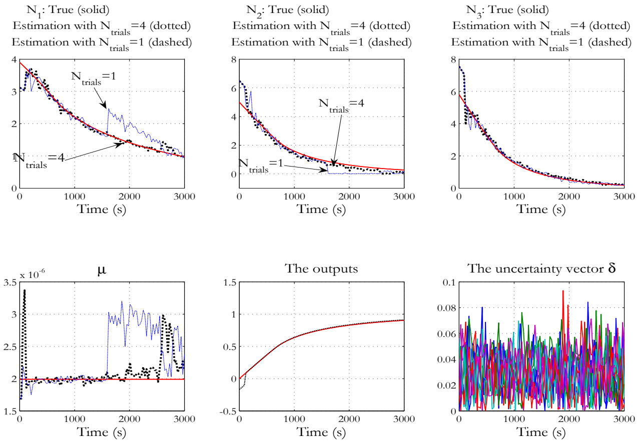


Figure: *Comparison between the observer behavior when $N_{trials} = 1$ and $N_{trials} = 4$ under the scenario depicted on figure ??. Note how the singularity cross mechanism enables to avoid drops in the estimation quality when the observer encounters a singular situation. This scenario uses a tolerance $\varepsilon = 10^{-8}$ for the optimization subroutine.*

Experimental results

Parameter	Value	Unit
ϕ_p^p	0.4	
MW_1	128.2	(g/mol)
MW_2	100.12	(g/mol)
MW_3	86.09	(g/mol)
ρ_1	0.89	(g/cm^3)
ρ_2	0.94	(g/cm^3)
ρ_3	0.93	(g/cm^3)
$\rho_{1,h}$	1.08	(g/cm^3)
$\rho_{2,h}$	1.15	(g/cm^3)
$\rho_{3,h}$	1.17	(g/cm^3)
k_{p11}	4.5×10^5	$(cm^3/mol/s)$
k_{p22}	1.28×10^6	$(cm^3/mol/s)$
k_{p33}	4.26×10^6	$(cm^3/mol/s)$
r_{12}	0.355	
r_{21}	1.98	
r_{13}	6.635	
r_{31}	0.037	
r_{23}	22.21	
r_{32}	0.07	

Table: Parameter values of the terpolymerization of BuA/MMA/VAc (used in the experimental validation)

Component	Charge (g)
Butyl acrylate	300
Methyl methacrylate	300
Vinyl acetate	60
Sodium dioctyl sulfosuccinate	3
Potassium persulfate	2
Water	2380

Table: Recipe of the terpolymerization of BuA/MMA/VAc

Experimental results: $N_{trials} = 10$

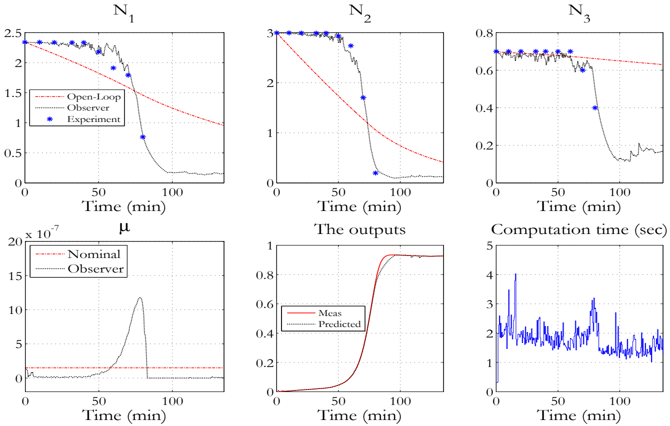


Figure: *Experimental validation with $N_{trials} = 10$ and tolerance threshold $\varepsilon = 10^{-3}$. The same scenario is depicted on figure 5 where $N_{trials} = 1$ is used. The computation time is given in seconds.*

Experimental results: $N_{trials} = 1$

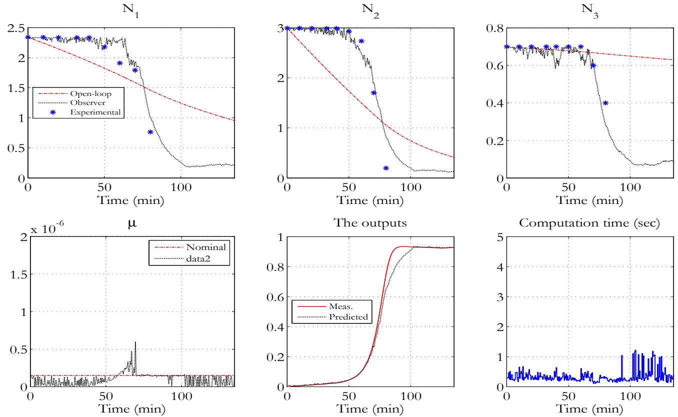


Figure: *Experimental validation with $N_{trials} = 1$ and tolerance threshold $\varepsilon = 10^{-3}$. The same scenario is depicted on figure 4 where $N_{trials} = 10$ is used. The computation time is given in seconds.*

Conclusion & Future work

Conclusion

- Moving-Horizon Observers is a suitable choice to handle
  - Nonlinearity
  - Complex (uncertain) dynamics
- The associated optimization problem is VERY PARTICULAR
- This enables a dedicated singularity avoidance heuristics

Future work

- Quality control by output feedback of terpolymerization processes
- More extensive (statistical) study of the singularity avoidance heuristic's efficiency

Example of a selection index

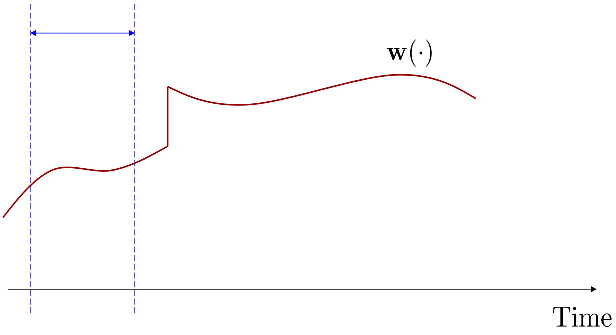
$$J(t,\xi,\mathbf{w}) := \Gamma(t,\xi-\xi^*(t)) + \int_{t-T}^{t} L\Big(\mathbf{w}(\sigma),\varepsilon_y(\sigma)\Big)$$

- $\varepsilon_y(\sigma) = y_{t-T}^{t}(\sigma) - Y(\sigma, t-T, \xi, \mathbf{w})$ output prediction error
- $\xi^*(t)$ condenses the past knowledge.
- For Kalman filter

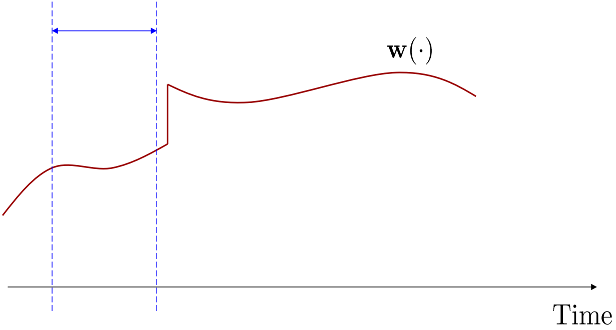
$$L(w,\varepsilon_y) = w^T Q^{-1} w + \varepsilon_y^T R^{-1} \varepsilon_y$$

$\xi^*(t)$ Induced by the past estimate (discrete KF)

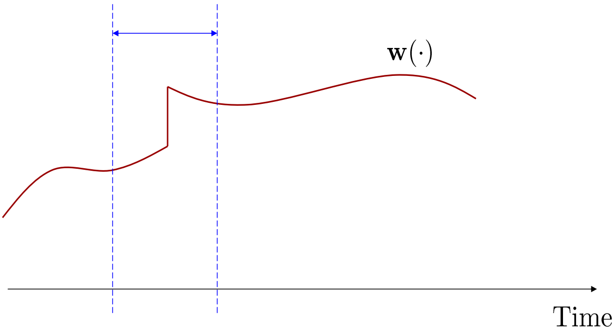
Handling abrupt behavior of uncertainties



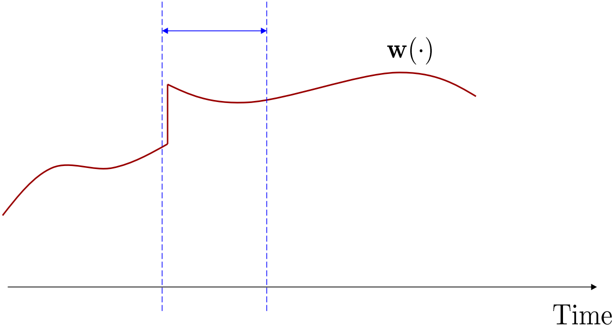
Handling abrupt behavior of uncertainties



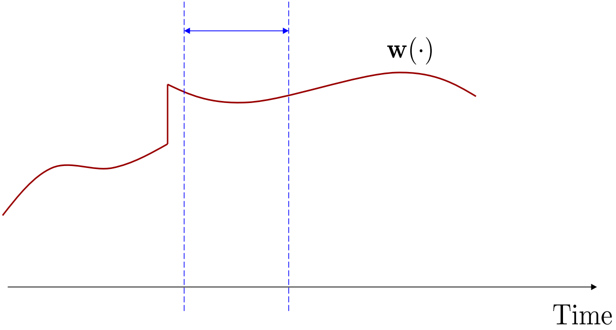
Handling abrupt behavior of uncertainties



Handling abrupt behavior of uncertainties

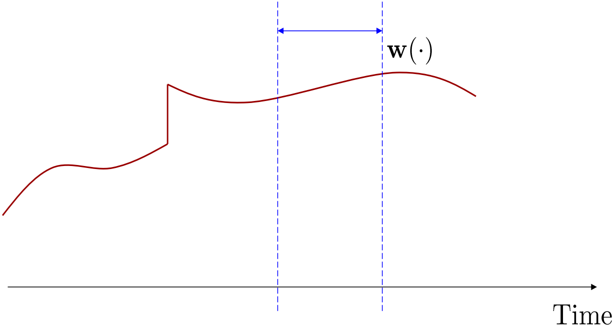


Handling abrupt behavior of uncertainties

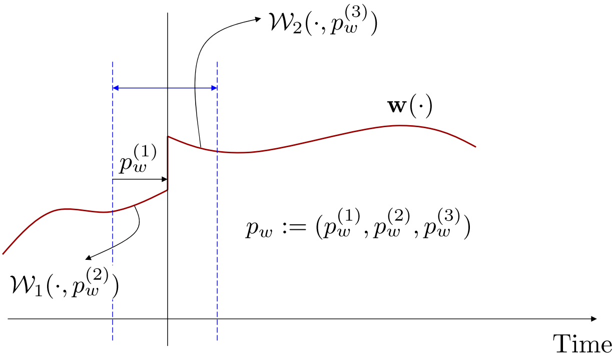


Alamir et al. (Nolcos 2007)

Handling abrupt behavior of uncertainties



Non smooth behaviors can be parametrized



$$\mathcal{W}(\cdot, p_w) := \begin{cases} \mathcal{W}_1(\tau, p_w^{(2)}) & \text{if } \tau \leq p_w^{(1)} \\ \mathcal{W}_2(\tau, p_w^{(3)}) & \text{otherwise} \end{cases}$$

Definition of the phase II: Existence of monomer droplets

$$N_1\delta_1 + N_2\delta_2 + N_3\delta_3 - \frac{(1-\phi_p^p)}{\phi_p^p}\sigma > 0 \tag{2}$$

where

$$\delta_i = MWi(\frac{1}{\rho_i} + \frac{(1-\phi_p^p)}{\rho_{i,h}\phi_p^p}) \ , \quad i = 1, 2, 3 \tag{3}$$

and

$$\sigma = \sum_{j=1}^{3} \frac{MW_j N_j^T}{\rho_j, h} \tag{4}$$

Example of dynamic evolution of μ