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Advances and selected recent developments in state and parameter estimation

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ABSTRACT

This paper deals with two topics from state and parameter estimation. The first contribution of this work provides an overview of techniques used for determining which parameters of a model should be estimated. This is a question that commonly arises when fundamental models are used as these models often contain more parameters than can be reliably estimated from data. The decision of which parameters to estimate is independent of the observer/estimator design, however, it is directly affected by the structure of the model as well as the available data. The second contribution is an overview of recent developments regarding the design of nonlinear Luenberger observers, with special emphasis on exact error linearization techniques, but also discussing more general issues, including observer discretization, sampled data observers and the use of delayed measurements.

1. Introduction

The use of fundamental models for process monitoring and control has become increasingly popular in recent years. However, the performance of a particular application does not only depend upon the algorithms used but also upon the quality of the model. This realization has led to several new research directions over the last few decades, two of which are reviewed in this work. One of these research areas focuses on the use of nonlinear models, and procedures required for dealing with these nonlinear models, to more appropriately describe a nonlinear system.

One type of approach for improving model accuracy, regardless if these are linear or nonlinear models, is to estimate model parameters from data. While there has been a significant interest in algorithms used for parameter estimation, the questions of how many and which parameters should be estimated have only been addressed more recently. The first part of this paper provides an overview of existing methods for selecting parameters for estimation.

The second part of this paper reviews theory and algorithms of nonlinear Luenberger observers for state and parameter estimation, focusing on recent methods and results from nonlinear systems theory. In a sense, this work complements a review paper presented at the previous CPC on particle filters and moving horizon estimators (Rawlings & Bakshi, 2006).

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2. Regularization techniques for parameter estimation of complex dynamic models

This section focuses on parameter estimation which plays an important role in process monitoring as well as mathematical modeling. Despite significant advances over the last few decades, this topic is still an active area of research and several review articles dealing with parts of this problem have been published in the last decade (Ashyraliyev, Fomekong-Nanfack, Kaandorp, & Blom, 2009; Chou & Voit, 2009; Dochain, 2003; Esposito & Floudas, 2000; Jimenez-Hornero, Santos-Duenas & Garcia-Garcia, 2009; Maria, 2004; McLean & McAuley, 2012; Moles, Mendes & Banga, 2003). Oftentimes, parameter estimation deals with the algorithms used for performing the estimation; in fact the second contribution of this work focuses on methodologies for estimating states and parameters. However, it is equally important to decide which parameters of a model should be estimated, why a particular subset of the parameters should be estimated, and also how accurate the estimation results will be based upon available data. This section provides a review of existing techniques that can answer these questions. One of the motivating factors behind these techniques is that complex systems, e.g., chemical reaction networks, can contain dozens to hundreds of parameters (Schoeberl, Eichler-Jonsson, Gilles, & Muller, 2002), however, it is often not possible to estimate more than a handful of these. In these cases, the accuracy of the estimates, and the model predictions resulting from these estimates, are strongly affected by the parameters chosen for estimation.

One challenge arising from estimation of complex systems is that the estimation problem is ill-conditioned. The reason for this is that a complex model contains a large number of parameters but not all of them are identifiable even if an unlimited amount of noise-free data would be available. Accordingly, the effects that changes in the parameters have on the outputs are correlated and the solution to the estimation problem is not unique. Furthermore, experimental data inevitably contain noise and the amount of available data is often limited. These limitations regarding the availability and quality of the data pose further challenges to the estimation problem since the optimal solution of the parameter values can be sensitive to variations in the data (Gutenkunst et al., 2007). Furthermore, similarly to what is widely known in system identification, parameters that best fit the training data are not necessarily the best ones from a practical point of view (Slezak, Suarez, Cecchi, Marshall, & Stolovitzky, 2010). Therefore, estimation of a complex system does not merely deal with determining the optimal solution to the data fitting problem but instead needs to focus on computing a solution which is robust to variations in the experimental data.

A second challenge that arises from estimation of a complex system is associated with the computational burden. Since a closed-form solution of the differential equations which describe a model is generally not available, it is only possible to evaluate the model via simulations. Since parameter estimation deals with solution of an optimization problem, the model needs to be evaluated repeatedly which can quickly result in estimation problems that are computationally prohibitive even for medium-scale problems.

A large number of techniques have been presented in the literature to address these problems in one way or another. A brief review of these techniques is provided in this section. The review is not meant to be comprehensive as this research area spans many different subtopics and is also an active area of research in many different fields of engineering. Instead, the work presented in this section focuses on techniques used for selecting a set of parameters for estimation. The reason for focusing on this area is that no review of existing techniques has previously been published in this field and that this approach aids regularizing ill-conditioned estimation problems.

This section is organized as follows. The formulation of the estimation problem for dynamic systems is presented next. After that, a general framework for regularization is proposed and three commonly used regularization techniques are compared. The following section focuses on the parameter selection procedure, which is one of the regularization approaches. As parameter selection encompasses a variety of methods, only the popular orthogonalization method is investigated further in the following section. This section concludes by presenting some suggestions for possible future research in this field.

2.1. Model formulation for estimation of dynamic systems

Parameter estimation aims to infer parameter values from available data so that the model predictions can accurately reflect the data (van den Bos, 2007). To estimate parameters of a dynamic system, a regression model is formulated that involves the differential equations. This formulation is presented in this subsection.

A time-invariant dynamic system is described by a set of ordinary differential equations as

$$\begin{cases} \dot{x}(t) = f(x(t), u(t), \theta) \\ y(t) = g(x(t), u(t), \theta) \end{cases} \quad (1)$$

where x is the state vector, u is the input vector, y is the output vector, and θ is the parameter vector.

The first step in parameter estimation is to derive an expression representing the parameter–output relationship. For the dynamic model shown in Eq. (1), the output y can be evaluated by model simulations, assuming that the initial state $x(0)$, the input profile $u(t)$, and the parameter vector θ are available. The resulting parameter–output relationship is denoted by $y(t, \theta)$ which is time-dependent, and generally lacks a closed-form solution expression.

The next step is to formulate the regression model by discretizing the output profiles and by including noise information. Given a set of time points $\{t_1, t_2, \cdots, t_m\}$, the output is sampled as

$$h(\theta) = \left[y_1(t_1, \theta), \ldots, y_1(t_m, \theta), \ldots, y_n(t_1, \theta), \ldots, y_n(t_m, \theta)\right]^T \quad (2)$$

where $y_1, y_2, \ldots, y_n$ are entries in the output vector y. After sampling, the continuous output profiles are discretized and the discretized output vector is only a function of the parameters, denoted by $h(\theta)$. Since all measurements contain some level of noise, the data available for estimation are given by

$$\tilde{y} = h(\theta) + \varepsilon \quad (3)$$

where $\tilde{y}$ is the data vector, $h(\theta)$ represents the model prediction, and $\boldsymbol{\varepsilon}$ denotes the noise vector. Apart from the model structure, information about the noise distribution plays an important role in parameter estimation. This distribution determines both formulation of the optimization problem for parameter estimation and the statistics of the estimated parameter values. In practice, a description of the noise is usually not accurately known and it is often assumed to be Gaussian, denoted by $\varepsilon \sim N(0, \sigma^2 I)$ where the mean vector is 0 and the covariance matrix is $\sigma^2 I$.

The third step in parameter estimation is to formulate an optimization problem which computes the parameter estimates as the optimal solution to the problem. Maximum likelihood estimation is commonly used, which estimates parameters by maximizing the likelihood function. In the case of Gaussian noise, maximum likelihood estimation reduces to least squares estimation, which computes the parameter estimates by minimizing the difference between the model prediction and the measured data as

$$\hat{\theta} = \arg\min_{\theta} (\tilde{y} - h(\theta))^T (\tilde{y} - h(\theta)) \quad (4)$$

where the difference is measured by the squared Euclidean norm.

It should be noted that estimation of a complex system is usually an ill-conditioned problem, i.e., the optimal least squares solution may be very sensitive to variations in the data. One approach to deal with this problem is to perform regularization to avoid ill-conditioning.

2.2. Regularization of ill-conditioned parameter estimation problems

When the estimation problem is ill-conditioned, a variety of regularization techniques can be applied to compute a robust solution. However, no detailed review of these regularization techniques exists in the literature and there is lack of a unified framework as part of which these regularization techniques can be viewed. Formulating such a general framework for regularization can provide insights into the commonalities but also into the differences that exist between the different techniques and, ultimately, help select an appropriate method. An attempt to present such a unified framework is made in this subsection where the framework combines three commonly used regularization techniques. Since regularization techniques for a nonlinear system are frequently extensions of those for a linear system, the linear case is investigated first.

The linear version of the regression model given by Eq. (3) is assumed be given by

$$\tilde{y} = H\theta + \varepsilon \quad (5)$$

The design matrix H is assumed to have a full column rank. If the design matrix is rank-deficient then the columns which are linearly dependent on others can be eliminated as well as the associated parameters. In this case, the reduced model will generate identical