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Development of moving window state and parameter estimators under maximum likelihood and Bayesian frameworks

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ABSTRACT

Estimation of slowly varying model parameters/unmeasured disturbances is of paramount importance in process monitoring, fault diagnosis, model based advanced control and online optimization. The conventional approach to estimate drifting parameters is to artificially model them as a random walk process and estimate them simultaneously with the states. However, this may lead to a poorly conditioned problem, where the tuning of the random walk model becomes a non-trivial exercise. In this work, the moving window parameter estimator of Huang et al. [1] is recast as a moving window maximum likelihood (ML) estimator. The state can be estimated within the window using any recursive Bayesian estimator. It is assumed that, when the model parameters are perfectly known, the innovation sequence generated by the chosen Bayesian estimator is a Gaussian white noise process and is further used to construct a likelihood function that treats the model parameters as unknowns. This leads to a well conditioned problem where the only tuning parameter is the length of the moving window, which is much easier to select than selecting the covariance of the random walk model. The ML formulation is further modified to develop a maximum a posteriori (MAP) cost function by including *arrival cost* for the parameter. Efficacy of the proposed ML and MAP formulations has been demonstrated by conducting simulation studies and experimental evaluation. Analysis of the simulation and experimental results reveals that the proposed moving window ML and MAP estimators are capable of tracking the drifting parameters/unmeasured disturbances fairly accurately even when the measurements are available at multiple rates and with variable time delays.

1. Introduction

The use of mechanistic dynamic models online for monitoring and control purpose has received a significant attention in the last two decades [2–4]. At the core of any model based monitoring and control scheme is a state estimator, which is used for online analysis or predictions. The predictive or diagnostic ability of any state estimation scheme critically depends on accuracy of the model parameters. While the model parameters may be known accurately in the beginning of a monitoring/control project, a common problem encountered in the implementation of state estimators is slow drifting of the model parameters from their initial (nominal) values. For example, in chemical processes, process parameters such as overall heat transfer coefficients change due to fouling in heat exchangers, catalysts deactivate over a period of time and feed quality may vary because of changes in the source of raw materials. If the parameters of the dynamic model are not changed to account for the variations in the process parameters, then the estimated state variables are biased. This, in turn, deteriorates the performance of the model based monitoring/control scheme. Thus, to maintain accuracy of the state estimates, parameters/unmeasured disturbances need to be estimated simultaneously with the states. Further, the state and parameter estimator can be used as a link between the real time optimization (RTO) and control layer that are used together for achieving adaptive and economically optimal operation in presence of drifting disturbances/parameters [5,6].

A widely used method for estimating the slowly drifting parameters/disturbances is filtering [6–8]. By this approach, the parameter variation is typically modelled as a random walk process and this model is combined with the process model. This augmented model is used for developing a nonlinear Bayesian estimation scheme, such as extended Kalman filter (EKF), unscented Kalman filter (UKF), ensemble Kalman filter (EnKF), particle filter (PF) or moving horizon estimation scheme (MHE) [9–16]. The

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random walk model artificially assumes that, like the state variables, the parameters change at each sampling instant while in reality they may be drifting very slowly. The main difficulty is in the selection of an appropriate distribution for the noise driving the random walk model. Even when the distribution of the noise term in the random walk model is assumed to be Gaussian, selecting the covariance of the parameter noise model is a non-trivial exercise. Moreover, if particle filters are used for simultaneous state and parameter estimation, then estimation of the transition probability density of the parameter vector based on straightforward application of the augmentation approach can lead to degeneracy [8]. Use of kernel approximation of the posterior density function of the parameters instead of particle approximation has been employed to address the degeneracy problem [7,15]. Recently, data driven approaches have been developed for identification of the noise density parameters when the parameters/disturbances are modelled as a random walk [17], or, even as a more general colored ARMA process [18]. However, these approaches are highly computationally intensive, and, as a consequence, are difficult to use for a system of moderately large dimension.

The other prominent approach in the literature for parameter estimation is based on the maximum likelihood principle [7,19,20]. While a significant section of the literature based on this approach is on estimation of the linear time series models, like ARMAX/Box-Jenkins model, or the innovation form of state space models [19,21,22], identifying parameters of general stochastic nonlinear differential equations (mechanistic or grey box models) have also been investigated by many researchers [20,23,24]. The key step here is approximating the data likelihood function. In the case of linear time invariant systems that are subjected to Gaussian state noise and Gaussian measurement noise, the innovation sequence generated using the Kalman filter forms a Gaussian white noise process. Thus, it is straight forward to construct a likelihood function using the Gaussianity and independence of the innovation sequence [20,22]. In the case of nonlinear grey box models, Bohlin and Graebe [23] and Kristensen et al. [24] have adopted a qualitatively similar approach for approximating the likelihood function. It is assumed that the innovation sequence generated by using the extended Kalman filter (EKF) is a Gaussian white noise process. This simplifying assumption facilitates construction of a computationally tractable likelihood function from the measured output data. In an alternate approach, similar to the linear state space model identification [22], Chitralekha et al. [14] and Gopaluni [25] construct the *complete* likelihood function, which involves unmeasured states and measured output data, for state and parameter estimation of nonlinear grey-box models. Unlike the conventional likelihood function which is based on only the measured data, this approach facilitates treatment of missing data. The resulting nonlinear non-convex optimization problem is solved using the expectation maximization (EM) approach. A recent article by Kantas et al. [7] reviews approaches based on particle filtering and maximum likelihood for estimating parameters of nonlinear state space models that are subjected to non-Gaussian disturbances.

A significant advantage of the maximum likelihood approach is that it does not require specification of a probability distribution function for the parameter vector. The maximum likelihood estimates are also asymptotically unbiased and consistent. However, most of the maximum likelihood methods available in the literature are meant for off-line estimation and for scenario where the true parameter vector is constant. The parameter estimation problem is formulated over a batch of data and the ML methods yield only a point estimate of the parameter vector [8]. However, if the true parameters are slowly time varying, then resorting to the moving time window based formulation can possibly be used to track the time varying parameters. A moving window formulation can track slowly changing parameters/disturbances while retaining the advantages of ML estimation. Jang et al. [10] and Liebman et al. [26] have proposed moving window based state and parameter estimation methods that have similar ideas. These approaches, however, uses the model as a simulator (i.e. as a *open loop observer* without output feedback) within the window. Huang et al. [1] proposed a moving window based state and parameter estimation approach that employs a nonlinear observer within the window for state estimation. This work primarily deals with stability properties of a broad class of nonlinear recursive estimators, including EKF, UKF and fixed gain observer, viewed as deterministic estimators. However, it also very briefly discusses the extension to estimating parameters over a moving horizon with embedded recursive estimators; this is demonstrated on a small case study. This approach, however, has been developed under the deterministic framework and can be viewed as a weighted least squares formulation. A major disadvantage of using the deterministic framework is that it does not provide a systematic basis for the selection of the weighting matrices appearing in the objective function. Recently, this moving window approach was re-cast under ML framework by Valluru et al. [27], which alleviates this difficulty.

This work aims at the development of moving window parameter estimation schemes under the stochastic framework that retains the advantages of the ML formulations and can track time varying parameters/unmeasured disturbances [27]. The preliminary version of moving window ML parameter estimator proposed by Valluru et al. [27] has been substantially enhanced. The parameters are assumed to be changing slowly (or at a very low frequency) and, thus, are assumed to remain constant in a time window in the immediate past. Given a set of model parameters, the state estimation is carried out using a recursive Bayesian estimator, such as EKF, UKF, EnKF or their respective constrained versions. The parameter estimators are developed under a simplifying assumption that, when the parameters are perfectly known, the innovation sequence generated by the chosen recursive estimator is a Gaussian white noise process. This assumption facilitates construction of a computationally tractable likelihood function. The only 'tuning parameter' in the proposed formulation is the length of the moving window, which is much easier to select than tuning the covariance of the random walk model. Another distinguishing feature of the proposed approach is that, unlike the majority of state and parameter estimation approaches available in the literature, which can handle only additive noise in the state dynamics, the proposed approach can accommodate non-additive noise, i.e. noise entering nonlinearly in the state dynamics. Efficacy of the proposed moving window formulations is demonstrated by conducting simulation studies on an ideal reactive distillation system and a CSTR system. Further, experimental verification of the proposed approach is carried out using the benchmark quadruple tank setup available at Automation Lab, Chemical Engineering, I.I.T. Bombay. With reference to Valluru et al. [27], the salient contributions of this work are as follows:

- In addition to ML formulation, a Bayesian or maximum a posteriori (MAP) version of the moving window estimator has been developed by incorporating prior information in the moving window ML formulation.
- Modifications necessary for dealing with measurements that are sampled at multiple sampling rates and that have time varying measurement delays have been incorporated.
- In addition to the sliding window formulation proposed in [1,27], the concept of shifting window based estimation has been introduced, which substantially reduce the on-line computations.
- Performances of the proposed moving window parameter estimators have been evaluated for (a) a multi-rate system with time varying measurement delays and (b) laboratory scale experimental data.

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