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Nonlinear state and parameter estimation using derivative information: A Lie-Sobolev approach

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ABSTRACT

The implementation of nonlinear control depends on the accuracy of the system model, which, however, is often restricted by parametric and structural uncertainty in the underlying dynamics. In this paper, we propose methods of estimating parameters and states that aim at matching the identified model and the true dynamics not only in the direct output measurements, i.e., in an L^2-sense, but also in the higher-order time derivatives of the output signals, i.e., in a Sobolev sense. A Lie-Sobolev gradient descent-based observer-estimator and a Lie-Sobolev moving horizon estimator (MHE) are formulated, and their convergence properties and effects on input–output linearizing control and model predictive control (MPC) respectively are studied. Advantages of Lie-Sobolev state and parameter estimation in nonlinear processes are demonstrated by numerical examples and a reactor with complex dynamics.

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1. Introduction

The development of nonlinear control methods has been one of the most important topics in process control due to the intrinsic nonlinearity of process systems. Examples include input–output linearization (Isidori, 1995), which uses state feedback to cancel out the nonlinearity and shape the output response, and model predictive control (MPC) (Rawlings et al., 2017), which generates control signals by optimizing a cost associated with the predicted trajectory. It is self-evident that the successful application of these nonlinear model-based control methods is intrinsically dependent on high-quality dynamic models. Process systems may be represented as white-box first-principles models, black-box models of completely unknown dynamics, or grey-box models in between (Sjöberg et al., 1995). Whenever a perfect white-box model is unavailable, the unknown parts of the underlying dynamics must be inferred through *system identification*, which is typically performed off-line, although on-line approaches such as adaptive control (Farrell and Polycarpou, 2006) or dual control (Filatov and Unbehauen, 2004) have also been proposed.In this paper, we focus on the off-line system identification problem, where perturbations are imposed on the system to generate data for identification and the controller is designed after the model is identified.

The specific formulations and procedures of system identification vary with the context. In general, system identification may refer to any regression or data-driven characterization of the unknown parts in dynamic models, e.g., state-space models, transfer function models, and autoregressive models (Schoukens and Ljung, 2019). A wide spectrum of approaches have been developed in this sense in the process control literature (Doyle III et al., 1995; Zhu, 1998; Favoreel et al., 2000; Simkoff and Baldea, 2019). In a broader sense, the identification can be performed in a model-free manner only to learn useful control-relevant information from data, such as optimal value/policy functions or dissipativity parameters (Tang and Daoutidis, 2018; 2019; 2021). The characterization of the unknown model structure along with the identification procedure can be categorized as parametric (Ljung, 1999) or nonparametric (Greblicki and Pawlak, 2008).

For nonlinear chemical processes, the aim of system identification is typically to estimate the unknown parameters, usually physical and chemical properties, in models of certain a-priori structures derived from first principles or approximations (Englezos and Kalogerakis, 2000; Zavala and Biegler, 2006). Also, for chemical processes there usually exist states that are not directly measurable and hence the parameter estimation needs to be combined with the simultaneous state observation, i.e., both dynamic states and model parameters should be estimated. Therefore, in this paper, we use the parametric formulation and consider system identification as the problem of designing such an *observer-estimator*. If the process dynamics can be represented by a parametric model without structural errors, the aim of such an observer-estimator (also

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known as adaptive observer in this context) design is to achieve both state and parameter convergence to the true values; otherwise, it is desirable that the identification results in only small deviations and the resulting control performance is not severely deteriorated (see, e.g., Marino et al., 2001; Liu, 2009; Zhang and Xu, 2015).

State observer design for dynamic systems is a classical problem in process control (Soroush, 1998; Dochain, 2003; Kravaris et al., 2013), which can be extended to combined observer-estimator design by viewing parameters as invariant states. The most common approach for nonlinear systems is to modify the Kalman filter for linear systems into an extended or unscented one (EKF, UKF) (Simon, 2006). For systems of specific structure, state observers can be designed through backstepping (Krstić et al., 1995) or based on the semilinear form obtained through input–output linearization (Farza et al., 2009; Tyukin et al., 2013). The latter approaches essentially employ high-gain output feedback and have led to elegant conditions under which the output-feedback control with state observer achieves desired performance (Khalil and Praly, 2014). As a generic result, Kazantzis and Kravaris (1998) proposed a nonlinear observer with assignable error dynamics based on the solution of partial differential equations, whose theoretical existence was established (Andrieu and Praly, 2006) but whose solution is hindered by computational considerations. In a different vein, implicit schemes based on nonlinear optimization, such as maximum likelihood estimation (MLE) (Schön et al., 2011) and especially moving horizon estimation (MHE) (Rao et al., 2003), have gained increasing applications. It should be noted that for generic nonlinear systems, a separation principle, either for state observer or for observer-estimator design, is lacking. In the present work, we will consider observer-estimators in a gradient descent and MHE form.

A key motivation for this work is the need for a *control-oriented approach* for nonlinear system identification. It is well known that any identified model is an approximation of the actual dynamics, and for a model used for the purpose of process control, the quality of system identification should be assessed by the resulting control performance (Ljung, 1999). However, the mismatch between the typical identification objective, e.g., least squares of regression residuals, and the control performance, makes system identification for truly optimal control performance an intrinsically challenging problem (Schrama, 1992; Gevers, 2005). Nevertheless, it is possible to develop control-oriented identification methods that account for certain aspects or information that are important for control (Rivera et al., 1992). To this end, we hereby focus on the role of directional derivatives (*Lie derivatives*) of the model functions in nonlinear control which capture information on the derivatives of the output functions. Their role is explicit in input–output linearizing control, where the control laws are directly constructed using Lie derivatives. For MPC, their impact is implied from the local Chen-Fliess series expansions (Isidori, 1995, Section 3.2) of the predicted trajectories, whose coefficients rely on the Lie derivatives of the nonlinear model. Typical estimation procedures such as MHE (Kühl et al., 2011) only seek to match the estimated model with the actual model in the directly measured output values and may not be effective in matching the output derivatives and thus the corresponding Lie derivatives, especially when structural errors exist, i.e., the true dynamics may not be exactly parameterized.

Motivated by the above, we propose a *Lie-Sobolev* framework for nonlinear state and parameter estimation. We develop constructive procedures for incorporating output derivative information in the combined observer-estimator design aiming to match the estimated model to the actual one in the corresponding Lie derivatives of the output functions. We establish well-characterized nominal convergence properties for the resulting estimators and boundedness in the presence of structural errors. We further illustrate how to proposed estimators can be combined with feedback linearizing controllers and model predictive controllers, and document their advantages through simulations. In related works, the regression of linearly parameterized functions accounting for first-order derivatives was discussed in (Novara et al., 2019), where the regression error bounds are derived through derivatives; Sobolev training of neural networks, where the errors together with error derivatives contribute to the back-propagation, was proposed by machine learning researchers (Pukrittayakamee et al., 2011; Czarnecki et al., 2017). The idea of accounting for output derivatives was also implicitly embodied in the design of state observers and adaptive observers based on input–output linearization for systems with specific structures (Afri et al., 2016), but to the best of our knowledge, was not considered explicitly in the identification of generic nonlinear systems and little used in schemes such as MHE.

The remainder of this paper is organized as follows. First, in Section 2, the general formulation of Lie-Sobolev estimation will be given. The Lie-Sobolev formulations of an explicit gradient descent observer-estimator and MHE are derived, and their convergence properties as well as their effects on nonlinear control are discussed in Sections 3 and 4, respectively. The advantages of the Lie-Sobolev approaches are demonstrated by the application to simple numerical examples and a glycerol etherification reactor with complex dynamics in Section 5. Conclusions are given in Section 6.

2. Lie-Sobolev estimation

2.1. System identification with observer-estimator

Consider a nonlinear dynamic model:

$$\begin{aligned} \dot{x}(t) &= f(x(t)) + g(x(t))u(t) \\ y(t) &= h(x(t)) \end{aligned} \tag{1}$$

where $x(t) \in \mathcal{X} \subseteq \mathbb{R}^{d_x}$, $u(t) \in \mathcal{U} \subseteq \mathbb{R}^{d_u}$ and $y(t) \in \mathbb{R}^{d_y}$ are the vectors of states, inputs and outputs, respectively. $f : \mathcal{X} \to \mathbb{R}^{d_x}$, $g : \mathcal{X} \to \mathbb{R}^{d_x \times d_u}$ and $h : \mathcal{X} \to \mathbb{R}^{d_y}$ are supposed to be smooth functions but may not be completely known, and hence need to be approximated within parameterized families of smooth functions $\{(\hat{f}(x|\theta), \hat{g}(x|\theta), \hat{h}(x|\theta))|\theta \in \Theta\}$, where $\theta \in \Theta \subseteq \mathbb{R}^{d_\theta}$ is a vector of parameters to be estimated. That is, we parameterize the system (1) as follows:

$$\begin{aligned} \dot{x}(t) &= \hat{f}(x(t)|\theta) + \hat{g}(x(t)|\theta)u(t) \\ y(t) &= \hat{h}(x(t)|\theta). \end{aligned} \tag{2}$$

When there is a value $\theta \in \Theta$ such that the parameterization keeps the model functions unchanged, i.e., $f(\cdot) = \hat{f}(\cdot|\theta)$, $g(\cdot) = \hat{g}(\cdot|\theta)$, and $h(\cdot) = \hat{h}(\cdot|\theta)$, then the parameterization (2) is said to be exact. Otherwise, we say that there exist *structural errors* in the parameterization.

Suppose that the estimates of θ are updated in continuous time based on measurements of the inputs u and outputs y. Specifically, at any time t, the historical measurements and past estimates in the time interval $[0, t]$ are available for deriving an estimation $\hat{\theta}(t)$ which is generally represented as

$$\hat{\theta}(t) = \Pi(\{y(s), u(s), \hat{\theta}(s)|0 \le s < t\}), \tag{3}$$

where Π is an adaptation (estimation) law (Yakubovich, 1968). Once the parameter estimation is completed, the nonlinear model is considered as identified and a control law

$$u(t) = \kappa(\{y(s), u(s), \hat{\theta}|0 \le s < t\}) \tag{4}$$

can be designed to shape the closed-loop trajectory.

Since the states x are not directly measured, the parameter estimation is realized with an accompanying state observer. We formulate the observer so as to estimate the state derivatives $\dot{x}$ in addition to the states x. We denote the observation law for $\dot{\hat{x}}$ as σ. The state observer and the parameter estimator are realized in the form of ordinary differential equations (ODEs) driven by historical information on y, derivatives of y (up to some order r_y), u and the current estimates:

$$\begin{aligned}
\dot{\hat{x}}(t) &= \hat{v}(t) \\
\dot{\hat{v}}(t) &= \sigma\left(\hat{x}(t), \hat{v}(t), \hat{\theta}(t), \left\{\{y^{(r)}(s)\}_{r=0}^{r_y}, u(s), \middle| 0 \le s < t\right\}\right) \\
\dot{\hat{\theta}}(t) &= \pi\left(\hat{x}(t), \hat{v}(t), \hat{\theta}(t), \left\{\{y^{(r)}(s)\}_{r=0}^{r_y}, u(s), \middle| 0 \le s < t\right\}\right).
\end{aligned} \tag{5}$$

The reason for using both $\hat{x}$ and $\dot{\hat{x}}$ is to allow a criterion that evaluates how well the first equation in (2), which involves $(\dot{x}, x, \theta)$, is satisfied by the estimates $(\dot{\hat{x}}, \hat{x}, \theta)$. As the control law κ is usually constructed based on the estimated model $(\hat{f}, \hat{g}, \hat{h})$, key to the construction of the observation and estimation laws (σ, π) is the matching of the trajectory of $\hat{x}(t)$, $\dot{\hat{x}}(t)$ and $\hat{\theta}(t)$ to the behavior of the parameterized model (2) under the measured historical data. A perfect identification refers to a pair (σ, π) that makes the following ODEs hold for all $t \ge 0$:

$$\begin{aligned}
\dot{\hat{x}}(t) &= \hat{f}(\hat{x}(t)|\hat{\theta}(t)) + \hat{g}(\hat{x}(t)|\hat{\theta}(t))u(t) \\
y(t) &= \hat{h}(\hat{x}(t)|\hat{\theta}(t)).
\end{aligned} \tag{6}$$

2.2. Lie-Sobolev state and parameter estimation

Before introducing the Sobolev-type state and parameter estimation of the dynamic system (1) from input and output historical trajectories, we review the definition of Lie derivatives in nonlinear control (Isidori, 1995, Chapter 4).

Definition 1 (Lie derivative)**.** The Lie derivative of the ith component of h, h_i, with respect to a vector field f is defined as

$$L_f h_i = \frac{\partial h_i}{\partial x} f \tag{7}$$

respectively, where $\partial h_i/\partial x \in \mathbb{R}^{1\times d_x}$. The Lie differentiation operators can be recursively composed to generate high-order or mixed Lie derivatives, e.g., $(L_{f_1} L_{f_2})h_i = L_{f_1}(L_{f_2} h_i)$. Denote $L_f^{k+1} = L_f L_f^k$, $k = 0, 1, \dots,$ with L_f^0 being identity. With a slight abuse of notation, we will denote by $L_g h_i$ a row vector of $L_{g_j} h_i$.

Definition 2 (relative degree)**.** The relative degree ρ_i for the ith output is the smallest positive integer r such that $L_g L_f^{r-1} h_i \neq 0$.

With relative degree ρ_i known, we have

$$\begin{aligned}
y_i(t) &= L_f^0 h_i(x(t)) \\
\dot{y}_i(t) &= L_f^1 h_i(x(t)) \\
&\dots \\
y_i^{(\rho_i)}(t) &= L_f^{\rho_i} h_i(x(t)) + L_g L_f^{\rho_i - 1} h_i(x(t))u(t)
\end{aligned} \tag{8}$$

which implies that the direct effect of inputs u falls on the ρ_ith time derivative of t. For controlling the system (1) by shaping the responses of y_i, accurately evaluating or managing the errors in approximating the Lie derivatives $L_f^r h_i(x)$, $r = 0, 1, \dots, \rho_i$ and $L_g L_f^{\rho_i - 1} h_i(x)$, $i = 1, \dots, d_y$ is thus of crucial importance. Therefore, for a control-oriented system identification, we propose that the state and parameter estimation should be performed such that not only the output values match the estimated ones, i.e., (6) is satisfied, but also the output time derivatives match the estimated ones up to an order equal to their relative degree, i.e.:

$$\begin{aligned}
y_i(t) &= L_{\hat{f}}^0 \hat{h}_i(\hat{x}(t)|\hat{\theta}(t)) \\
\dot{y}_i(t) &= L_{\hat{f}}^1 \hat{h}_i(\hat{x}(t)|\hat{\theta}(t)) \\
&\dots \\
y_i^{(\rho_i)}(t) &= L_{\hat{f}}^{(\rho_i)} \hat{h}_i(\hat{x}(t)|\hat{\theta}(t)) + L_{\hat{g}} L_{\hat{f}}^{\rho_i - 1} \hat{h}_i(\hat{x}(t)|\hat{\theta}(t))u(t).
\end{aligned} \tag{9}$$

We refer to such a scheme as *Lie-Sobolev state and parameter estimation (or identification).*[1]

In the next two sections, we formulate the Lie-Sobolev observer-estimator for nonlinear systems based on the gradient descent method, which underlies the majority of adaptive parameter estimation schemes (Fradkov, 1979). Specifically, a real-valued criterion J is defined based on the state observations $\hat{x}(t)$, their time derivatives $\hat{v}(t) = \dot{\hat{x}}(t)$ and parameter estimates $\hat{\theta}(t)$, given the measured inputs, outputs and output derivatives. The update rules are designed such that the time derivative of J is made as negative as possible. Depending on the way that $J(t)$ is defined, we formulate two different Lie-Sobolev estimation schemes.

- In the first type, $J(t)$ is defined based only on the current estimates and measurements. We view this explicit gradient-based identification scheme as a prototype approach, for which theoretical properties can be analyzed with classical Lyapunov arguments.
- The second type – MHE, is an implicit observer-estimator formulated as an optimization problem involving the current and past measurements. Its convergence properties are established in a similar way to the ordinary MHE whose analysis has been covered in the recent literature.

In addition to the constructive design procedures, we provide formal statements for the convergence and boundedness properties and their impact on control.

3. Lie-Sobolev gradient descent observer-estimator

3.1. Derivation

Consider the following function $J(t)$, which accounts for the residuals of the parameterized model (2) evaluated based on the estimations and measurements of inputs, outputs and output derivatives:

$$\begin{aligned}
J(t) &= Q(\hat{x}(t), \dot{\hat{x}}(t), \hat{\theta}(t)) \\
&= \frac{1}{2}\left\| \dot{\hat{x}}(t) - \hat{f}(\hat{x}(t)|\hat{\theta}(t)) - \hat{g}(\hat{x}(t)|\hat{\theta}(t))u(t) \right\|^2 \\
&+ \frac{1}{2}\sum_{i=1}^{d_y}\left[\sum_{r=0}^{\rho_i - 1} w_i^r \left\| y_i^{(r)}(t) - L_{\hat{f}}^r \hat{h}_i(\hat{x}(t)|\hat{\theta}(t)) \right\|^2 \right. \\
&\left. + w_i^{\rho_i}\left\| y_i^{(\rho_i)}(t) - L_{\hat{f}}^{\rho_i}\hat{h}_i(\hat{x}(t)|\hat{\theta}(t)) - L_{\hat{g}} L_{\hat{f}}^{\rho_i - 1}\hat{h}_i(\hat{x}(t)|\hat{\theta}(t))u(t) \right\|^2 \right]
\end{aligned} \tag{10}$$

where the weights w_i^r corresponding to the response of $y_i^{(r)}$, $r = 0, 1, \dots, \rho_i$, $i = 1, \dots, d_y$ are positive constants. If the terms in the brackets (involving y and y derivatives) are all removed except for the one corresponding to $r = 0$ (involving y), then J reduces to the one used in classical gradient descent methods. The criterion function $J(t)$ equals zero whenever the estimated model is equivalent to the true model and the state observation is error-free. J lends itself to the following performance measure that captures the distance between the estimated model functions $(\hat{f}(\cdot|\theta), \hat{g}(\cdot|\theta), \hat{h}(\cdot|\theta))$ and actual dynamics (f, g, h), which we refer to as the Lie-Sobolev norm.

[1] A Sobolev space, conventionally denoted as $W^{p,k}$, refers to a vector space of functions equipped with a Sobolev norm that is defined based on the L^p-norms of the function and its derivative functions up to order k.

Definition 3 (Lie-Sobolev norm)**.** For the identified model $\hat{f}(x|\hat{\theta})$, $\hat{g}(x|\hat{\theta})$, $\hat{h}(x|\hat{\theta})$, the squared Lie-Sobolev norm of the model error $(\Delta f, \Delta g, \Delta h) = (f, g, h) - (\hat{f}, \hat{g}, \hat{h})$ is

$$\|\Delta(f,g,h)\|_W^2 = \int_{\mathcal{X}\times\mathcal{U}} \|\Delta f + \Delta g u\|^2 + \sum_{i=1}^{d_y}\left[\sum_{r=0}^{\rho_i-1} w_i^r \left\|L_f^r h_i - L_{\hat{f}}^r \hat{h}_i\right\|^2 + w_i^{\rho_i}\left\|L_f^{\rho_i} h_i + L_g L_f^{\rho_i-1} h_i u - L_{\hat{f}}^{\rho_i}\hat{h}_i - L_{\hat{g}} L_{\hat{f}}^{\rho_i-1}\hat{h}_i u\right\|^2\right] dxdu \quad (11)$$

Here we assume that $\mathcal{U}$ contains a d_u-dimensional (i.e., full-dimensional) neighborhood of 0 and that the characteristic matrix

$$A(x) = \begin{bmatrix} L_{g_1} L_f^{\rho_1} h_1(x) & \cdots & L_{g_{d_u}} L_f^{\rho_1} h_1(x) \\ \vdots & \ddots & \vdots \\ L_{g_1} L_f^{\rho_{d_y}} h_{d_y}(x) & \cdots & L_{g_m} L_f^{\rho_{d_y}} h_{d_y}(x) \end{bmatrix} \quad (12)$$

is nonsingular, so that $\|(\Delta f, \Delta g, \Delta h)\|_W = 0$ only when $\Delta f(x)$, $\Delta g(x)$, $\Delta h(x)$ as well as the differences in the Lie derivatives involved in (11) are equal to 0 in $\mathcal{X}$. Thus, (11) gives a well-defined (positive definite) norm and $Q(\hat{x}(t), \dot{\hat{x}}(t), \hat{\theta}(t))$ can be regarded as an approximate evaluation of the Lie-Sobolev norm on the snapshot at time t. Hence, the observer-estimator should be designed with an aim to reduce the value of Q with time.

Assuming that the input signals are differentiable and the output signals are differentiable up to the order of relative degrees with respect to t,

$$\begin{aligned}\dot{Q} = {} & (\dot{\hat{x}} - \hat{f} - \hat{g}u)^\top\left[\ddot{\hat{x}} - \left(\frac{\partial \hat{f}}{\partial \hat{x}} + \sum_{j=1}^{d_u} u_j \frac{\partial \hat{g}_j}{\partial \hat{x}}\right)\dot{\hat{x}} + \left(\frac{\partial S}{\partial \hat{x}}\right)^\top - \hat{g}\dot{u}\right] \\ & + \left[\frac{\partial S}{\partial \hat{\theta}} - (\dot{\hat{x}} - \hat{f} - \hat{g}u)^\top\left(\frac{\partial \hat{f}}{\partial \hat{\theta}} + \sum_{j=1}^{d_u} u_j \frac{\partial \hat{g}_j}{\partial \hat{\theta}}\right)\right]\dot{\hat{\theta}} \\ & + \frac{\partial S}{\partial \hat{x}}(\hat{f} + \hat{g}u) + \frac{\partial S}{\partial u}\dot{u} + \sum_{i=1}^{d_y}\sum_{r=0}^{\rho_i} \frac{\partial S}{\partial y_i^{(r)}} y_i^{(r+1)},\end{aligned} \quad (13)$$

where

$$\begin{aligned} S = {} & S\left(\hat{x}, \hat{\theta}\middle| u, y_1, \dot{y}_1, \ldots, y_1^{(\rho_1)}, \ldots, y_{d_y}, \dot{y}_{d_y}, \ldots, y_{d_y}^{(\rho_{d_y})}\right) \\ = {} & \frac{1}{2}\sum_{i=1}^{d_y}\left[\sum_{r=0}^{\rho_i-1} w_i^r \left\|y_i^{(r)}(t) - L_{\hat{f}}^r \hat{h}_i(\hat{x}(t)|\hat{\theta}(t))\right\|^2 \right. \\ & \left. + w_i^{\rho_i}\left\|y_i^{(\rho_i)}(t) - L_{\hat{f}}^{\rho_i}\hat{h}_i(\hat{x}(t)|\hat{\theta}(t)) - L_{\hat{g}} L_{\hat{f}}^{\rho_i-1}\hat{h}_i(\hat{x}(t)|\hat{\theta}(t))u(t)\right\|^2\right] \end{aligned} \quad (14)$$

represents the part of Q after the first term in (10). In (13), $\dot{\hat{x}}$ and $\dot{\hat{\theta}}$ can be designed through the laws of the state observer σ and parameter estimator π in Eq. (5). We construct the state observer σ and parameter estimator π as follows:

$$\begin{aligned} \sigma &= -\Gamma_\sigma(v - \hat{f} - \hat{g}u) + \left(\frac{\partial \hat{f}}{\partial \hat{x}} + \sum_{j=1}^{d_u} u_j \frac{\partial \hat{g}_j}{\partial \hat{x}}\right)v - \left(\frac{\partial S}{\partial \hat{x}}\right)^\top + \hat{g}\dot{u} \\ \pi &= -\Gamma_\pi\left[\frac{\partial S}{\partial \hat{\theta}} - (\dot{\hat{x}} - \hat{f} - \hat{g}u)^\top\left(\frac{\partial \hat{f}}{\partial \hat{\theta}} + \sum_{j=1}^{d_u} u_j \frac{\partial \hat{g}_j}{\partial \hat{\theta}}\right)\right]. \end{aligned} \quad (15)$$

where $\Gamma_{\hat{x}}$ and $\Gamma_{\hat{\theta}}$ are tunable positive definite matrices of order d_x and d_θ, respectively.

3.2. Convergence properties

Substituting the observer-estimator law (15) into the expression of $\dot{Q}$ (13) according to (5), we can characterize the convergence property of the observer-estimator (15) based on Lyapunov stability analysis. To begin with, we consider the case with exact parameterization, i.e., there exists a true value of θ such that the errors between the functions f, g, h and Lie derivatives vanish. The following proposition gives the conditions for the nominal convergence of (15).

Proposition 1 (Nominal convergence of the gradient descent observer-estimator)**.** *Assume that*

- *$\hat{f}, \hat{g}, \hat{h}$, the Lie derivative functions and their partial derivatives with respect to $\hat{x}$ and $\hat{\theta}$ are bounded and Lipschitz in $\hat{x}$;*
- *Q is strongly convex in $\hat{\theta}$;*
- *$u, \dot{u}$ and $\hat{g}(\hat{x})$ are bounded;*
- *The errors in state observations are linearly bounded by the errors in their estimated dynamics and the parameter estimations, i.e., $\|\hat{x} - x\| \le c_1\|\dot{\hat{x}} - \hat{f} - \hat{g}u\| + c_2\|\hat{\theta} - \theta\|$ for some $c_1, c_2 > 0$.*

Under the observer-estimator (15), if the tunable matrices Γ_σ and Γ_π are chosen such that their smallest eigenvalues are large enough, then $\dot{Q} \le 0$ and the equality holds when $\dot{\hat{x}} = \hat{f}(\hat{x}) + \hat{g}(\hat{x})u$ and $\hat{\theta} = \theta$.

Remark 1 (Satisfiability of assumptions)**.** Among the above assumptions, the first and third are rather mild and can be satisfied as long as $\mathcal{X}$ and $\mathcal{U}$ are bounded sets and the input signals are generated with a bounded rate of change. Since Q is a weighted sum of squares of estimation errors, the strong convexity condition on Q essentially requires that the parameterization should be such that these estimation errors are strictly monotonically dependent on the parameters. In nonlinear process systems, such parameterizations can often be satisfied (at least locally), e.g., the conversion or flux quantities in transport-reaction systems usually have monotonic relations with the corresponding rate or activation energy constants. The last condition, however, usually can be verified only a-posteriori. If the errors in $\dot{x}$ grow with time, then the errors in x will grow on a higher order, and hence the linear bounding condition can not be satisfied by any constant c_1. Hence to meet the last condition, it is necessary to make the errors bounded, e.g., by designing the input signals such that the resulting state trajectory oscillates around the origin.

Remark 2 (Implication of nonlinear observability condition)**.** In the case of exact parameterization, the simultaneous state and parameter estimation is equivalent to the state observation of the following system of augmented states $\bar{x} = (x, \theta)$:

$$\begin{bmatrix}\dot{x} \\ \dot{\theta}\end{bmatrix} = \begin{bmatrix} f(x,\theta) \\ 0\end{bmatrix} + \begin{bmatrix} g(x,\theta) \\ 0 \end{bmatrix}u \\ y = h(x,\theta). \quad (16)$$

Denoting the corresponding model functions of the augmented states as $(\bar{f}, \bar{g}, \bar{h})$, we know from nonlinear control theory that the system (16) is observable if the observability co-distribution

$$\mathcal{O} = \operatorname{span}\left(dL_{\bar{g}_{j_1}}\ldots L_{\bar{g}_{j_k}}\bar{h}_i \middle| 0 \le j_1, \ldots, j_k \le d_u, 1 \le i \le d_y, k < \infty\right) \quad (17)$$

is of full rank (where $\bar{g}_0 = \bar{f}$). It then suffices if a restricted subspace of $\mathcal{O}$, which can be denoted as $\mathcal{O}'$, where the recursive Lie derivatives in its definition only contain the Lie derivatives that are involved in (10):

$$\mathcal{O}' = \operatorname{span}\left(dL_f^r h_i, dL_g L_f^{\rho_i-1} h_i \middle| 0 \le r \le \rho_i, 1 \le i \le d_y\right) \quad (18)$$

is also of full rank. This full-rank condition is in fact implied by the second and the fourth assumptions in Proposition 1, which guarantee that the convergence of the state observations and parameter estimations in (15) can be driven by $\partial S/\partial \bar{x} = (\partial S/\partial x, \partial S/\partial \theta)$, and hence $\partial S/\partial \bar{x}$ is of full rank. Examining the form of S in (14), it can be found that $(\partial S/\partial\bar{x})d\bar{x}\in\mathcal{O}'$. Therefore, $\mathcal{O}'$ must be a full-rank codistribution.

In general, when there exist structural errors, i.e., there is a non-vanishing distance between the parameterized and true dynamics even when $\hat{\theta}=\theta$ (for some "good" parameter estimate θ) and $\hat{x}=x$, the asymptotic convergence property is replaced with ultimate boundedness, if the structural errors are also bounded. This is stated in the following proposition.

Proposition 2 (Boundedness of errors of the gradient descent observer-estimator under structural uncertainty)**.** *Assume that*

- *$\hat{f},\hat{g},\hat{h}$, Lie derivatives and their partial derivatives are bounded linearly in the nominal parameter errors, state observation errors plus bounded quantities, i.e., for $\psi=f,g,h$, $L_f^r h_i$, $L_g L_f^{\rho_i-1}h_i$, $r=0,1,\dots,\rho_i$, $i=1,\dots,d_y$, there exists $m_\psi,\ell_\psi,c_\psi>0$, such that*

$$\|\psi(x)-\hat{\psi}(\hat{x}|\hat{\theta})\|\le m_\psi\|\theta-\hat{\theta}\|+\ell_\psi\|x-\hat{x}\|+c_\psi; \tag{19}$$

- *Q is strongly convex in $\hat{\theta}$ with a bounded deviation, i.e., $\partial Q/\partial\hat{\theta}=(\partial Q/\partial\hat{\theta})_0+\epsilon_Q^\top$, with $(\partial Q/\partial\hat{\theta})_0(\hat{\theta}-\theta)\ge\mu\|\hat{\theta}-\theta\|^2$ for some $\mu>0$ and $\|\epsilon_Q\|\le c_Q$ for some $c_Q>0$;*
- *$u,\dot{u}$ and $\hat{g}(\hat{x})$ are bounded;*
- *The errors in state observations are linearly bounded by the errors in their estimated dynamics and the parameter estimations, i.e., $\|\hat{x}-x\|\le c_1\|\dot{\hat{x}}-\hat{f}-\hat{g}u\|+c_2\|\hat{\theta}-\theta\|+c_0$ for some $c_1,c_2,c_0>0$.*

Under (15), the errors in state observations and parameter estimations will be ultimately bounded.

Assuming that the trajectory on which state and parameter estimation is performed is informative in the sense that it can be rendered close enough to any point in $\mathcal{X}\times\mathcal{U}$, and that the sensitivity of errors to such a distance is limited, the boundedness property can be generalized from the trajectory to $\mathcal{X}\times\mathcal{U}$.

Proposition 3 (Boundedness of identification error under the gradient descent observer-estimator)**.** *Suppose that the assumptions in Proposition 2 hold, and assume that*

- *For some $\epsilon>0$ and a corresponding $T_\epsilon>0$, there exists $t_1,\dots,t_{n_k}>T_\epsilon$ and $\eta>0$ such that for any $(x,u)\in\mathcal{X}\times\mathcal{U}$, $\|(x(t_k)-x,u(t_k)-u\|\le\eta$;*
- *$L_f^r h_i(x)-L_{\hat{f}}^r\hat{h}_i(x|\hat{\theta})$ and $L_g L_f^{\rho_i-1}h_i(x)-L_{\hat{g}}L_{\hat{f}}^{\rho_i-1}\hat{h}_i(x|\hat{\theta})$, $r=0,1,\dots,\rho_i$, $i=1,\dots,d_y$ are uniformly Lipschitz in x for all $\hat{\theta}\in\Theta$.*

Then there is an upper bound $B(\epsilon,\eta)>0$ such that

$$\|(\Delta f,\Delta g,\Delta h)\|_W^2\le B(\epsilon,\eta). \tag{20}$$

The proofs of the 3 propositions in this subsection are provided in Appendix A.

Remark 3 (Tuning of the matrices. Γ_σ and Γ_π**)** Under exact parameterization and the assumptions in Proposition 1, the nominal convergence is guaranteed for any positive definite Γ_σ and Γ_π, and hence using high-gain observers and estimators helps to accelerate the convergence. However, when the assumptions do not hold globally on $\mathcal{X}\times\mathcal{U}$, but rather locally in a neighborhood of zero errors, arbitrarily large matrices Γ_σ and Γ_π may not be allowed. When the parameterization induces structural errors, from the end of the proof of Proposition 2 in A.2 we see that the ultimate bound of errors has a lower bound that is independent of Γ_σ and Γ_π, which implies that the use of high-gain observers and estimators can not eliminate the intrinsic uncertainties.

3.3. Effect on input–output linearizing control

Assuming that the characteristic matrix $A(x)$ is nonsingular, then there exist vector fields $\zeta_k(x)$, $k=1,\dots,d_\zeta=d_x-\sum_{i=1}^{d_y}\rho_i$ to complement the Lie derivatives, satisfying $L_g\zeta_k=0$ ($k=1,\dots,d_\zeta$), such that the following nonlinear change of coordinates Φ is nonsingular (Isidori, 1995):

$$(\zeta,\xi)=\Phi(x)=[\zeta_1(x),\dots,\zeta_{d_\zeta}(x),L_f^0h_1(x),\dots,L_f^{\rho_1-1}h_1(x),\\ \dots,L_f^0h_{d_y}(x),\dots,L_f^{\rho_{d_y}-1}h_{d_y}(x)]^\top, \tag{21}$$

and thus an inverse transformation $x=\Phi^{-1}(\zeta,\xi)$ exists. Under the transformed coordinates, the original system (1) is expressed as

$$\begin{aligned}&\dot{\zeta}=Z(\zeta,\xi)\\&\dot{\xi}_i^0=\xi_i^1\\&\dots\\&\dot{\xi}_i^{\rho_i-1}=L_f^{\rho_i}h_i(x)+L_gL_f^{\rho_i-1}h_i(x)u\\&(i=1,\dots,d_y)\end{aligned} \tag{22}$$

where $\xi_i^0,\dots,\xi_i^{\rho_i-1}$ correspond to $y_i,\dots,y_i^{\rho_i-1}$, respectively. In the zero dynamics, ξ can be considered as the inputs to the partial states ζ. For the input–output linearizing control of system (22), if the states are accurately known, then the inputs can be specified as such that the output trajectories are shaped to satisfy

$$\sum_{i=1}^{d_y}\sum_{r=0}^{\rho_i}\beta_{ir}\frac{d^r y_i}{dt^r}(t)=\omega(t) \tag{23}$$

for a d_y-dimensional reference signal ω, in which $\beta_{ir}\in\mathbb{R}^{d_y}$ with $[\beta_{1\rho_1},\dots,\beta_{d_y\rho_{d_y}}]$ being a nonsingular matrix. In other words, the control law is designed as

$$u=\begin{bmatrix}\sum_{i=1}^{d_y}\beta_{i\rho_i}L_{g_1}L_f^{\rho_i-1}h_i(x) & \dots & \sum_{i=1}^{d_y}\beta_{i\rho_i}L_{g_{d_u}}L_f^{\rho_i-1}h_i(x)\end{bmatrix}^{-1}\\ \left[\omega-\sum_{i=1}^{d_y}\sum_{r=0}^{\rho_i}\beta_{ir}L_f^r h_i(x)\right]=:B(x)^{-1}b(x,\omega). \tag{24}$$

With observation and estimation errors, the terms in the ideal control law above are then replaced with the corresponding observed and estimated terms $B(\hat{x}|\hat{\theta})$ and $b(\hat{x}|\hat{\theta})$. This results in an additional term $\Delta\omega=B(B+\Delta B)^{-1}\Delta b-\Delta B(B+\Delta B)^{-1}b$ to the right-hand side of (23), where $\Delta B=B(\hat{x}|\hat{\theta})-B(x)$ and Δb is defined analogously. If the outputs and Lie derivatives are subject to bounded errors, then $\Delta\omega$ is bounded by their errors, as long as the nonsingularity of $B(x)$ is retained. Usually the reference response should be shaped such that the eigenvalues of the left-hand side of (23) should be negative in real parts. Hence the errors in outputs and output derivatives are bounded in terms of $\Delta\omega$ and thereafter in terms of the errors. That is, there exist positive constants c_ψ for $\psi=L_f^r h_i$, $r=0,\dots,\rho_i$ and $L_gL_f^{\rho_i-1}h_i$, $i=1,\dots,d_y$, such that a bound on the deviation of ξ from the reference trajectory (23) can be written as $\|\Delta\xi\|\le\sum_\psi c_\psi\|\psi(x)-\hat{\psi}(\hat{x}|\hat{\theta})\|$.

Then consider the deviation of the zero dynamics states ζ from its reference trajectory. Since the zero dynamics takes ξ as its input, as long as the incremental zero dynamics

$$\Delta\dot{\zeta}=Z(\zeta+\Delta\zeta,\xi+\Delta\xi)-Z(\zeta,\xi) \tag{25}$$

is input–state stable (ISS), then there exists $c'_\psi>0$ such that

$$\|\Delta\zeta\|\le\sum_\psi c'_\psi\|\psi(x)-\hat{\psi}(\hat{x}|\hat{\theta})\|. \tag{26}$$

The above discussion is summarized as follows.

Proposition 4 (Performance of input–output linearizing control under the gradient descent observer-estimator)**.** *Suppose that the assumptions in Proposition 2 hold, and also assume that*

- *The eigenvalues for the left-hand side of reference trajectory (23) are all negative in the real part.*
- *The incremental zero dynamics with $\Delta\xi$ as inputs and $\Delta\zeta$ as states is ISS.*

Then the input–output linearizing control based on the observer-estimator given by (15) gives a trajectory with bounded deviations from the reference (23).

4. Lie-Sobolev moving horizon estimator

4.1. Formulation

Different from the previous explicit observer-estimator, the Lie-Sobolev MHE determines the state observation $\hat{x}(t)$ and parameter estimation $\hat{\theta}(t)$ based on the historical measurements in the past time period of length T, by solving the following dynamic optimization problem about $\hat{\theta}$ and $\hat{x}(s)$ for $s \in [t-T, t]$:

$$\min \int_{t-T}^{t} Q(\hat{x}(s), \hat{\theta} | u(s), y(s)) ds + R(\hat{x}(t-T), \hat{\theta}) \tag{27}$$

The objective accounts for the discrepancies between the estimated outputs along with their time derivatives and the measured values. A regulation term $R(\hat{x}(t-T), \hat{\theta})$ accounts for the truncation before the time instant $t-T$ and the allowed range of parameters θ. The non-Lie-Sobolev counterpart takes the same form with the exception that Q does not involve output derivatives-related terms (see Eq. (10)). By solving the above problem, the obtained $\hat{x}(t)$ and $\dot{\hat{x}}(t)$ are the observed states and state derivatives at the current time t, respectively, and $\hat{\theta}$ is the current estimated parameters $\hat{\theta}(t)$. Although the practical approximate solution of the problem requires discretization, here we use the original formulation for analysis.

Applying variational calculus, one can verify that the optimal solution of the observation-estimation pair $(\{\hat{x}(s)|s \in [t-T, t]\}, \hat{\theta})$ should be specified by the following first-order optimality conditions:

$$\begin{aligned}
0 &= \frac{d}{ds}(\dot{\hat{x}}(s) - \hat{f}(\hat{x}(s)|\hat{\theta}) - \hat{g}(\hat{x}(s)|\hat{\theta})u(s)) - \frac{\partial S}{\partial \hat{x}}(\hat{x}(s), \hat{\theta}) \\
&\quad - (\dot{\hat{x}}(s) - \hat{f}(\hat{x}(s)|\hat{\theta}) - \hat{g}(\hat{x}(s)|\hat{\theta})u(s))^\top \\
&\quad \left(\frac{\partial \hat{f}}{\partial \hat{x}}(\hat{x}(s)|\hat{\theta}) + \sum_j u_j \frac{\partial \hat{g}_j}{\partial \hat{x}}(\hat{x}(s)|\hat{\theta})\right), s \in [t-T, t] \\
0 &= \dot{\hat{x}}(t-T) - \hat{f}(\hat{x}(t-T)|\hat{\theta}) \\
&\quad - \hat{g}(\hat{x}(t-T)|\hat{\theta})u(t-T) - \frac{\partial R}{\partial \hat{x}}(\hat{x}(t-T), \hat{\theta}) \\
0 &= \dot{\hat{x}}(t) - \hat{f}(\hat{x}(t)|\hat{\theta}) - \hat{g}(\hat{x}(t)|\hat{\theta})u(t) \\
0 &= \int_{t-T}^{t} \frac{\partial S}{\partial \hat{\theta}}(\hat{x}(s), \hat{\theta}) + (\dot{\hat{x}}(s) - \hat{f}(\hat{x}(s)|\hat{\theta}) - \hat{g}(\hat{x}(s)|\hat{\theta})u(s))^\top \\
&\quad \left(\frac{\partial \hat{f}}{\partial \hat{\theta}}(\hat{x}(s)|\hat{\theta}) + \sum_j u_j \frac{\partial \hat{g}_j}{\partial \hat{\theta}}(\hat{x}(s)|\hat{\theta})\right) ds + \frac{\partial R}{\partial \hat{\theta}}(\hat{x}(t-T), \hat{\theta}).
\end{aligned} \tag{28}$$

As the time t flows for an infinitesimal time δt, there will be infinitesimal changes in the inputs, outputs and output derivatives in the time horizon $[t-T, t]$, which are the parameters needed by the optimization problem (27). This will then result in changes $\delta\ddot{\hat{x}}, \delta\dot{\hat{x}}, \delta\hat{x}, \delta\hat{\theta}$ to guarantee that the first-order optimality conditions still hold. The procedure to find the changes in the optimal solution originating from changes in the parameters is known as *sensitivity analysis* (Fiacco, 1983).

Specifically, under appropriate regularity assumptions, the variation of the first equation in (28) can be expressed as

$$\delta\hat{\theta} = \pi\left(\left\{\delta\dot{\hat{x}}(s), \delta\hat{x}(s), \delta u(s), \delta Y(s) | s \in [t-T, t]\right\}\right) \tag{29}$$

for some linear functional π, and the variation of the third equation is

$$\delta\dot{\hat{x}}(t) = \sigma\left(\delta\hat{x}(t), \delta\hat{\theta}, \delta u(t), \delta Y(t)\right) \tag{30}$$

for some linear functional σ, in which $Y(s)$ is the collection of $y_i^{(r)}(s)$ for $r = 0, 1, \dots, \rho_i$, $i = 1, \dots, d_y$. The variations in the states and their derivatives during the horizon are determined by the variations of the fourth equation of (28) as second-order ODEs, and the variations of the second and third equations of (28) as two boundary conditions. This results in $\delta\hat{x}(s)$ and $\delta\dot{\hat{x}}(s)$ as linear functionals of $\{\delta u(s), \delta Y(s) | s \in [t-T, t]\}$ depending on the current solution. Therefore we can rewrite the above two formulas as

$$\begin{aligned}
\delta\hat{\theta} &= \pi\left(\left\{\dot{\hat{x}}(s), \hat{x}(s), u(s), Y(s), \delta u(s), \delta Y(s) | s \in [t-T, t]\right\}\right), \\
\delta\dot{\hat{x}}(t) &= \sigma\left(\hat{x}(t), \hat{\theta}, u(s), Y(s), \delta u(t), \delta Y(t)\right),
\end{aligned} \tag{31}$$

with functionals π and σ linear in $\delta u(s)$ and $\delta Y(s)$. Since $\delta u(s) = \dot{u}(s)\delta t$ and $\delta Y(s) = \dot{Y}(s)\delta t$, we finally have

$$\begin{aligned}
\dot{\hat{\theta}} &= \pi\left(\left\{\dot{\hat{x}}(s), \hat{x}(s), u(s), Y(s), \dot{u}(s), \dot{Y}(s) | s \in [t-T, t]\right\}\right), \\
\ddot{\hat{x}}(t) &= \sigma\left(\hat{x}(t), \hat{\theta}, u(s), Y(s), \dot{u}(t), \dot{Y}(t)\right).
\end{aligned} \tag{32}$$

This indicates that the MHE is an implicit dynamic system of an observer-estimator.[2]

4.2. Convergence properties

Due to the implicitness of MHE, the convergence properties need to be considered in a roundabout way. The key idea is to establish the conditions under which the objective function of (27) is a Lyapunov function, and the descent or boundedness of such a Lyapunov function implies convergence or boundedness of the distance to nominal parameters and true states. Such properties have been well studied in the literature (Rao et al., 2003; Ji et al., 2015; Müller, 2017). Here we rephrase the conditions for the convergence of MHE for state observation given in (Müller, 2017, Theorem 14). Compared to the original theorem, we simply augment the outputs with their derivatives, augment the states with time-invariant model parameters, and reformulate the conditions in continuous time.

Definition 4. A function α is said to belong to class $\mathcal{K}_\infty$ if it is defined on $[0, +\infty)$, strictly increasing, and such that $\alpha(0) = 0$ and $\alpha(r) \to \infty$ as $r \to \infty$. A function $\beta : [0, +\infty) \times [0, +\infty) \to [0, +\infty]$ is said to belong to class $\mathcal{KL}$ if it is strictly increasing in the first variable with $\beta(0, s) = 0$ for any s, and decreasing in the second variable with $\beta(r, s) \to 0$ as $s \to +\infty$.

Proposition 5 (Convergence properties of Lie-Sobolev MHE)**.** *Assume that*

[2] In many works on MHE (e.g., Kühl et al. (2011)), the consistency with the identified dynamic model is imposed as a hard constraint, which is the case with $w_i^r \to 0$. Bounds for $\hat{x}$ and $\hat{\theta}$ can also be imposed. Under such formulations, the above analysis of variations and sensitivities can be extended by incorporating the flow of the Lagrangian multipliers of equality constraints, known as co-states $\lambda(s)$, $s \in [t-T, t]$. Optimality conditions can be derived in a similar appearance to the equations in the Pontryagin maximum principle.

- *The system represented as the estimation model under nominal parameter values θ with structural errors w, v:*

$$\begin{aligned}&\dot{x} = \hat{f}(x|\theta) + \hat{g}(x|\theta)u + w\\ &y_i^{(r)} = \begin{cases} L_{\hat{f}}^r \hat{h}_i(x|\theta) + v_i^r, r = 0, 1, \dots, \rho_i - 1 \\ L_{\hat{f}}^{\rho_i}\hat{h}_i(x|\theta) + L_{\hat{g}} L_{\hat{f}}^{\rho_i}\hat{h}_i(x|\theta)u + v_i^{\rho_i}, r = \rho_i \end{cases}\end{aligned} \tag{33}$$

is incrementally input-to-state stable (ISS) and output-to-state stable (OSS). That is, there exists a $\mathcal{KL}$-class function β and two $\mathcal{K}_\infty$-class functions α_w and α_v, such that if the two systems (33) starts at time 0 from two different states $x(0)$ and $x'(0)$, then at any time t, their states $x(t)$ and $x'(t)$ have a distance bounded by

$$\begin{aligned}&\|x(t) - x'(t)\| \le \beta(\|x(0) - x'(0)\|, t)\\ &+\alpha_w(\|w - w'\|_{[0,t]}) + \alpha_v(\|v - v'\|_{[0,t]}).\end{aligned} \tag{34}$$

- *The function β satisfies $\beta(r, s) \le c_\beta r^{p_r} s^{-p_s}$ for some $c_\beta > 0$, $p_r \ge 1$, and $p_s > 0$. The functions α_w and α_v satisfy $\alpha_w(r) \le c_w r^{q_w}$ and $\alpha_v(r) \le c_v r^{q_v}$, respectively, for some $c_w, c_v, q_w, q_v > 0$.*
- *The regulation term $R(\hat{x}, \hat{\theta})$ is restricted by*

$$R(\hat{x}, \hat{\theta}) \in \left\| \begin{bmatrix} \hat{x}(t-T) - \hat{x}^*(t-T) \\ \hat{\theta} - \hat{\theta}^* \end{bmatrix} \right\|^q [m_R, M_R], \tag{35}$$

where $\left(\{\hat{x}^*(s) | s \in [t-T, t]\}, \hat{\theta}\right)$ is the optimal solution to (27), $M_R \ge m_R > 0$, and $\max(1/q_w, 1/q_v, 2p_r/p_s) \le q \le 2/\max(q_w, q_v)$.
- *The initial observation-estimation error and structural errors are bounded.*

Then the observation-estimation errors of the MHE (27) remain bounded. Furthermore in the absence of structural error in the model, $\hat{x}(t) - x(t) \to 0$, $\hat{\theta}(t) - \theta \to 0$.

4.3. Effect on nonlinear MPC

The nonlinear MPC of the system (1) is such a control strategy where at each time instant t, the control signal $u(t)$ is determined by solving the following optimization problem

$$\begin{aligned}&\min \int_t^{t+T} \ell(\tilde{x}(s), \tilde{u}(s))ds + \ell_f(\tilde{x}(t+T))\\ &\text{s.t.}\dot{\tilde{x}}(s) = f(\tilde{x}(s)) + g(\tilde{x}(s))\tilde{u}(s), s \in [t, t+T],\\ &\tilde{x}(t) = x(t)\end{aligned} \tag{36}$$

and extracting the first piece of the input signal $\tilde{u}(s)$ in the receding horizon $[t, t+T]$ (the horizon length T may be different from the one in MHE). The functions ℓ and ℓ_f are called stage cost and terminal cost, respectively. For simplicity we consider the case without process constraints. The stability conditions for nonlinear MPC have been well established in the literature, where the objective function of (36), denoted as V, is considered as a control-Lyapunov function. Specifically, if there exists a control policy $u = \kappa(x)$ such that

$$\frac{d\ell_f}{dx}(f(x) + g(x)\kappa(x)) \le -\ell(x, \kappa(x)) \tag{37}$$

then the asymptotic stability towards the origin follows from the descent property $\dot{V}(t) \le -\ell(x(t), u(t))$ under appropriate assumptions on the choice of the relevant functions (Mayne and Falugi, 2019).

When the model and the states are not precisely known, $(f(\cdot), g(\cdot))$ in (36) should be replaced by $(\hat{f}(\cdot|\hat{\theta}), \hat{g}(\cdot|\hat{\theta}))$, and $x(t)$ should be replaced by the observed state $\hat{x}(t)$. The effect of the accuracy of Lie derivatives on the solution of the MPC problem is implicit. First, the predicted states are related to the predicted outputs, output derivatives and states of the zero dynamics through the nonlinear transformation (21): $\tilde{x} = \Phi^{-1}(\tilde{\zeta}, \tilde{\xi})$, which transforms the MPC problem into the following form:

$$\begin{aligned}&\min \int_t^{t+T} \ell\big(\tilde{\zeta}(s), \tilde{\xi}(s), \tilde{u}(s)\big)ds + \ell_f\big(\tilde{\zeta}(t+T), \tilde{\xi}(t+T)\big)\\ &\text{s.t.}\dot{\tilde{\zeta}}(s) = Z\big(\tilde{\zeta}(s), \tilde{\xi}(s)\big), s \in [t, t+T]\\ &\dot{\tilde{\xi}}_i^r(s) = \tilde{\xi}_i^{r+1}(s), r = 0, \cdots, \rho_i - 2, s \in [t, t+T]\\ &\dot{\tilde{\xi}}_i^{\rho_i - 1}(s) = L_f^{\rho_i} h_i(\tilde{x}(s)) + L_g L_f^{\rho_i - 1} h_i(\tilde{x}(s))\tilde{u}(s), s \in [t, t+T]\\ &\tilde{x}(t) = x(t)\end{aligned} \tag{38}$$

where the Lie derivatives appear in the prediction of the transformed state trajectories. Alternatively, if only the outputs are accounted for in the objective function, one may use Chen-Fliess series expansion to express the outputs (Isidori, 1995, Section 3.2):

$$y_i(s) = h_i(x(t)) + \sum_{k=0}^{\infty} \sum_{j_0, \dots, j_k = 0}^{d_u} L_{g_{j_0}} \dots L_{g_{j_k}} h_i(x(t)) \int_t^s d\chi_{j_k} \dots d\chi_{j_0} \tag{39}$$

where

$$\begin{aligned}&g_0 = f, \chi_0(s) = s,\\ &\chi_j(s) = \textstyle\int_t^s u_j(s')ds', j = 1, \dots, d_u,\\ &\textstyle\int_t^s d\chi_{j_k} \dots d\chi_{j_0} = \int_t^s d\chi_{j_k}(s') \int_t^{s'} d\chi_{j_{k-1}} \dots d\chi_{j_0}.\end{aligned} \tag{40}$$

Again in (39) we see the presence of Lie derivatives.

We formalize the impact of the observation-estimation errors on the MPC performance by considering its perturbation on the stability conditions (37) and hence on the Lyapunov descent. The coordinate-transformed MPC formulation is used, with the dynamics abbreviated as $(\dot{\zeta}, \dot{\xi}) = \Lambda_0(\zeta, \xi) + \Lambda(\zeta, \xi)u$. Suppose that there exists a control policy $u = \kappa(\zeta, \xi)$ such that

$$\left(\frac{d\ell_f}{d\zeta}, \frac{d\ell_f}{d\xi}\right)(\Lambda_0(\zeta, \xi) + \Lambda(\zeta, \xi)\kappa(\zeta, \xi)) \le -\ell(\zeta, \xi, \kappa(\zeta, \xi)). \tag{41}$$

When the information of Λ_0 and Λ is erroneous, the right-hand side above needs to be added with a term to bound such errors. We may assume that structural errors are linearly bounded by $\|\hat{\theta} - \theta\|$ plus a positive constant. Then the change in the Lyapunov function becomes

$$\dot{V}(t) \le -\ell(\hat{x}(t), u(t)) + c_\theta\|\hat{\theta} - \theta\| + c_0 \tag{42}$$

for some $c_\theta, c_0 > 0$. Then, as long as the $\hat{x}(t)$ entry in the ℓ term above can be replaced by $x(t)$ with an additional term linear in the observation error $\|x(t) - \hat{x}(t)\|$, and the observation-estimation errors are ultimately bounded, it follows that

$$\dot{V}(t) \le -\ell(x(t), u(t)) + \epsilon \tag{43}$$

for some $\epsilon > 0$, which implies the ultimate boundedness of the states in the closed-loop system (Mayne and Falugi, 2019). The conditions are summarized in the following proposition.

Proposition 6 (Performance of MPC under the Lie-Sobolev MHE)**.** *Assume that*

- *the state observation and parameter estimation errors $(x - \hat{x}, \theta - \hat{\theta})$ are ultimately bounded, e.g., under the conditions of Proposition 5;*
- *the stage cost $|\ell(x) - \ell(\hat{x})| \le c_x\|x - \hat{x}\|$ for some $c_x > 0$;*
- *the structural errors in the transformed dynamics (22) are bounded by $c_\theta\|\hat{\theta} - \theta\| + c_0$ for some $c_\theta, c_0 > 0$;*
- *there exist $\mathcal{K}_\infty$-class functions α and α_f such that $\ell_f(x) \le \alpha_f(x)$ and $\ell(x, u) \ge \alpha(x)$.*

Then $\|x\|$ is ultimately bounded.

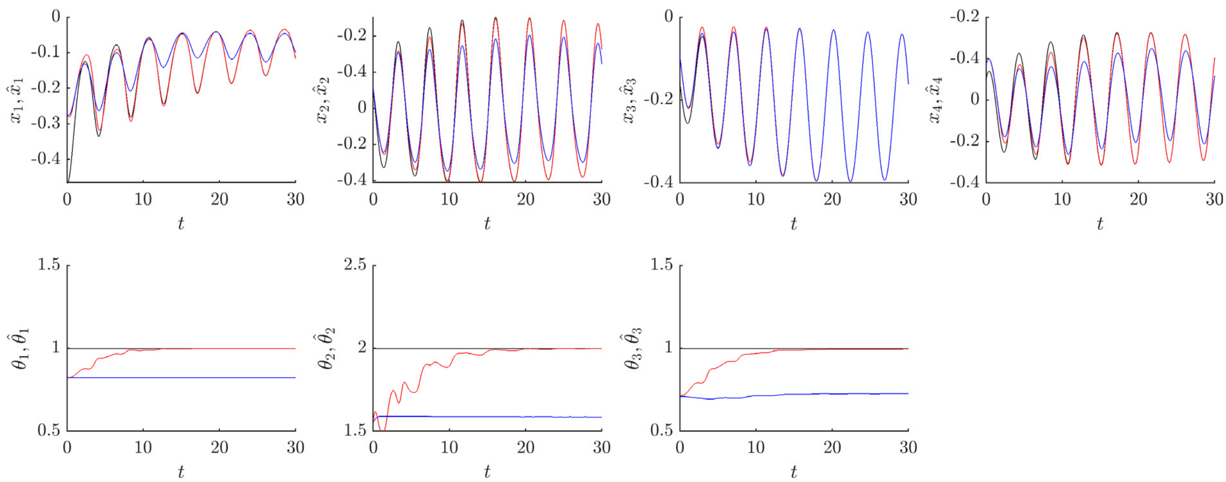

Fig. 1. Observed states and estimated parameters for (44) under the Lie-Sobolev (red) and non-Lie-Sobolev (blue) approaches compared to the true values (black). (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)

5. Applications

We apply the proposed Lie-Sobolev state and parameter estimation approaches to several examples. First, we use the explicit observer-estimator proposed in Section 3 on two numerical examples, one with exact parameterization, and the other with structural error in the parameterized model. Then we apply the Lie-Sobolev MHE in Section 4 to a complex chemical reactor system. Through these case studies, improved convergence of the estimated parameters, smaller structural errors, and better performance of the resulting nonlinear control can be seen in the Lie-Sobolev approaches compared to the non-Lie-Sobolev ones.

5.1. Example without structural errors

Consider the following system (Isidori, 1995, Example 4.1.5):

$$\dot{x} = \begin{bmatrix} \theta_1 x_1 x_2 - x_1^3 \\ x_1 \\ -x_3 \\ \theta_3 x_1^2 + x_2 \end{bmatrix} + \begin{bmatrix} 0 \\ \theta_2(1+x_3) \\ 1 \\ 0 \end{bmatrix} u, \quad y = x_4 \tag{44}$$

with true parameter values $\theta_1 = 1$, $\theta_2 = 2$ and $\theta_3 = 1$. By choosing the control input as a proportional feedback from the output, the resulting state trajectories appear to be oscillatory around the origin for a considerable time span, and hence this is considered as a suitable condition to perform system identification.

For the Lie-Sobolev approach, the weight constants w^0, w^1, w^2 are all set as 1. For the non-Lie-Sobolev one, w^1 and w^2 become 0. The tunable semidefinite matrices in the observer-estimator are empirically determined as $\Gamma_\sigma = \mathrm{diag}(5, 2, 2, 1)$, $\Gamma_\pi = \mathrm{diag}(1, 5, 1.5)$, under which the observed states and estimated parameters of the Lie-Sobolev approach converge to the true values.[3] The trajectories of $(\hat{x}, \hat{\theta})$ during a simulation time span of $T = 30$ are shown in Fig. 1. For non-Lie-Sobolev observation and estimation, the lack of convergence to the nominal values does not appear to be improved by choosing different tunings of Γ_σ and Γ_π. The reason for this limitation of the non-Lie-Sobolev approach is that when the output derivatives are not explicitly considered, the objective function can be insensitive to some of the parameters. After a short incipient time, the trajectories of the observed states become consistent with the estimated parameters that deviate from the true values. Afterwards, the updates on the estimated parameters are driven only by the difference between the output y and the observed $\hat{x}_4$, which results in changes significant only in $\hat{\theta}_3$.

5.2. Example with structural errors

Consider the following system (Isidori, 1995, Example 4.1.4):

$$\dot{x} = \begin{bmatrix} -x_1 \\ x_1 x_2 \\ x_2 \end{bmatrix} + \begin{bmatrix} \phi(x_2) \\ 1 \\ 0 \end{bmatrix} u, y = x_3 \tag{45}$$

where $\phi(x_2) = \exp(x_2)$ unknown a priori and parametrized as $\hat{\phi}(x_2|\theta) = \theta_0 + \theta_1 x_2 + \frac{1}{2}\theta_2 x_2^2$. A nominal estimation according to the Maclaurin series would be $\theta_0 = 1$, $\theta_1 = 1$, $\theta_2 = 1$. The tuning of the observer-estimator (15) is determined as $\Gamma_\sigma = I$, and $\Gamma_\pi = \mathrm{diag}(4, 1, 10)$. The resulting trajectories[4] within $T = 20$ are shown in Fig. 2, where one can observe that the Lie-Sobolev approach results in apparently smaller state observation errors, while under the non-Lie-Sobolev estimation, the state observation error does not appear to vanish. To quantify the performance of parameter estimation, we may calculate the integrated errors on the identified function ϕ: $\int_0^T (\phi(x(t)) - \hat{\phi}(\hat{x}(t)|\hat{\theta}(t)))^2 dt$, which equals 0.7131 for Lie-Sobolev estimation and 7.0140 for non-Lie-Sobolev estimation. This result confirms the advantage of using Lie-Sobolev estimation in the presence of structural errors.

A non-trivial problem involved in the Lie-Sobolev approach is how to numerically find the derivatives of y_i up to order ρ_i at any time instant $t > 0$. Generally, numerical derivatives will result in noise inevitably, and typically higher-order derivatives will be noisier than lower-order ones. If the assumptions in the propositions presented earlier still hold, then the theoretical convergence properties can be established. Here we use a sliding-mode differentiator proposed by (Levant, 2003), which was found to result in smaller noises compared to several other classical differentiators in numerical studies (Listmann and Zhao, 2013). The sliding mode

[3] The initial state for simulation $x(0)$ is chosen according to a uniform distribution in the hypercube $[-0.5, 0.5]^4$. The initialized observation error for x, $\hat{x}(0) - x(0)$ is randomized in $[-0.25, 0.25]^4$, and for $\dot{x}$, $\dot{\hat{x}}(0) - \dot{x}(0)$ is randomized in $[-0.25^2, 0.25^2] \times [-0.25, 0.25]^3$. The initial guess for the parameters, $\hat{\theta}(0)$, is randomly chosen in $[0.5, 1.5] \times [1.5, 2.5] \times [0.5, 1.5]$.

[4] The initial guess of parameters are chosen under a uniform distribution in $[0.5, 1.5]^3$. The initial state is chosen randomly in $[-0.5, 0.5]^3$, and the initial guess of states and state derivatives are perturbed from their true values respectively by $[-0.5, 0.5]^3$.

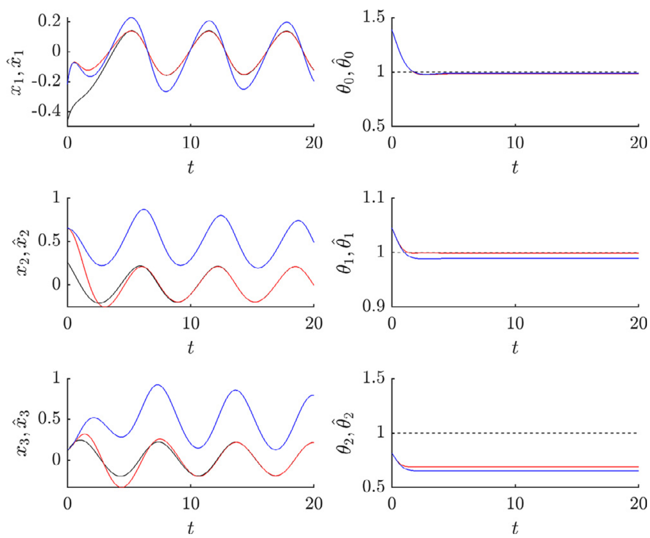

Fig. 2. Observed states and estimated parameters for (45) under Lie-Sobolev (red) and ordinary (blue) identification, respectively. The solid curves and dashed lines in black are true states and nominal parameter values, respectively. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)

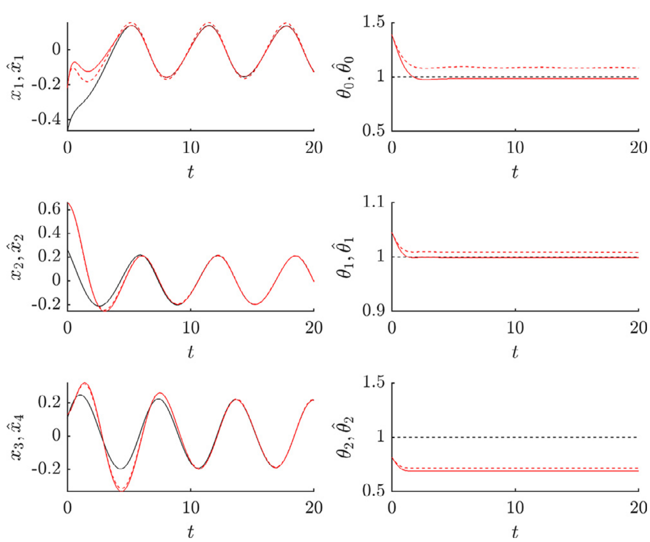

Fig. 3. Observed states and estimated parameters for (45) under the Lie-Sobolev approach with exact output derivatives (red solid) and sliding mode numerical differentiation (red dash). (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)

differentiator is written as

$$\begin{aligned} \dot{z}_i^0 &= -\lambda_i^0 \gamma_i^{\frac{1}{\rho_i+1}} |z_i^0 - y_i|^{\frac{\rho_i}{\rho_i+1}} \mathrm{sign}(z_i^0 - y_i) + z_i^1 \\ \dot{z}_i^r &= -\lambda_i^r \gamma_i^{\frac{1}{\rho_i-r+1}} |z_i^r - \dot{z}_i^{r-1}|^{\frac{\rho_i-r}{\rho_i-r+1}} \mathrm{sign}(z_i^r - \dot{z}_i^{r-1}) + z_i^{r+1} \\ (r &= 1, \dots, \rho_i - 1) \\ \dot{z}_i^{\rho_i} &= -\lambda_i^{\rho_i} \gamma_i \mathrm{sign}(z_i^{\rho_i} - \dot{z}_i^{\rho_i-1}) \end{aligned} \tag{46}$$

where the parameters are recommended as $\lambda_i^0 = 12$, $\lambda_i^1 = 8$, $\lambda_i^2 = 5$, with γ_i being a tunable Lipschitz estimate of the y_i signal. z_i^r is thus an estimate of $y_i^{(r)}$. For faster ODE solution, we approximate sign$(\cdot)$ with tanh$(\cdot/0.01)$.

Assuming an initial deviation of z from $(y, \dot{y}, \ddot{y})$ randomized according to a uniform distribution in $[0.5, 0.5]^3$, under the Levant sliding mode differentiator ($\gamma = 1$), the trajectories of the observed states and estimated parameters are shown in Fig. 3. It is observed that the trajectories under the sliding mode differentiator are asymptotically close to the trajectories with exact output derivatives. The integrated errors for the numerical differentiation-based estimation is 0.8993, 26.1% larger than the exact case. It is thus concluded that due to the capability of sliding mode differentiator to give accurate estimations of output derivatives, the performance of numerical differentiation-based Lie-Sobolev state and parameter estimation remains satisfactory.

Remark 4 (Filtering differentiation of noisy signals)**.** Practically, the output measurements usually contain noise. Signal preprocessing and filtering techniques need to be applied in this case. For example, in the Laplace domain, the differentation operator s can be modified as $s/(1+\lambda s)$ with a time constant $\lambda > 0$ which should be much larger than that of the noise dynamics while much shorter than the dynamics of the differentiated signal.

5.3. A glycerol etherification reactor

We consider a glycerol etherification reactor (Liu et al., 2016) with 6 states, 1 input and 1 output, and a relative degree of 1. The true dynamics involving the thermodynamics of non-ideal mixtures is approximated by a 6-parameter ideal mixture model. It is desirable to handle such structural errors with Lie-Sobolev estimation, in which the time derivative of the output accounts for the sensitivity of reaction rates on component concentrations. A detailed description of the system is given in Appendix B.

For the estimation, a sinusoidal excitation is imposed on the input F_1 with an amplitude of 50 kmol/h and a period of 1 h. The output derivatives are obtained by Levant's sliding mode differentiator (46). The horizon length for MHE is set as 1.5 h. The trajectories of observed states, estimated parameters, and the correspondingly inferred outputs and output derivatives of the Lie-Sobolev and non-Lie-Sobolev MHEs[5] are compared to the actual states and nominal parameters in Fig. 4. It is observed that due to the structural error in the parametric model assuming ideal liquid mixture, the observed states and estimated parameters inevitably have deviations from the true values of states and nominal kinetic parameters. By using the Lie-Sobolev MHE, the observation and estimation result in significantly smaller deviations in the output derivative. Comparing the trajectories of the Lie-Sobolev MHE to those of the non-Lie-Sobolev MHE, we note that the different decisions made by the two identification schemes include primarily the estimation of θ_3 and secondarily the estimation of θ_2, namely the pre-exponential factors of the two main reactions occurring in the system – the reactions of IB with DE (with a molar fraction of about 0.1045) and with ME (with a molar fraction of approximately 0.0436).

To examine the impact of Lie-Sobolev MHE on nonlinear control, MPC simulations are then performed based on the identified model starting from initial points randomly sampled around the steady state within the state bounds of the MHEs. The MPC is activated after one MHE horizon is passed, before which the control signal is fixed at zero. The prediction horizon length and the discretization scheme is the same as those of MHE, and the sampling time is 0.1 h, during which the control input is held constant. Fig. 5 shows the closed-loop trajectories of inputs and states using MPC based on MHE as the state observer and the models

[5] The MHE is discretized by 30 finite elements. The weights for output and output derivative are 10^2 and 1, respectively. The MHEs are coded using the `pyomo.dae` module (Nicholson et al., 2018) in Python 3.6 in Anaconda 3 with IPOPT 3.11.1 as the solver. The computational performance is improved by providing a lower bound $(-5, -5, 1, 1, 5, 1)$ and an upper bound $(-0.5, -1, 10, 10, 15, 5)$ on the parameters. The observed states are bounded within a proportion of $(0.1, 0.025, 0.1, 0.1, 0.1, 0.1)$ of their respective steady-state values, and the quadratic inverse of these bounds are used as the weights of the states.

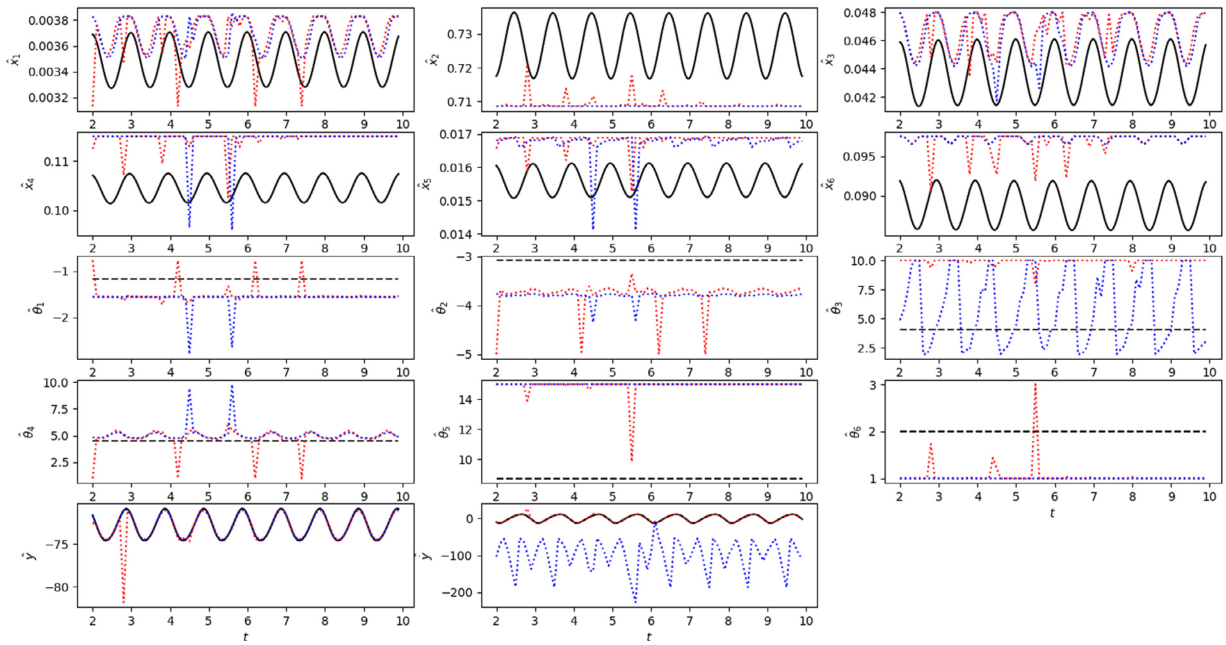

Fig. 4. Observed states and estimated parameters for the glycerol etherification reactor under Lie-Sobolev (red dotted) and ordinary (blue dotted) MHE, respectively. The solid curves and dashed lines in black are true states and nominal parameter values, respectively. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)

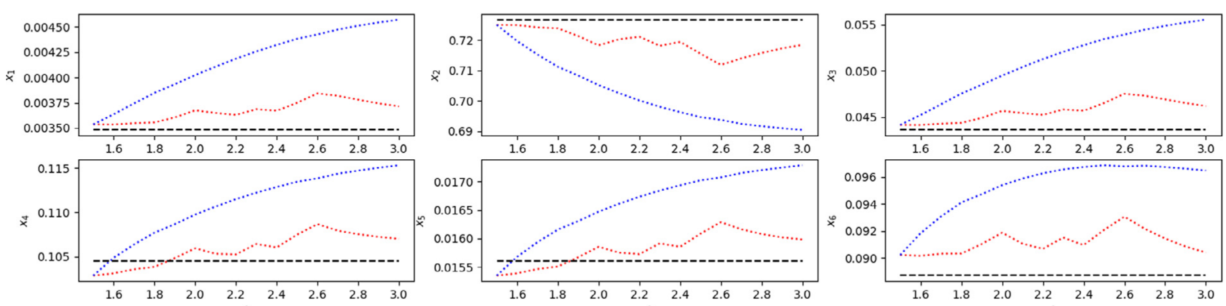

Fig. 5. Closed-loop trajectories of MHE-MPC based on Lie-Sobolev (red) and non-Lie-Sobolev estimation (blue) compared to the steady state (black). (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)

determined by the Lie-Sobolev and non-Lie-Sobolev identification. Clearly, the model predictive controller using the Lie-Sobolev estimated model parameters and Lie-Sobolev MHE better stabilizes the process near the steady state in the presence of structural errors, while the non-Lie-Sobolev controller steers the molar fractions away from the steady state. In other words, nonlinear system identification using the Lie-Sobolev MHE results in improved MPC control performance.

It should be noted, however, that the incorporation of Lie derivative terms significantly increases the computational difficulty of solving the MHE problem. The total computational time for MHE in the above MPC simulation is 372.3 and 116.4 seconds with Lie-Sobolev and non-Lie-Sobolev state observation, respectively. Solver failures are also more frequently encountered.

6. Conclusions

In this paper we have proposed that for nonlinear control, it is desirable to perform state and parameter estimation following a Lie-Sobolev procedure, where the state observations and parameter estimates aim to match not only the predicted outputs but also the output time derivatives to the measurements. We have discussed the Lie-Sobolev formulations and their convergence properties for explicit gradient descent-based and implicit moving horizon-based estimation schemes. Their effects on input–output linearizing control and MPC have also been discussed, respectively. The improved performance of Lie-Sobolev state and parameter estimation was demonstrated by two numerical examples and a case study on a glycerol etherification reactor.

We note that classical observer and estimator designs tend to avoid using time derivatives of output variables due to the view that the derivative estimates are usually inaccurate with noisy output signals. On the other hand, as shown in this work, Lie-Sobolev schemes that exploit derivative information can play a significant role in improving the identification and control performance, assuming that the outputs are accurately measured and appropriate numerical differentiators are used. How these two aspects can be reconciled towards better practice in a general setting remains an open question.

Declaration of Competing Interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

CRediT authorship contribution statement

Wentao Tang: Conceptualization, Formal analysis, Investigation, Methodology, Software, Validation, Visualization, Writing - original draft. **Prodromos Daoutidis:** Conceptualization, Funding acquisition, Project administration, Resources, Supervision, Writing - review & editing.

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Appendix A. Proofs of Propositions 1–3

A1. Proof of Proposition 1

The design of the gradient descent-based observer-estimator results in the time derivative of Q equal to

$$\dot{Q} = -\left\|\dot{\hat{x}} - \hat{f} - \hat{g}u\right\|^2_{\Gamma_\sigma} - \left\|\frac{\partial Q}{\partial \hat{\theta}}\right\|^2_{\Gamma_\pi} + \frac{\partial S}{\partial \hat{x}}(\hat{f} + \hat{g}u) + \frac{\partial S}{\partial u}\dot{u} + \sum_{i=1}^{d_y}\sum_{r=0}^{\rho_i}\frac{\partial S}{\partial y_i^{(r)}}y_i^{(r+1)}. \tag{A.1}$$

The first two terms are negative whenever $\dot{\hat{x}}(t) = \hat{f}(\hat{x}(t)|\hat{\theta}(t)) + \hat{g}(\hat{x}(t)|\hat{\theta}(t))u(t)$ and $\partial Q/\partial\hat{\theta} = 0$ are not satisfied, i.e., when there exist state observer errors and the parameter estimates are not at their temporal stationary values, respectively. The remaining three terms are not manipulable by the construction of σ and π, in which the first term is the change of S resulted from the flow of the state observations, and the other two terms are resulted from the exogenous changes in the input and output and output derivative signals, respectively. For convergence, these non-manipulable terms should be small enough compared to the negative definite terms.

By finding the partial derivatives of S and substituting them into (A.1), after simplifications we have

$$\begin{aligned}\dot{Q} = &-\left\|\dot{\hat{x}} - \hat{f} - \hat{g}u\right\|^2_{\Gamma_\sigma} - \left\|\frac{\partial Q}{\partial \hat{\theta}}\right\|^2_{\Gamma_\pi} \\ &+ \sum_{i=1}^{d_y}\left\{\sum_{r=0}^{\rho_i-1} w_i^r \Delta(L_f^r h_i)\left[\Delta\left(\frac{\partial L_f^r h_i}{\partial x}\right)(f+gu) + \frac{\partial L_f^r h_i}{\partial x}(\Delta f + \Delta g u)\right]\right. \\ &+ w_i^{\rho_i}\left[\Delta(L_f^{\rho_i}h_i) + \Delta(L_g L_f^{\rho_i}h_i)u\right]\left[\Delta\left(\frac{\partial L_f^{\rho_i}h_i}{\partial x} + \frac{\partial L_g L_f^{\rho_i-1}h_i}{\partial x}u\right)(f+gu)\right. \\ &\left.\left.+\left(\frac{\partial L_f^{\rho_i}h_i}{\partial x} + \frac{\partial L_g L_f^{\rho_i-1}h_i}{\partial x}u\right)(\Delta f + \Delta g u) + \Delta(L_g L_f^{\rho_i-1}h_i)\dot{u}\right]\right\}. \end{aligned} \tag{A.2}$$

where Δ denotes the differences between the true dynamics evaluated at true states $x(t)$ and the estimated dynamics at observed states $\hat{x}(t)$. Under the assumptions of Proposition 1, there exist constants $c_\sigma, c_\pi > 0$ such that

$$\dot{Q} \le -c_\sigma\|\dot{\hat{x}} - \hat{f} - \hat{g}u\|^2 - c_\pi\|\hat{\theta} - \theta\|^2, \tag{A.3}$$

and hence the criterion $Q(t)$ becomes a Lyapunov function. As $t \to \infty$, we have $\dot{\hat{x}}(t) - \hat{f}(\hat{x}(t)|\hat{\theta}(t)) - \hat{g}(\hat{x}(t)|\hat{\theta}(t))u(t) \to 0$ and $\hat{\theta}(t) - \theta \to 0$, and therefore $\hat{x}(t) - x(t) \to 0$.

A2. Proof of Proposition 2

Under the first two assumptions, we may specify constants $M_{11}, M_{12}, M_{22}, M_0 > 0$ such that

$$\begin{aligned}\dot{Q} \le &-\|\dot{\hat{x}} - \hat{f} - \hat{g}u\|^2_{\Gamma_\sigma} - \left\|\left(\frac{\partial Q}{\partial\hat{\theta}}\right)_0 + \epsilon_Q^\top\right\|^2_{\Gamma_\pi} + M_{11}\|\dot{\hat{x}} - \hat{f} - \hat{g}u\|^2 \\ &+ 2M_{12}\|\dot{\hat{x}} - \hat{f} - \hat{g}u\|\,\|\hat{\theta} - \theta\| + M_{22}\|\hat{\theta} - \theta\|^2 + M_0,\end{aligned} \tag{A.4}$$

where the second term on the right hand side is further bounded by $-\mu\lambda_{\min}(\Gamma_\pi)\|\hat{\theta} - \theta\|^2 + 2c_Q\lambda_{\max}(\Gamma_\pi)(\partial Q/\partial\hat{\theta})$, where $\partial Q/\partial\hat{\theta}$ can be bounded linearly with $m_Q, \ell_Q, c_Q > 0$ as in the first assumption. It follows that

$$\begin{aligned}\dot{Q} \le \quad &-M_2\left(\left\|\dot{\hat{x}} - \hat{f} - \hat{g}u\right\|^2 + \mu\|\hat{\theta} - \theta\|^2\right) \\ &+M_1\left(\left\|\dot{\hat{x}} - \hat{f} - \hat{g}u\right\|^2 + \mu\|\hat{\theta} - \theta\|^2\right)^{1/2} + M_0,\end{aligned} \tag{A.5}$$

where

$$\begin{aligned}M_1 &= 2c_Q\lambda_{\max}(\Gamma_\pi)\left(\ell_Q + \tfrac{m_Q}{\mu}\right)\max(\ell_Q, m_Q), \\ M_2 &= \min\left(\lambda_{\min}(\Gamma_\sigma) - M_{11} - \tfrac{M_{12}}{\mu}, \lambda_{\min}(\Gamma_\pi) - M_{12} - \tfrac{M_{22}}{\mu}\right).\end{aligned} \tag{A.6}$$

Therefore Q is guaranteed to decrease unless

$$\left\|\dot{\hat{x}} - \hat{f} - \hat{g}u\right\|^2 + \mu\|\hat{\theta} - \theta\|^2 \le \left(\frac{M_1 + (M_1^2 + 4M_0M_2)^{1/2}}{2M_2}\right)^2. \tag{A.7}$$

When this inequality is satisfied, according to the first assumption, there will be a corresponding upper bound $Q_{\max} > 0$ of Q. In other words, whenever $Q \ge Q_{\max}$, $\dot{Q} < 0$, implying that Q is ultimately bounded, and hence the errors are ultimately bounded. Thus we have proved the proposition. We note that the right-hand side expression above is always lower-bounded by a constant:

$$M_1/M_2 \ge c_Q(\ell_Q + m_Q/\mu)\max(\ell_Q, m_Q). \tag{A.8}$$

A3. Proof of Proposition 3

Having assumed the Lipschitz continuity of f, g, h and Lie derivatives, we can claim that the difference between the estimated model and the true dynamics and their Lie derivatives will be ultimately bounded. That is, $\exists B > 0$, $\forall\epsilon > 0$, $\exists T_\epsilon > 0$ such that $\forall t > T_\epsilon$,

$$\begin{aligned}&\|f(x(t)) - \hat{f}(x(t)|\hat{\theta}(t)) + g(x(t))u(t) - \hat{g}(x(t)|\hat{\theta}(t))u(t)\|^2 \\ &+\textstyle\sum_{i=1}^{d_y}\left[\sum_{r=0}^{\rho_i-1} w_i^r\|L_f^r h_i(x(t)) - L_{\hat{f}}^r\hat{h}_i(x(t)|\hat{\theta}(t))\|^2\right. \\ &+w_i^{\rho_i}\|L_f^{\rho_i}h_i(x(t)) - L_{\hat{f}}^{\rho_i}\hat{h}_i(x(t)|\hat{\theta}(t)) + L_g L_f^{\rho_i-1}h_i(x(t))u(t) \\ &\left.-L_{\hat{g}}L_{\hat{f}}^{\rho_i-1}\hat{h}_i(x(t)|\hat{\theta}(t))u(t)\|^2\right] \le B + \epsilon.\end{aligned} \tag{A.9}$$

Under the assumptions of Propositions 2 and 3, replacing the $x(t)$ and $u(t)$ with any $x \in \mathcal{X}$ and $u \in \mathcal{U}$ leads to an increase linearly bounded by η on the right-hand side of the above formula. That is, $\forall x \in \mathcal{X}$, $\forall u \in \mathcal{U}$,

$$\begin{aligned}&\|f(x) - \hat{f}(x|\theta) + g(x)u - \hat{g}(\hat{x}|\theta)u\|^2 \\ &+\textstyle\sum_{i=1}^{d_y}\left[\sum_{r=0}^{\rho_i-1} w_i^r\|L_f^r h_i(x) - L_{\hat{f}}^r\hat{h}_i(x|\theta)\|^2\right. \\ &+w_i^{\rho_i}\|L_f^{\rho_i}h_i(x) - L_{\hat{f}}^{\rho_i}\hat{h}_i(x|\theta) \\ &\left.+L_g L_f^{\rho_i-1}h_i(x)u - L_{\hat{g}}L_{\hat{f}}^{\rho_i-1}\hat{h}_i(x|\theta)u\|^2\right] \le B(\epsilon, \eta).\end{aligned} \tag{A.10}$$

Thus proving the proposition.

Table B1
Parameters related to the reaction kinetics.

E_1	21.3 kJ/mol	k_1°	2.56×10^2 kmol/(h · mol H)
E_2	39.1 kJ/mol	k_2°	1.14×10^5 kmol/(h · mol H)
E_3	25.6 kJ/mol	k_3°	7.52×10^3 kmol/(h · mol H)
E_4	39.9 kJ/mol	k_4°	5.59×10^3 kmol/(h · mol H)
ΔH_1	−49.4 kJ/mol	ΔS_1	−119.1 J/(mol · K)
ΔH_2	−6.0 kJ/mol	ΔS_2	−36.9 J/(mol · K)
ΔH_3	−27.1 kJ/mol	ΔS_3	−89.8 J/(mol · K)
ΔH_{a1}	−7.6 kJ/mol	K_{a1}°	2.51×10^{-1}
ΔH_{a2}	−12.3 kJ/mol	K_{a2}°	2.24×10^{-4}
w_1	92 kg/mol	ρ_1	1261 kg/m^3
w_2	56 kg/mol	ρ_2	588 kg/m^3
w_3	148 kg/mol	ρ_3	1015 kg/m^3
w_4	204 kg/mol	ρ_4	920 kg/m^3
w_5	260 kg/mol	ρ_5	880 kg/m^3
w_6	112 kg/mol	ρ_6	718 kg/m^3
w_7	18 kg/mol	ρ_7	1000 kg/m^3
ρ_{cat}	60 kg/m^3	q	4.7 mol H/kg

Appendix B. Dynamics of the etherification reactor

In the glycerol etherification process, glycerol reacts with isobutene to yield mono-, di-, and tri-*tert*-butyl ethers of glycerol with a side dimerization reaction of isobutene:

G + IB <=> ME, ME + IB <=> DE,

DE + IB <=> TE, 2 IB − > DIB.

Apart from these components, water (W) exists in the system as the solvent. The stoichiometric constants ν_{ij} of the 7 species (1=G, 2=IB, 3=ME, 4=DE, 5=TE, 6=DIB, 7=W, subscripted by i) in the 4 reactions (subscripted by j) are given as

$$\begin{aligned}&\nu_{11}=-1, \nu_{21}=-1, \nu_{31}=1, \nu_{22}=-1, \nu_{32}=-1,\\&\nu_{42}=1, \nu_{23}=-1, \nu_{43}=-1, \nu_{53}=1, \nu_{24}=-2,\\&\nu_{64}=1, \text{other } \nu_{ij}=0.\end{aligned} \tag{B.1}$$

The rates of the 4 reactions, in terms of total extent per unit time per mole of active catalytic site (kmol · h^{-1} · (mol H)$^{-1}$), are

$$r_1=\frac{k_1(a_1a_2-a_3/K_{e1})}{(1+K_{a1}a_1+K_{a2}a_2)^2},\quad r_2=\frac{k_2(a_2a_3^2-a_4/K_{e2})}{1+K_{a1}a_1+K_{a2}a_2},$$
$$r_3=\frac{k_3(a_2a_4^2-a_5/K_{e3})}{1+K_{a1}a_1+K_{a2}a_2},\quad r_4=\frac{k_4a_2^2}{(1+K_{a1}a_1+K_{a2}a_2)^2}, \tag{B.2}$$

where k and K_e stands for the rate constants, related to pre-exponential factors and activation energies, and equilibrium constants, related to the enthalpy and entropy changes, respectively. The adsorption equilibrium constants K_a follow similar rules:

$$\begin{aligned}&k_j=k_j^\circ\exp(-E_j/RT), K_{ej}=\exp(-\Delta H_j/RT+\Delta S/R),\\&K_{ai}=K_{ai}^\circ\exp(-\Delta H_{ai}/RT).\end{aligned} \tag{B.3}$$

The reaction rate for each species is therefore

$$R_i=\textstyle\sum_{j=1}^4\nu_{ij}r_jV\rho_{cat}q,\quad V=M\sum_{j=1}^7\frac{w_jx_j}{\rho_j}. \tag{B.4}$$

with q being the quantity of active sites in moles per mass of catalyst, ρ_{cat} the density of catalyst, and V the volume of reacting liquid linked to the total molar holdup M and molar fractions x_j by densities ρ_j and molar weights w_j. The true values of these constants are listed in Table B.1. We assume that the thermodynamic constants E_j, ΔH_j, ΔS_j, ΔH_{ai} are known exactly, while the pre-exponential factors k_j° ($j=1,2,3,4$) for the reaction rates and K_{ai}° ($i=1,2$) for adsorption equilibria are to be estimated.

For the activity of the chemical species in the multicomponent liquid mixture, the NRTL model is used:

$$a_i=\gamma_ix_i,$$
$$\ln\gamma_i=\frac{\sum_j x_j\frac{A_{ji}}{RT}\exp\left(-\frac{\alpha_{ji}A_{ji}}{RT}\right)}{\sum_j x_j\exp\left(-\frac{\alpha_{ji}A_{ji}}{RT}\right)}+\sum_j\frac{x_j\exp\left(-\frac{\alpha_{ij}A_{ij}}{RT}\right)}{\sum_k x_k\exp\left(-\frac{\alpha_{ik}A_{ik}}{RT}\right)}$$
$$\times\left(\frac{A_{ij}}{RT}-\frac{\sum_k x_kA_{kj}\exp\left(-\frac{\alpha_{kj}A_{kj}}{RT}\right)}{\sum_k x_k\exp\left(-\frac{\alpha_{kj}A_{kj}}{RT}\right)}\right), i=1,\dots,7. \tag{B.5}$$

Table B2
Parameters in the NRTL model.

A_{12}	6000.6295	A_{21}	7790.3843	α_{12}	0.2
A_{13}	5093.9878	A_{31}	−261.0596	α_{13}	0.2
A_{14}	15394.2024	A_{41}	3470.2636	α_{14}	0.2
A_{15}	18947.6060	A_{51}	9748.1650	α_{15}	0.2
A_{16}	10108.9095	A_{61}	16721.0340	α_{16}	0.2
A_{17}	−2280.9459	A_{71}	2145.9265	α_{17}	1.011
A_{23}	10225.3886	A_{32}	−2579.3354	α_{23}	0.2
A_{24}	−3867.1740	A_{42}	−6172.8956	α_{24}	0.2
A_{25}	−3867.1740	A_{52}	−6172.8956	α_{25}	0.2
A_{26}	−735.1239	A_{62}	472.8172	α_{26}	0.329
A_{27}	11654.4821	A_{72}	11799.1457	α_{27}	0.255
A_{34}	−4605.9560	A_{43}	8587.5306	α_{34}	0.2
A_{35}	7737.8398	A_{53}	−1327.7458	α_{35}	0.2
A_{36}	2163.8848	A_{63}	10377.8670	α_{36}	0.275
A_{37}	−3457.2938	A_{73}	13410.9808	α_{37}	0.392
A_{45}	9937.7242	A_{54}	−3728.8290	α_{45}	0.2
A_{46}	−1867.1581	A_{64}	8318.6558	α_{46}	0.286
A_{47}	−168.9405	A_{74}	20784.1686	α_{47}	0.345
A_{56}	−3141.0292	A_{65}	6209.7266	α_{56}	0.398
A_{57}	−386.1022	A_{75}	20784.9169	α_{57}	0.202
A_{67}	9981.2064	A_{76}	20784.9169	α_{67}	0.2

Table B3
Parameters and steady states in the reactor dynamics.

x_1	0.0035	x_2	0.7267	x_3	0.0436
x_4	0.1045	x_5	0.0156	x_6	0.0887
$x_{1,1}$	0.0000	$x_{1,2}$	0.9198	$x_{1,3}$	0.0000
$x_{1,4}$	0.0000	$x_{1,5}$	0.0000	$x_{1,6}$	0.0584
$x_{2,1}$	0.0000	$x_{2,2}$	0.9731	$x_{2,3}$	0.0000
$x_{2,4}$	0.0000	$x_{2,5}$	0.0000	$x_{2,6}$	0.0192
$x_{3,1}$	0.7674	$x_{3,2}$	0.0000	$x_{3,3}$	0.2294
$x_{3,4}$	0.0001	$x_{3,5}$	0.0000	$x_{3,6}$	0.0000
F_1	185.4900	F_2	1.7267	F_3	40.1762

The parameters in the NRTL model is listed in Table B.2. For $i=1,\dots,7$, $A_{ii}=0$ and $\alpha_{ii}=0$. For $i,j=1,\dots,7$, $\alpha_{ij}=\alpha_{ji}$. We assume that the NRTL model is unknown, and in the identification the mixture is considered ideal, i.e., $\gamma_i=1$, $\forall i$.

For simplicity we consider an isothermal reactor with constant temperature $T=353$ K and constant molar holdup M. The inlet stream to the reactor is mixed by 4 streams, in which one is the fresh feed of pure isobutene, whose molar flow rate is considered as the manipulated input. The flow rates and compositions of other 3 streams to the reactor are fixed. The molar flow rate of the outlet stream is adjusted accordingly to keep the molar holdup constant. Hence the dynamic model has 6 states standing for the molar fractions of the previous 6 components (with the 7th one dependent). Let the controlled output be the total reaction rate $R=\sum_{i=1}^7R_i$, namely the difference between the molar flow rates of the inlet stream and the outlet, which are assumed measurable. Hence the model is

$$\dot{x}_i=\frac{F_0+u}{M}(x_{0,i}-x_i)+\sum_{l=1}^3\frac{F_l}{M}(x_{l,i}-x_i)+\frac{R_i(x)}{M}, y=\sum_{i=1}^7R_i(x). \tag{B.6}$$

Under the nominal input $u=0$, the steady states along with the parameters are given in Table B.3. The approximate model is the one with R_i in the above accurate model substituted with an ideal mixture (with all $\gamma_i=1$) and kinetic coefficients $k_1^\circ/10^4$, $k_2^\circ/10^3$, $k_3^\circ/10^3$, $k_4^\circ/10^3$, K_{a1}, $K_{a2}/10^{-4}$ (scaled by orders of magnitudes that are assumed to be known) left as 5 unknown parameters, represented as $\hat{R}(x|\theta)$.

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