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Moving Horizon Estimator Design for a Nonlinear Diffusion-Reaction System with Sensor Dynamics ⋆

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Abstract: Moving horizon estimation (MHE) is applied to estimate the spatial-temporal evolution of the state of nonlinear diffusion-reaction system with linear sensor dynamics. A late-lumping approach is introduced, which exploits directly the partial differential equation (PDE) and the ordinary differential equation (ODE) of the sensor dynamics to solve the optimal estimation problem. This leads to the determination of an adjoint PDE-ODE system, whose solution yields a gradient that is used for the implementation of a line search approach to achieve fast convergence to the minimum of the cost functional. The initial state of the MHE herein serves as decision variable and is determined on a receding horizon. Simulation results for in-domain measurement illustrate the performance of the approach.

Keywords: Moving horizon estimation, late-lumping, sensor dynamics, optimal estimation.

1. INTRODUCTION

The aim of the moving horizon estimation approach is to estimate the state trajectory from only the measurement of the output by using dynamic optimization on fixed-size time horizons Muske et al. (1993); Robertson et al. (1996); Kühl et al. (2011); Rawlings (2013). Subsequently moving horizon estimation is applied to a distributed parameter system governed by a nonlinear diffusion-reaction equation with in-domain, locally averaged measurement subject to additive noise. The sensor dynamics is explicitly included in terms of a linear ordinary differential equation (ODE). Such a dynamical formulation becomes relevant in applications, where the sensor dynamics and the process dynamics evolve approximately on the same time scale or when the sensor rise time has implications for the estimator performance.

Partial differential equations (PDEs) are widely used to model systems with high dynamic complexity, e.g., in chemical engineering Jensen and Ray (1982), mechatronics Preumont (1997); Meurer (2013a), heating-cooling processes Moura et al. (2013); Schaum et al. (2018) or formation control for multi-agent systems Frihauf and Krstic (2010); Freudenthaler and Meurer (2019). Herein, the complete knowledge of the spatial-temporal state of the system is needed to address feedback stabilization and closed-loop (optimal) control.

Observers are designed for PDE systems by making use of early- or late-lumping. For early-lumping the problem is discretized / approximated first to obtain a set of ODEs so that established finite-dimensional techniques can be applied. This approach has already been successfully introduced and applied to design moving horizon estimators (MHEs), see, e.g., Rhein et al. (2013); Jang et al. (2014). Late-lumping directly exploits the infinite-dimensional PDE formulation for the control and observer design. In the context of moving horizon estimation, this implies to first determine the necessary optimality conditions with respect to the decision variables using variational calculus before imposing approximation schemes for their numerical evaluation. Hence, this requires to introduce Lagrange multipliers which are governed by the so-called adjoint system, see, e.g., Troeltzsch (2010) for related results in the context of PDE-constrained optimal control and, e.g., Nguyen et al. (2016) for adjoint-based state and parameter estimation approaches applied to a switched hyperbolic overland flow model.

In this contribution, the late-lumping approach is used to address nonlinear PDE-based moving horizon estimation. The corresponding PDE-ODE-constrained optimization problem to minimize the difference between measured and estimated output is formulated and the necessary optimality conditions are deduced. The resulting adjoint system has to be solved backward in time to determine the gradient needed to set up a line search approach for the decision variable. The latter is given by the initial state of the observer system, which is solved forward in time. The problem is solved on a moving (receding) horizon taking into account the measurement updates. Tailored gradient-based line search is presented and applied so that a fast convergence of the estimator for a diffusion-reaction PDE-based system under disturbances with sensor dynamics is guaranteed.

The paper is organized as follows. In Section 2, the nonlinear system model is summarized to motivate the

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moving horizon estimation problem introduced in Section 3, where also the necessary optimality conditions are deduced. Section 4 covers the discretization of the obtained PDEs and an algorithm is introduced for the numerical solution. In Section 5 simulation results are presented and the paper closes with some final remarks in Section 6.

2. PROBLEM FORMULATION

Consider the nonlinear diffusion-reaction system

$$\partial_t x(z,t) = d\partial_z^2 x(z,t) + r(z,t,x(z,t)) \tag{1a}$$

on $z \in (0,1)$ for $t > 0$ with boundary conditions

$$\begin{aligned} b\partial_z x(0,t) + x(0,t) &= u(t) \\ \partial_z x(1,t) &= 0 \end{aligned} \tag{1b}$$

for $t \geq 0$ and initial state

$$x(z,0) = x_0(z), \qquad z \in [0,1] \tag{1c}$$

Herein d is the diffusion coefficient and the function $r(z,t,x)$ is assumed continuous in z, continuously differentiable in t and locally Lipschitz continuous in x uniformly in t on bounded intervals. This implies the existence and uniqueness of a mild solution of (1), see, e.g., (Pazy, 1992, Thm. 6.1.4). The parameter $b \in \mathbb{R}$ is used to model Dirichlet ($b = 0$) or mixed ($b \neq 0$) boundary conditions. The system output is determined via the ODE

$$\dot{w}(t) = \frac{1}{T}(y(t) - w(t)), \qquad t > 0,\ w(0) = w_0 \tag{1d}$$

with time constant $T > 0$ and

$$y(t) = (Cx)(t) + v(t), \qquad t \geq 0, \tag{1e}$$

where $(Cx)(t) = \int_0^1 c(z)x(z,t)\mathrm{d}z$ denotes the in-domain, spatially averaged measurement with the spatial characteristics $c(z)$ and $v(t)$ is the additive noise. The properties of $v(t)$ will be further characterized in the simulation examples in Section 5.

The basic idea of the moving horizon estimator design is to reformulate the estimation problem as a (quadratic) optimization problem that has to be solved on a fixed-size estimation time windows to minimize the distance between the output $w(t)$ and its estimate $\hat{w}(t)$ Rao et al. (2003). This implies accounting for a fixed amount of data to compute the best approximate of the output based on the measurement data on the current horizon.

3. PDE-BASED MOVING HORIZON ESTIMATION

In the following the moving horizon estimation problem is set up and variational calculus is applied to determine the necessary optimality conditions in terms of the adjoint PDE-ODE system.

3.1 Dynamic optimization problem

The MHE is obtained by solving repeatedly the dynamic optimization problem

$$\min_{\hat{x}_{t_k-\tau}(z),\hat{w}_{t_k-\tau}} J = \frac{1}{2}\int_{t_k-\tau}^{t_k} \big(\Delta w(t)\big)^2 \mathrm{d}t \tag{2a}$$

for $\Delta w(t) = w(t) - \hat{w}(t)$ subject to

$$\begin{aligned} \partial_t \hat{x}(z,t) &= d\partial_z^2 \hat{x}(z,t) + r(z,t,\hat{x}(z,t)), \\ &\quad z \in (0,1),\ t \in (t_k-\tau, t_k) \\ \dot{\hat{w}}(t) &= \frac{1}{T}((C\hat{x})(t) - \hat{w}(t)),\ t \in [t_k-\tau, t_k) \\ b\partial_z \hat{x}(0,t) + \hat{x}(0,t) &= u(t) \text{ and} \\ \partial_z \hat{x}(1,t) &= 0, \quad t \geq t_k - \tau \\ \hat{x}(z,t_k-\tau) &= \hat{x}_{t_k-\tau}(z), \qquad z \in [0,1] \\ \hat{w}(t_k-\tau) &= \hat{w}_{t_k-\tau} \end{aligned} \tag{2b}$$

with $\tau > 0$ the estimation horizon. Herein, $\hat{x}_{t_k-\tau}(z)$ and $\hat{w}_{t_k-\tau}$ denote the decision variables for fixed end time t_k. The cost functional $J(\hat{x}_{t_k-\tau}(z), \hat{w}_{t_k-\tau})$ measures the quadratic difference between the actual and the observed output after processing by the sensor and is defined in such a way that the optimal initial state $\hat{x}_{t_k-\tau}(z)$ and initial sensor value $\hat{w}_{t_k-\tau}$ coincide with its (local) minimum. The estimated state $\hat{x}(z,t)$ and sensor output $\hat{w}(t)$ for $z \in [0,1]$ and $t \in [t_k - \tau, t_k)$ are governed by the system (2b), which is subsequently called the forward system.

3.2 Optimality conditions

By applying variational calculus, see, e.g., Troeltzsch (2010), the necessary optimality conditions are obtained in terms of the adjoint PDE-ODE system

$$\begin{aligned} \partial_t p(z,t) &= -d\partial_z^2 p(z,t) - \partial_{\hat{x}} r(z,t,\hat{x}(z,t))p(z,t) \\ &\quad - \frac{q(t)}{T}c(z),\ z\in(0,1),\ t\in(t_k-\tau, t_k) \\ \dot{q}(t) &= \frac{q(t)}{T} + \Delta w(t),\ t\in[t_k-\tau, t_k) \\ b\partial_z p(0,t) + p(0,t) &= \partial_z p(1,t) = 0, \quad t \geq t_k - \tau \\ p(z,t_k) &= p_{t_k}(z) = 0, \qquad z \in [0,1] \\ q(t_k) &= q_{t_k} = 0, \end{aligned} \tag{3}$$

where $p(z,t)$ and $q(t)$ are Lagrange multipliers. This equation is derived from the first variation of the Lagrange functional

$$\begin{aligned} L = J + \int_{t_k-\tau}^{t_k}\int_0^1 p(z,t)\big(d\partial_z^2 \hat{x}(z,t) \\ + r(z,t,\hat{x}) - \partial_t \hat{x}(z,t)\big)\mathrm{d}z\mathrm{d}t \\ + \int_{t_k-\tau}^{t_k} q(t)\Big(\frac{1}{T}\big((C\hat{x})(t) - \hat{w}(t)\big) - \dot{\hat{w}}(t)\Big)\mathrm{d}t \end{aligned} \tag{4}$$

related to the dynamic optimization problem (2). The derivation of (3) from (4) is summarized in Appendix A. Equation (3) is subsequently called backward system since it has to be solved backward in time taking into account terminal conditions $p(z,t_k) = 0$, $z \in [0,1]$ and $q(t_k) = 0$. The adjoint states $p(z,t_k-\tau)$ and $q(t_k-\tau)$ can be interpreted as the gradients of the cost functional (2a), which will be used to update the initial states $\hat{x}_{t_k-\tau}(z)$ and $\hat{w}_{t_k-\tau}$ until (2a) reaches a (local) minimum and (2b) provides the estimate.

It is a rather standard procedure to re-cast the forward and the backward system into a form that is easier to handle for numerical purposes by introducing the change of coordinates $s := s(t) = t-(t_k-\tau)$ so that $\hat{x}(\cdot,t) \mapsto \hat{x}(\cdot,s)$, $p(\cdot,t) \mapsto p(\cdot,s)$, $q(t) \mapsto q(s)$. This yields

$$
\begin{aligned}
&\partial_s \hat{x}(z,s) = d\partial_z^2 \hat{x}(z,s) + \bar{r}(z,s,\hat{x}(z,s)),\\
&\qquad z \in (0,1),\ s \in (0,\tau)\\
&\partial_s \hat{w}(s) = \frac{1}{T}((C\hat{x})(s) - \hat{w}(s)),\ s \in (0,\tau)\\
&b\partial_z \hat{x}(0,s) + \hat{x}(0,s) = \bar{u}(s),\ \partial_z \hat{x}(1,s) = 0, \quad s \geq 0\\
&\hat{x}(z,0) = \hat{x}_0(z), \qquad z \in [0,1]\\
&\hat{w}(0) = \hat{w}_0
\end{aligned} \tag{5a}
$$

with $\bar{r}(z,s,\hat{x}(z,s)) = r(z,t(s),\hat{x}(z,t(s)))$, $\bar{u}(s) = u(t(s))$, $\Delta\bar{w}(s) = \Delta w(t(s))$ for $t(s) = s + (t_k - \tau)$ and

$$
\begin{aligned}
&\partial_s p(z,s) = -d\partial_z^2 p(z,s) - \partial_{\hat{x}} \bar{r}(z,s,\hat{x}(z,s))p(z,s)\\
&\qquad - \frac{q(s)}{T} c(z),\ z \in (0,1),\ s \in (0,\tau)\\
&\partial_s q(s) = \frac{q(s)}{T} + \Delta\bar{w}(s),\ s \in (0,\tau)\\
&b\partial_z p(0,s) + p(0,s) = \partial_z p(1,s) = 0, \quad s \geq 0\\
&p(z,\tau) = 0, \qquad z \in [0,1]\\
&q(\tau) = 0.
\end{aligned} \tag{5b}
$$

Herein, $(\hat{x}_0(z), \hat{w}_0)$ denotes the minimizer of (2a) with $\Delta\bar{w}(s) = (w(t(s)) - \hat{w}(s))$ given $\hat{w}(s) = \int_0^1 c(z)\hat{x}(z,s)\mathrm{d}z$.

Remark 1. The adjoint PDE (5b) can be re-formulated as an initial-boundary-value problem by reversing the time coordinate. Hence, let $\alpha := \alpha(s) = \tau - s$ or $s(\alpha) = \tau - \alpha$, respectively, and $p(\cdot,s) \mapsto p(\cdot,\alpha)$, $q(s) \mapsto q(\alpha)$, then (5b) reads

$$
\begin{aligned}
&\partial_\alpha p(z,\alpha) = d\partial_z^2 p(z,\alpha) + \partial_{\hat{x}} \bar{r}(z,s(\alpha),\hat{x}(z,s(\alpha)))p(z,\alpha)\\
&\qquad + \frac{q(\alpha)}{T} c(z),\ z \in (0,1),\ \alpha \in (0,\tau)\\
&\partial_\alpha q(\alpha) = -\frac{q(\alpha)}{T} - \Delta\bar{w}(s(\alpha)),\ \alpha \in (0,\tau)\\
&b\partial_z p(0,\alpha) + p(0,\alpha) = \partial_z p(1,\alpha) = 0, \quad \alpha \geq 0\\
&p(z,0) = 0, \qquad z \in [0,1]\\
&q(0) = 0.
\end{aligned} \tag{6}
$$

In this case the solution $\hat{x}(z,s)$ of (5a) has to be mapped accordingly.

3.3 Estimation algorithm

The optimization problem is solved based on (5) by means of gradient iteration and line search by carrying out the following steps:

(1) Obtain the output $w(t)$ from the system governed by (1) involving the sensor dynamics.

(2) Initialize the decision variables $(\hat{x}_0^{(i)}(z),\ \hat{w}_0^{(i)})$, then repeat the following gradient iteration until a suitable stopping criteria is fulfilled:

- (a) Solve (5a) forward in time to obtain the state and output trajectories $(\hat{x}^{(i)}(z,s), \hat{w}^{(i)}(s))$ at the ith iteration on the current horizon on the basis of the initial state $(\hat{x}_0^{(i)}(z),\ \hat{w}_0^{(i)})$;
- (b) Solve (5b) backward in time or solve respectively (6) to obtain the adjoint state trajectory $(p^{(i)}(z,s), q^{(i)}(s))$ for the considered horizon;
- (c) Compute the gradients $g_{\hat{x}_0}^{(i)}(z) = p^{(i)}(z,0)$ and $g_{\hat{w}_0}^{(i)} = q^{(i)}(0)$;
- (d) Update the estimated state and output

$$
\begin{aligned}
\hat{x}_0^{(i+1)}(z) &= \hat{x}_0^{(i)}(z) - \alpha_{\hat{x}}^{(i)} g_0^{(i)}(z)\\
\hat{w}_0^{(i+1)} &= \hat{w}_0^{(i)} - \alpha_{\hat{w}}^{(i)} g_{\hat{w}_0}^{(i)}
\end{aligned} \tag{7}
$$

with the step sizes $\alpha_{\hat{x}}^{(i)} > 0$ and $\alpha_{\hat{w}}^{(i)} > 0$.

Using the steepest descent avoids the need to compute the Hessian related to $g_{\hat{x}_0}^{(i)}(z)$ and $g_{\hat{w}_0}^{(i)}$, which is in general computationally demanding. However, steepest descent is robust enough to achieve convergence for randomly chosen initial values. Alternatively conjugated gradients could be used. For the determination of the step sizes $\alpha_{\hat{x}}^{(i)}$ and $\alpha_{\hat{w}}^{(i)}$ a Wolfe condition, nested intervals or some adaptive procedure can be used Nocedal and Wright (2006).

For moving horizon estimation the aforementioned optimization problem is repeatedly computed on the introduced receding horizon. Due to the considered change of coordinates this refers to update $w(t)$, $u(t)$ and $r(\cdot,t,\cdot)$ with time. Note that the previously introduced late-lumping approach for the general formulation is independent of the particular choice of numerical approximation method. Subsequently, (5a) and (5b) or (6), respectively, are approximated exemplarily using the finite differences method for the PDE parts of the equations and are solved recursively using adequate numerical tools. The spatial discretization step is chosen small enough to remain as close as possible to the covered infinite dimensional systems. This helps reducing the numerical dispersion due to the discretization and thus increases the applicability of the designed MHE.

Remark 2. If we consider the time constant T of the sensor dynamics as an additional decision variable, then its variation, see, Appendix A, leads to the constraint that $\hat{w}(t) = (C\hat{x})(t)$. Hence the $\hat{x}$-part of the MHE setting reduces to

$$
\begin{aligned}
&\partial_t \hat{x}(z,t) = d\partial_z^2 \hat{x}(z,t) + r(z,t,\hat{x}(z,t)),\\
&\qquad z \in (0,1),\ t \in (t_k - \tau, t_k)\\
&b\partial_z \hat{x}(0,t) + \hat{x}(0,t) = u(t) \text{ and}\\
&\partial_z \hat{x}(1,t) = 0, \quad t \geq t_k - \tau\\
&\hat{x}(z, t_k - \tau) = \hat{x}_{t_k-\tau}(z), \qquad z \in [0,1].
\end{aligned} \tag{8}
$$

The variation of T leads to the cancellation of the sensor dynamics so that the spatially averaged estimated state $(C\hat{x})(t)$ is directly used in the adjoint sensor dynamics. This influences in turn the adjoint state and the computation of the respective gradient.

4. NUMERICAL APPROXIMATION

To solve the forward and backward PDE-ODE systems numerically, a finite difference discretization is applied as an example. Note that any other technique such as weighted residuals, collocation techiques or Galerkin's method can be considered similarly. The resulting finite-dimensional approximation is composed of two coupled sets of ODEs, where the first set is solved forward and the second backward in time, respectively.

4.1 Finite differences discretization of PDE subsystems

The spatial coordinate z is discretized using a uniform grid of $n+1$ nodes $z_j = (j-1)\Delta z$, $j \in \{1,\ldots,n+1\}$ for $\Delta z = 1/n$. Let $\hat{x}_j(\cdot) = \hat{x}(z_j,\cdot)$, $p_j(\cdot) = p(z_j,\cdot)$ so that $\hat{\boldsymbol{x}}(\cdot) = [\hat{x}_2(\cdot), \ldots, \hat{x}_n(\cdot)]^T$, $\boldsymbol{p}(\cdot) = [p_2(\cdot), \ldots, p_n(\cdot)]^T$ and consider centered finite differences to approximate the second order derivative

$$\partial_z^2 \hat{x}(z,\cdot) \approx \frac{\hat{x}_{j+1}(\cdot) - 2\hat{x}_j(\cdot) + \hat{x}_{j-1}(\cdot)}{(\Delta z)^2}. \tag{9}$$

Then (5) can be approximated according to

$$\partial_s \hat{\boldsymbol{x}}(s) = A\hat{\boldsymbol{x}}(s) + \boldsymbol{b}\bar{u}(s) + \boldsymbol{f}(s, \hat{\boldsymbol{x}}(s)) \tag{10a}$$

$$\partial_s \hat{w}(s) = \frac{1}{T}\big((C\hat{x})(s) - w(s)\big) \tag{10b}$$

$$\partial_s \boldsymbol{p}(s) = -A\boldsymbol{p}(s) - \boldsymbol{g}(s, \hat{\boldsymbol{x}}(s), \boldsymbol{p}(s)) - \frac{q(s)}{T}\boldsymbol{c} \tag{10c}$$

$$\partial_s q(s) = \frac{q(s)}{T} + \Delta\bar{w}(s) \tag{10d}$$

for $s \in (0, \tau)$ with initial and terminal conditions

$$\hat{\boldsymbol{x}}(0) = \hat{\boldsymbol{x}}_0, \quad \hat{w}(0) = \hat{w}_0, \quad \boldsymbol{p}(\tau) = \boldsymbol{0}, \quad q(\tau) = 0 \tag{10e}$$

and

$$A = \frac{d}{(\Delta z)^2}\begin{bmatrix} -\frac{2-\nu}{1-\nu} & 1 & 0 & \cdots & 0 & 0 \\ 1 & -2 & 1 & \cdots & 0 & 0 \\ \vdots & & & & & \vdots \\ 0 & 0 & 0 & \cdots & 1 & -1 \end{bmatrix}$$

$$\boldsymbol{b} = \begin{bmatrix} \frac{d}{(\Delta z)^2(1-\nu)} \\ 0 \\ \vdots \\ 0 \end{bmatrix} \quad \boldsymbol{c} = \begin{bmatrix} c(z_2) \\ c(z_3) \\ \vdots \\ c(z_n) \end{bmatrix}$$

$$\boldsymbol{f} = \begin{bmatrix} \bar{r}(z_2, s, \hat{x}_2(s)) \\ \vdots \\ \bar{r}(z_n, s, \hat{x}_n(s)) \end{bmatrix}, \quad \boldsymbol{g} = \begin{bmatrix} \partial_{\hat{x}}\bar{r}(z_2, s, \hat{x}_2(s))p_2(s) \\ \vdots \\ \partial_{\hat{x}}\bar{r}(z_n, s, \hat{x}_n(s))p_n(s) \end{bmatrix}$$

for $\nu = b/\Delta z$. Using first order forward and backward finite differences the boundary values follow as

$$\hat{x}_1(s) = \frac{\bar{u}(s) - \nu\hat{x}_2(s)}{1-\nu}, \qquad \hat{x}_{n+1}(s) = \hat{x}_n(s)$$

$$p_1(s) = -\frac{\nu}{1-\nu}p_2(s), \qquad p_{n+1}(s) = p_n(s).$$

Note that Remark 1 can be applied to re-formulate the final-value problems for $\boldsymbol{p}(s)$ and $q(s)$ into an initial-value problems on a reverse time scale.

4.2 Discretization-based estimation algorithm

The numerical solution process is based on the gradient algorithm developed in Section 3.3 and is implemented as follows:

(1) Obtain the output $w(t)$ from the system governed by (1) involving the sensor dynamics.
(2) Initialize the decision variables $(\hat{\boldsymbol{x}}_0^{(i)}, \hat{w}_0^{(i)})$ for each iteration i and execute the following steps until a stopping condition is reached:
   (a) Solve (10a) and (10b) forward in time and determine the corresponding states $(\hat{\boldsymbol{x}}^{(i)}(s), \hat{w}^{(i)}(s))$ on the current horizon $s \in [0, \tau]$.
   (b) Solve (10c) and (10d) backward in time to obtain $(\boldsymbol{p}^{(i)}(s), q^{(i)}(s))$ and evaluate the gradients $\boldsymbol{g}_{\hat{\boldsymbol{x}}_0}^{(i)} = \boldsymbol{p}^{(i)}(0)$ and $g_{\hat{w}_0}^{(i)} = q^{(i)}(0)$.
   (c) Update the initial state and output

$$\begin{aligned} \hat{\boldsymbol{x}}_0^{(i+1)} &= \hat{\boldsymbol{x}}_0^{(i)} - \alpha_{\hat{x}}^{(i)}\boldsymbol{g}_{\hat{\boldsymbol{x}}_0}^{(i)} \\ \hat{w}_0^{(i+1)} &= \hat{w}_0^{(i)} - \alpha_{\hat{w}}^{(i)}g_{\hat{w}_0}^{(i)} \end{aligned} \tag{11}$$

   with suitable step lengths $\alpha^{(i)}$ and $\alpha_{\hat{w}}^{(i)}$.

5. SIMULATION RESULTS

Subsequently simulation results are presented for the moving horizon estimation problem given by (1) with measurements corrupted by noise.

5.1 Implementation

The set of PDEs (5) is solved numerically using the discretization introduced in (10) at each iteration step. For this MATLAB is used, where the gradient descent algorithm described in Section 3.3 or 4.2, respectively, is applied. To determine the nominal solution of (1) the solver `pdepe` is used to compute $x(z,t)$. The output $w(t)$ defined in (1d) is evaluated numerically and the in-domain output $y(t)$ is determined utilizing an adaptive quadrature rule to evaluate the integral of $c(z)x(z,t)$ over $z \in [0,1]$. The spatial measurement characteristics is assigned as a square pulse

$$c(z) = \sigma(z - \xi_1) - \sigma(z - \xi_2) \tag{12}$$

with $0 < \xi_1 < \xi_2 < 1$ and $\sigma(\cdot)$ denoting the Heaviside function. The additive output disturbance $v(t)$ is assumed to be normally distributed with zero mean. The parameters are assigned as $d = 1$, $b = 1$ and the external boundary input is set to zero, i.e., $u(t) = 0$.

The considered horizon interval is $[t_k - \tau, t_k]$, where $\tau = 0.2$ is chosen as horizon length and t_k is the upper bound of the current horizon interval. At the beginning of the simulation $t_k = \tau$ holds true and t_k is incremented by τ at the end of each horizon. Each horizon $[t_k - \tau, t_k]$ is discretized in time using 10 grid elements. The spatial discretization was carried out with $n = 21$ grid points and the MHE was evaluated using (10). The time constant T is chosen as a multiple of τ.

For the evaluation of the MHE performance, we consider the L^2-norm of the estimation error

$$\|e\|_{L^2}(t) = \|x(z,t) - \hat{x}(z,t)\|_{L^2}. \tag{13}$$

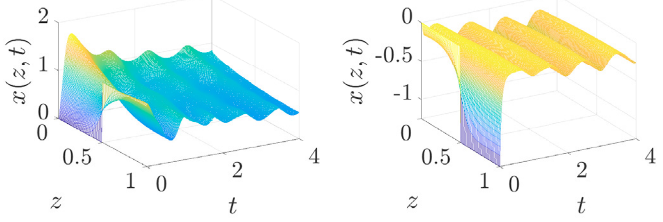
The line search algorithm summarized in Section 4.2 is evaluated using an adaptive line search Englert et al. (2019) for the computation of the step length.

5.2 Bistable diffusion-reaction system

The reaction term in (1) is chosen as

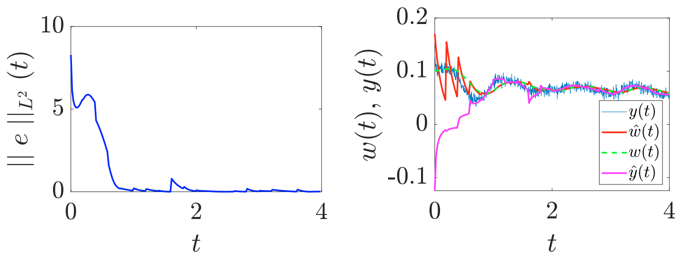
$$r(z,t,x(z,t)) = \beta_0 x(z,t)(\beta_1(z,t) - x(z,t)) \times (x(z,t) - \beta_2(t)) \tag{14}$$

with $\beta_0 = 10$, $\beta_1(z,t) = 1/2 + \cos(5\pi z t/2)$ and $\beta_2(t) = \sin(2\pi t)/2$, see also Pesin and Yurchenko (2004); Meurer (2013b). With this, (1) represents a bistable semilinear PDE. The initial state of the nominal system is assigned as $x_0(z) = 5/4\sigma(z - 1/2)$ with the Heaviside function $\sigma(\cdot)$. The MHE is initialized with $\hat{x}_0(z) = -x_0(z)$. Due to the bistability induced by (14) the solution of (1) for the initial states $x_0(z)$ and $-x_0(z)$, respectively, converges



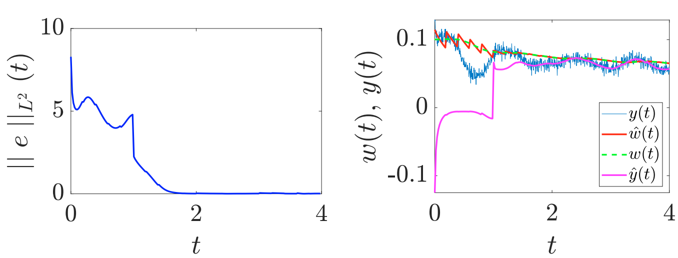
a) $x_0(z) = 5/4\sigma(z-1/2)$. b) $\hat{x}_0(z) = -5/4\sigma(z-1/2)$.

Fig. 1. Evolution of $x(z,t)$ for $x(z,0) = x_0(z)$ and $x(z,0) = \hat{x}_0(z)$ used for the initialization of the system dynamics and the MHE, respectively. The resulting convergence to different final states due to the bistability becomes visible.



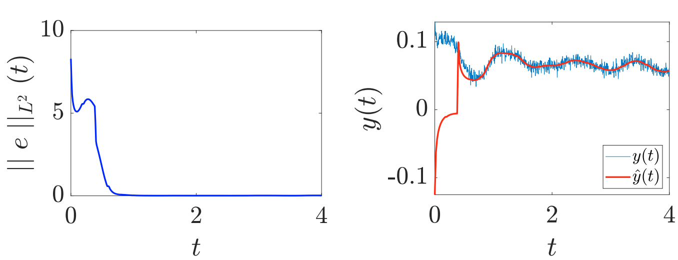
a) Time evolution of L^2-norm of state estimation error $\|e\|_{L^2}(t)$ according to (12). b) Estimated measurement $\hat{y}(t)$ and sensor value $\hat{w}(t)$ compared to simulated values.

Fig. 2. MHE with time constant $T = \tau$.



a) Time evolution of L^2-norm of state estimation error $\|e\|_{L^2}(t)$ according to (12). b) Estimated measurement $\hat{y}(t)$ and sensor value $\hat{w}(t)$ compared to simulated values.

Fig. 3. MHE with time constant $T = 5\tau$.



a) Time evolution of L^2-norm of state estimation error $\|e\|_{L^2}(t)$ according to (12). b) Estimated measurement $\hat{y}(t)$ compared to simulated value.

Fig. 4. MHE with time constant $T = 5\tau$ with sensor time constant as decision variable according to Remark 2.

to different stable (transient) operation profiles, see, Fig. 1. The measurement characteristics (12) is parametrized using $\xi_1 = 0.6$ and $\xi_2 = 0.7$.

The simulation results are computed for the nominal model of the system. Hereby, the observer system remains in its original form (2b) and the initial state of the sensor dynamics $\hat{w}_{t_k-\tau}$ is updated at the end of each estimation horizon by the gradient $\partial_{\delta\hat{w}_{t_k-\tau}} L = q_{t_k-\tau}$ according to the algorithm introduced in Section 3.3. Based on this algorithm, the simulation results depicted in Fig. 2 and Fig. 3 are obtained for two different values of the time constant T taking into account the same noise level $v(t)$. For the smaller time constant $T = \tau = 0.2$ (Fig. 2) the MHE is able to follow the measurement quickly and precisely. The convergence of the estimation error is fast with minor local perturbations due to the added noise. The estimation $\hat{w}(t)$ similarly converges to $w(t)$ with initial transients due to the determination of the initial value on each receding horizon. In Fig. 3 determined for $T = 5\tau = 1$ the initial transient phase is extended but convergence of the estimation error is achieved similarly. Both cases have an average computational time of $0.182s$ per iteration step considering an `Intel Core i5-8265U CPU`.

If Remark 2 is applied and $\hat{w}(t) = (C\hat{x})(t)$ is imposed, then the performance of the resulting MHE is shown in Fig. 4 for the scenario of Fig. 3, i.e. $T = 1$. This in particular provides a better estimation performance as the rather slow sensor dynamics considered in this example is omitted in the MHE evaluation.

6. CONCLUSIONS

A moving horizon estimator for a nonlinear diffusion-reaction system with sensor dynamics is designed using a late-lumping approach by directly exploiting the PDE-ODE formulation of the system. The necessary optimality conditions are evaluated and are used to formulate a line search approach involving the solution of the adjoint PDE-ODE system defining the gradient. Based on this, a finite differences discretization is presented and utilized for the evaluation of the MHE. Simulation results for a bistable diffusion-reaction system with measurements subject to additive noise and processed via a linear sensor dynamics confirm the applicability of the PDE-ODE-based moving horizon estimation.

Current research addresses the proper selection of the optimization horizon in view of optimality, sampling times and computational time, the connection of the sensor placement and the performance of the MHE as well as the inclusion of noise estimation into the MHE setup. This in addition includes the comparison with early-lumping MHE for nonlinear PDE systems.

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Appendix A. FIRST VARIATION OF LAGRANGE FUNCTIONAL

The optimality conditions (3) are deduced evaluating the first variation or Gâteaux derivative, respectively, for (2). To this end, the Lagrange functional (4) is evaluated taking into account also T as additional decision variable (see Remark 2). Hence, integration by parts of the Lagrangian yields

$$
\begin{aligned}
L = J &- \int_0^1 \Big[p(z,t)\hat{x}(z,t)\Big]_{t_k-\tau}^{t_k} \mathrm{d}z \\
&+ \int_{t_k-\tau}^{t_k} d\Big[p(z,t)\partial_z\hat{x}(z,t) - \partial_z p(z,t)\hat{x}(z,t)\Big]_0^1 \mathrm{d}t \\
&+ \int_{t_k-\tau}^{t_k}\int_0^1 \Big(\hat{x}(z,t)\big(d\partial_z^2 p(z,t) + \partial_t p(z,t)\big) \\
&\qquad\qquad + r(z,t,\hat{x}(z,t))p(z,t)\Big)\mathrm{d}z\mathrm{d}t \\
&- \Big[q(t)\hat{w}(t)\Big]_{t_k-\tau}^{t_k} \\
&+ \int_{t_k-\tau}^{t_k} \left(\hat{w}(t)\Big(\dot{q}(t) - \frac{q(t)}{T}\Big) + \frac{q(t)}{T}(C\hat{x})(t)\right)\mathrm{d}t.
\end{aligned}
$$

The Gâteaux derivative of the Lagrangian can be formulated as $\delta L = \delta L_{\hat{x}} + \delta L_{\hat{w}} + \delta L_T$, whereby $\delta J = -\int_{t_k-\tau}^{t_k} \big(w(t) - \hat{w}(t)\big)\delta\hat{w}(t)\mathrm{d}t$ such that

$$
\begin{aligned}
\delta L_{\hat{x}} &= -\int_0^1 \Big[p(z,t)\delta\hat{x}(z,t)\Big]_{t_k-\tau}^{t_k}\mathrm{d}z \\
&\quad + \int_{t_k-\tau}^{t_k} d\Big[p(z,t)\delta\partial_z\hat{x}(z,t) - \partial_z p(z,t)\delta\hat{x}(z,t)\Big]_0^1\mathrm{d}t \\
&\quad + \int_{t_k-\tau}^{t_k}\int_0^1 \delta\hat{x}(z,t)\Big(\partial_t p(z,t) + d\partial_z^2 p(z,t) \\
&\qquad\qquad + \partial_{\hat{x}} r(z,t,\hat{x}(z,t))p(z,t) + \frac{q(t)}{T}c(z)\Big)\mathrm{d}z\mathrm{d}t, \\
\delta L_{\hat{w}} &= -\Big[q(t)\delta\hat{w}(t)\Big]_{t_k-\tau}^{t_k} \\
&\quad + \int_{t_k-\tau}^{t_k} \delta\hat{w}(t)\Big(\dot{q}(t) - \frac{q(t)}{T} - \big(w(t) - \hat{w}(t)\big)\Big)\mathrm{d}t, \\
\delta L_T &= \int_{t_k-\tau}^{t_k} \frac{q(t)}{T^2}\big(\hat{w}(t) - (C\hat{x})(t)\big)\delta T\mathrm{d}t.
\end{aligned}
$$

Taking into account the fundamental lemma of variational calculus for admissible directions $\delta\hat{x}(z,t)$, $\delta\hat{w}(t)$, and δT the evaluation of the first order necessary optimality condition $\delta L = 0$ implies (2) and (3). In addition, the gradients

$$
\partial_{\hat{x}(z,t_k-\tau)} L = \int_0^1 p(z,t_k-\tau)\mathrm{d}z, \quad \partial_{\hat{w}(t_k-\tau)} L = q(t_k-\tau)
$$

are obtained, which are used in Section 3.3. Furthermore, the evaluation of $\delta L_T = 0$ implies $\hat{w}(t) = (C\hat{x})(t)$, see also Remark 2.