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On-line state estimation of nonlinear dynamic systems with gross errors

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ABSTRACT

State estimation is a crucial part of the monitoring and/or control of all chemical processes. Among various approaches for this problem, moving horizon estimation (MHE) has the advantage of directly incorporating nonlinear dynamic models within a well-defined optimization problem. Moreover, advanced step moving horizon estimation (asMHE) substantially reduces the on-line computational expense associated with MHE. Previously, MHE and asMHE have both been shown to perform well when measurement noise follows some known Gaussian distribution. In this study we extend MHE and asMHE to consider measurements that are contaminated with large errors. Here standard least squares based estimators generate biased estimates even with relatively few gross error measurements. We therefore apply two robust M-estimators, Huber's fair function and Hampel's redescending estimator, in order to mitigate the bias of these gross errors on our state estimates. This approach is demonstrated on dynamic models of a CSTR and a distillation column. Based on this comparison we conclude that the asMHE formulation with the redescending estimator can be used to get fast and accurate state estimates, even in the presence of many gross measurement errors.

1. Introduction

Improvement of on-line operation of chemical processes requires accurate knowledge of the current state of the system. This is particularly true for strategies that rely on first-principles models of the chemical plant, such as model predictive control (Rawlings & Mayne, 2009) or real-time optimization (Forbes & Marlin, 1996). Complicating factors that make real time state estimation challenging include the impracticality or infeasibility of measuring every state of a process directly, and delays that arise from measurements that take a significant amount of time to obtain.

Assuming that sufficient plant measurements can be obtained in real-time, one now needs to use these measurements to obtain the states of the system. This can be done by developing a model of the process which includes relationships between the measured and unmeasured state variables along with variables to estimate plant-model mismatch, unknown disturbances, and measurement noise. With this model several state estimation approaches can be applied; these approaches differ by assumptions they make about the linearity or nonlinearity of the plant model and the probability distribution of the error and noise variables. State estimation and the closely related topic of data reconciliation have been studied under a broad variety of assumptions. For nonlinear systems, the extended Kalman filter (EKF) (Bryson & Ho, 1975) is commonly applied in practice. While EKF is relatively easy to implement, it has been shown to have poor performance for highly nonlinear systems (Daum, 2005; Prakash, Patwardhan, & Shah, 2010). Related estimation methods that also deal with nonlinear systems include the unscented Kalman filter (Julier, Uhlmann, & Durrant-Whyte, 2000), the ensemble Kalman filter (Burgers, van Leeuwen, & Evensen, 1998; Evensen, 1994; Houtekamer & Mitchell, 1998), and the particle filter (Arulampalam, Maskell, Gordon, & Clapp, 2002; Chen, 2003). While each of these methods has pros and cons, one common drawback is their inability to deal with bounds on the states. Ignoring these constraints can lead to an increase in the estimation error or the divergence of the estimator (Haseltine & Rawlings, 2005). On the other hand, heuristic strategies, such as clipping, can greatly reduce the performance of the estimator. Other remedies to handle constrained nonlinear state estimation include nonlinear recursive dynamic data reconciliation (Vachhani, Rengaswamy, Gangwal, & Narasimhan, 2004), unscented recursive nonlinear dynamic data reconciliation (Vachhani et al., 2004; Vachhani, Narasimhan, & Rengaswamy, 2006), the constrained ensemble Kalman filter (Prakash et al., 2010), and the constrained particle filter (Prakash, Shah, & Patwardhan, 2008).

In contrast to the above estimators, the state estimation problem can be formulated directly as a nonlinear programming (NLP) problem. Here we consider moving horizon estimation (MHE) (Michalska & Mayne, 1995; Muske & Rawlings, 1993; Rao, 2000;

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Nomenclature

M_i	molar hold-up on tray i
V_i	vapor flow rate leaving tray i
L_i	liquid flow rate leaving tray i
F_i	feed flow rate entering tray i
D	distillate flow rate from condenser
B	bottoms flow rate from reboiler
R	reflux ratio
x_i	mole fraction of methanol in liquid on tray i
y_i	mole fraction of methanol in vapor on tray i
$z_{f,i}$	mole fraction of methanol in feed entering tray i
P_i	total pressure on tray i
$P^s_{i,j}$	vapor pressure of component j on tray i
T_i	temperature on tray i
A_j, B_j, C_j	Antoine's equation constants for component j
α_i	tray i efficiency
h^L_i	liquid enthalpy on tray i
h^V_i	vapor enthalpy on tray i
$\bar{h}^L_{i,j}$	liquid enthalpy for pure component j on tray i
$\bar{h}^V_{i,j}$	vapor enthalpy for pure component j on tray i
Q_R	reboiler heat duty
Q_{loss}	reboiler heat loss
Q_C	condenser heat duty
n^v_i	liquid volume holdup on tray i
V^m_i	molar volume of liquid on tray i
$\bar{V}^m_{i,j}$	molar volume of pure component j on tray i
W_i	Weir constant for tray i
$n^{v,\mathrm{ref}}_i$	volume of tray i

Robertson, Lee, & Rawlings, 1996), which uses a batch of past measurements to find the optimal state estimates. MHE has been shown to have very desirable asymptotic stability properties (Rao, Rawlings, & Mayne, 2003) and often performs better than EKF (Haseltine & Rawlings, 2005). In addition, constraints and bounds on plant states are handled directly by the NLP solver. On the other hand, computational delay is a major drawback for implementing MHE in an industrial setting (Ramlal, Allsford, & Hedengren, 2007).

A nice overview of methods for state estimation is given in Rawlings and Bakshi (2006), where it is noted that computational complexity still remains a significant challenge. Efficient algorithms for MHE include work done by Ohtsuka and Fujii (1996) and Tenny and Rawlings (2002). More recently, an MHE based real-time iteration approach has been investigated in Kühl, Diehl, Kraus, Schlöder, and Bock (2011). Additionally, Abrol and Edgar (2011) applied an in situ adaptive tabulation based MHE for on-line state estimation. In this work we make use of a fast MHE strategy based on NLP sensitivity developed by Zavala, Laird, and Biegler (2008a).

Another important factor for state estimation is the robustness of our estimate. Sensors can fail or be contaminated in such a way that their measurements are vastly different from the true plant state. In this work we reduce the influence of bad measurements in state estimation through a data reconciliation and gross error detection framework. A summary of early work done in this field is given in Crowe (1996). Recent reviews of the state of the art in outlier detection can be found in Hodge and Austin (2004), Kadlec, Gabrys, and Strandt (2009) and Chandola, Banerjee, and Kumar (2009). General approaches to gross error detection include principal component analysis (Tong & Crowe, 1995), cluster analysis (Chen & Romagnoli, 1998), artificial neural networks (Vachhani, Rengaswamy, & Venkatasubramanian, 2001), and robust statistics (Özyurt & Pike, 2004).

Related work has also been done in the process control literature, including investigating sensor faults and fault tolerance. A thorough review of work in this area can be found in Zhang and Jiang (2008). Of particular relevance to this work is the study of Chen and You (2008) that considers fault-tolerant sensor system for noisy or drifting sensors. However, it should be noted that in this work we are considering strategies to mitigate the effects of gross error measurements and not to explicitly detect or identify bad measurements.

In this study we consider the moving horizon estimation (MHE) formulation (Rao, 2000) as well as its extension called advanced step moving horizon estimation (asMHE) (López Negrete, 2011; Zavala et al., 2008a). Both strategies are described in more detail in Section 2. The main contribution of this work is to extend these formulations using robust M-estimators in order to mitigate the effect of gross errors and make our state estimates more robust. A brief overview of robust statistics and M-estimators is given in Section 3. Section 4 provides details on how the simulations done in this study were implemented. In Section 5 we compare the performance of various MHE formulations on a small dynamic model of a non-isothermal CSTR. Section 6 then examines a much larger example of a binary distillation column. Finally, a summary and conclusions are given in Section 7.

2. State estimation formulation

As mentioned in Section 1, there are many ways to approach the state estimation problem. In this paper we focus on its formulation as a nonlinear optimization problem. The formulations used in this work are briefly described below.

2.1. Moving horizon estimation

Moving horizon estimation (MHE) (Rao, 2000) is a well known strategy for constrained state estimation. The overall idea with MHE is to estimate the current state of the system using only the last N states and measurements directly, where we refer to N as the horizon length. In other words, we split time into two sets $T_1 = \{l | 0 \le l < k - N\}$ and $T_2 = \{l | k - N \le l \le k\}$ where k is the current time step. The NLP associated with this formulation is shown below. Notice that the summation terms in the objective function are only over T_2.

$$
\begin{aligned}
\{\hat{z}_{k-N|k}, \ldots, \hat{z}_{k|k}\} = \arg \min_{\{z_{k-N}, \ldots, z_k\}} \Phi(z_{k-N}) &+ \frac{1}{2} \sum_{l=k-N}^{l=k} v_l^T R_l^{-1} v_l \\
&+ \frac{1}{2} \sum_{l=k-N}^{l=k-1} w_l^T Q_l^{-1} w_l \\
\text{s.t.} \quad z_{l+1} &= f(z_l) + w_l, \\
y_l &= h(z_l) + v_l \\
z^{LB} \le z_l &\le z^{UB}, \quad l \in T_2 \qquad (1)
\end{aligned}
$$

where $\{\hat{z}_{k-N|k}, \ldots, \hat{z}_{k|k}\}$ refers to the optimal state estimates at each time step in the horizon. Also, $\Phi(z_{k-N}) = ||z_{k-N} - \hat{z}_{k-N|k-1}||^2_{\hat{\Pi}^{-1}_{k-N|k-1}}$ is the arrival cost and represents all the information in T_1, which is not included in the horizon. v_l is the vector of measurement noise, R_l is the covariance matrix of the measurement noise, w_l is the vector of unknown disturbances, and Q_l is the covariance matrix of the unknown disturbances. Also, the equality constraints are a state-space model of the plant where $h(z_l)$ is the measurement model and $f(z_l)$ is the system model. Additionally, bounds can be added to the states. A key assumption behind this formulation is that the measurement noise and unmeasured disturbances