Applied Mathematical Modelling 38 (2014) 5407–5420

Contents lists available at ScienceDirect

Applied Mathematical Modelling

journal homepage: www.elsevier.com/locate/apm

Observability analysis and model formulation for nonlinear state estimation

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ARTICLE INFO

Article history:
Received 16 April 2013
Received in revised form 14 January 2014
Accepted 28 March 2014
Available online 13 April 2014

Keywords:
Nonlinear state estimation
System observability
Process modeling strategies

ABSTRACT

A suitable design of state estimators for advanced control requires a detailed and representative mathematical model for capturing the nonlinear process behavior. The system observability, i.e. when the set of measurements provides enough information to estimate all the system states, is not a premise of the derivation of the Kalman filter. However, this propriety can improve the state estimator performance. On the basis of these design tasks, we outline a state estimation tuning strategy for different model formulations and present an algorithm to select the smallest number of measured variables to guarantee the system observability. The Williams–Otto semi-batch reactor was selected as case study, since its model formulation can be represented by two different set of states: (a) a mass basis states set and (b) a mass fraction basis states set. While the process-noise covariance matrix Q in the state estimator can be a diagonal and constant for the first model formulation, the matrix Q is not diagonal and time-varying for the second one due to their highly correlated states. Our results have shown how to convert the tuning matrices between different state definitions so that similar estimation results can be achieved.

1. Introduction

The success of employing on-line optimization in control as demonstrated by the industrial success of model-predictive control cf. Qin and Badgwell [1] provided the initial motivation for process modeling and better use of model uncertainty estimates.

Currently, in a direct optimizing control approach, accurate dynamic nonlinear process models are needed. For the computation of economically optimal process trajectories based upon a rigorous nonlinear process model, the state variables of the process at the beginning of the prediction horizon must be known. As not all states will be measured in a practical application, state estimation is a key ingredient of a directly optimizing controller [2]. Hence, a suitable design of state estimators with the purpose of improving advanced control applications requires rigorous models usually based on first principles. A systematization of the modeling process to support control system design, evaluation, and implementation is suggested by Marquardt [3]. Yip and Marlin [4] have discussed the issue of model fidelity in detail. Their paper investigates the crucial factors in deciding the model structure to be used in Real-Time Optimization (RTO) systems, since the RTO performance

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http://dx.doi.org/10.1016/j.apm.2014.03.053

depends on the accuracy of the plant model. In general, the use of a rigorous model based on first principles is recommended. All of aforementioned studies stressed the importance of accurate rigorous models based on first principles for the use of sophisticated nonlinear model-based advanced control techniques. Nevertheless, nothing is discussed about the model representation.

Concerning stochastic grey-box models, Kristensen et al. [5] have presented a systematic framework for improving the quality of continuous time models of dynamic systems based on experimental data. The framework is based on interplay between stochastic differential equation modeling, statistical tests and nonparametric modeling and provides features that allow model deficiencies to be pinpointed and their structural origin to be uncovered.

Differently from previous works, we have considered the case where the same nonlinear dynamic model can be defined using different state definitions. Here, two different model formulations based on first principles are evaluated to decide which one is more suited to be implemented into the state estimator. The Williams-Otto semi-batch reactor as introduced by Forbes [6] was selected as case study, since its model can be naturally formulated by two different set of states. The first model formulation holds a mass basis states set and the second one holds a mass fraction basis states set. Considering the state and parameter estimation problem, the first contribution of this work is shown the influence of these two model formulations in the tuning of state estimators. Afterwards, a state estimator tuning strategy is proposed to obtain comparable results with both model formulations.

In literature are found several techniques for measurements selection to be used in the state estimation problem, for instance, techniques based on minimum singular value [7–9], techniques based on optimization problem [10] and techniques based on data reconciliation metrics [11].

Oisiovici and Cruz [7] have applied the SVD analysis for selecting the sensor locations in high-purity multicomponent batch distillation columns. Their methodology consists of performing the singular value decomposition on a steady-state gain matrix that describes the temperature sensitivity on each tray with respect to changes in load variables. The authors claimed that one difficulty with applying the singular value decomposition (SVD) analysis in selecting the best sensor locations for inferential control of batch columns is that, because of the unsteady behavior of batch distillation systems, the matrix of gains is time-varying and the most sensitive tray locations vary along the batch cycle.

Other limitations of SVD based methods are reported by Bian and Henson [8] such as: (1) the number of selected measurements must be equal to the number of estimated variables; and (2) the algorithm is not designed to allow a priori inclusion of preselected measurements. To overcome the mentioned limitations, the authors have proposed an interesting approach for selecting stage composition/temperature measurements in high purity distillation columns for online estimation of wave model parameters. The proposed measurement selection method is an extension of the parameter selection procedure developed by Li et al. [12] presenting as limitation the fact of being based entirely on the steady-states sensitivity matrix, whose shortcomings include: (1) the actual information content of the candidate measurements under typical operating conditions is not considered; (2) the obtained measurement rankings are local and dependent on the steady state chosen as the base case; and (3) dynamic and nonlinear effects are neglected.

Singh and Hangh [9] have presented a methodology for determining optimal sensor locations for stable nonlinear systems for state and parameter estimation. Further, the authors have analyzed several different observability measures used for sensor location and concluded that methods mainly influenced by the largest singular value of the observability covariance matrix provide better results than methods based upon maximizing the observability of the least observable direction (magnitude of the smallest singular value is often very close to zero). Afterwards, the authors [10] have extended the methodology to the multiple sensor case which implies on sensor cost and measurement redundancy. Both proprieties are addressed via the formulation of an optimization problem with genetic algorithm.

Bagajewicz and Jiang [13] proposed a sensor-placement strategy based on the precision of the reconciled variables, including performance specifications with regard to gross error detectability, resilience to undetected gross errors, as well as precision bounds during sensor fault situations (residual precision). Such formulations of this problem have resulted in the definition of a mixed-integer nonlinear program (MINLP) with dimensions dependent on the value of the integer decision variables. Afterwards, Chmielewski et al. [11] have proposed an equivalent reformulation of the design problem such that the dimension of the NLP is independent of all decision variables. Both works are not concerned with state and parameter estimation problem.

The proposed algorithm aims to establish the smallest number of required measurements to guarantee the system observability taking into account: (1) nonlinear dynamic models based on first principles; and (2) the state and parameter estimation problem. The focus of our work is not on performance comparison of techniques found in the literature but on proposal of an alternative and simple algorithm based on the rank test to select the best and smallest number of measured variables to guarantee the system observability. Considering a specific set of system data in combination with the linearized time-variant system model, the approach can guarantee the best numerical performance in selecting the best measured variables under such conditions.

Since the choice of the more suited model formulation depends on issues such as system observability and state estimator tuning, the performance of the observability analysis algorithm is compared in both model formulations presented in this manuscript.