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Development of a Moving Window Maximum Likelihood Parameter Estimator and its Application on Ideal Reactive Distillation System

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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 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. Recently, Huang et al. (2010) has proposed a novel moving window weighted least squares parameter estimation approach, which is capable of simultaneous estimation of states and slowly drifting parameters/unmeasured disturbances. The slowly drifting parameters are assumed to remain constant in a time window in the immediate past and are estimated by solving a constrained minimization problem formulated over the window. In this work, the moving window parameter estimator of Huang et al. (2010) is recast as a moving window maximum likelihood (ML) estimator. It is assumed that the innovation sequence generated by the DAE-EKF is a Gaussian white noise process and further used to construct a likelihood function that treats the drifting 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. Efficacy of the proposed ML formulation has been demonstrated by conducting simulation studies on an ideal reactive distillation system. Analysis of the simulation results reveals that the proposed moving window ML estimator is capable of tracking the drifting unmeasured parameter fairly accurately using only the tray temperature measurements.

Keywords: State and Parameter Estimation, Maximum Likelihood Estimation, Extended Kalman Filter, Reactive Distillation

1. INTRODUCTION

Over the last two decades, there is a significant increase in research activity in the area of monitoring and control approaches that make use of mechanistic dynamic models online (Qin and Badgwell (2003), Venkatasubramanian et al (2003)). 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 might vary with effect of fouling in heat exchanger, catalysts deactivate over a period of reaction 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 model 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 (Valluru et al. (2015), Soroush (1998)).

To estimate the slowly drifting parameters/disturbances along with the states, the most common method used in the literature is to assume that the dynamic behavior of the model parameters/unmeasured disturbances can be

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modelled as a random walk process. The dynamic model for the process is combined with the random walk model, resulting in augmented state and parameter model, which is then used for developing a suitable estimation algorithm such as EKF/UKF or MHE. The difficulty in this particular approach is in selecting an appropriate distribution of the parameter noise of the random walk model (Patwardhan et al. (2012)). Even when the distribution of the noise term in the random walk model is assumed to be Gaussian, selecting the covariance of the noise model is a non-trivial exercise.

Recently, Huang et al. (2010) has proposed a moving window weighted least squares parameter estimation approach, which is capable of simultaneous estimation of states and slowly drifting parameters/unmeasured disturbances online. This approach, however, has been developed under the deterministic framework. The disadvantage of using the deterministic framework, however, is that it does not provide a systematic basis for the selection of the weighting matrices appearing in the objective function. Recasting the moving window formulation through probabilistic/stochastic viewpoint can alleviate this difficulty and provide much better insight into its working. In this work, the moving window parameter estimator of Huang et al. (2010) is recast as a moving window maximum likelihood estimator. The state estimation is carried out using the extended Kalman filter. It is assumed that the innovation sequence generated by the EKF is Gaussian white noise and further used to construct the likelihood function. The parameters are assumed to be changing slowly and are assumed to remain constant in a time window in the immediate past. Under this assumption, the parameters are estimated by minimizing the log-likelihood function over the time window. 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. Efficacy of the proposed ML formulation is demonstrated by conducting simulation studies on an ideal reactive distillation system. A version of EKF (Mandela et al. (2010)) for differential algebraic systems (DAE) is used for estimating the states of the ideal RD system. The performance of the proposed moving window ML approach is compared with the conventional DAE-EKF approach.

The rest of the paper is organized as follows. Section 2 develops the proposed ML approach for state and parameter estimation. Section 3 presents the results of the simulation case study conducted using the ideal RD system. The conclusions reached from the analysis of the simulation results are discussed in Section 4.

2. STATE AND PARAMETER ESTIMATION

2.1 Model for state and parameter estimation

Consider a process represented by a set of semi-explicit differential algebraic equations (DAEs) of index one

$$\frac{d\mathbf{x}}{dt} = \mathbf{f}(\mathbf{x}(t), \mathbf{z}(t), \mathbf{m}(t), \boldsymbol{\theta}, \mathbf{d}(t)) \tag{1}$$

$$\bar{0} = \mathbf{G}[\mathbf{x}(t), \mathbf{z}\,(t)] \tag{2}$$

$$\mathbf{y}_T = [\mathbf{C}_x \;\; \mathbf{C}_z] \begin{bmatrix} \mathbf{x}(t) \\ \mathbf{z}(t) \end{bmatrix} \tag{3}$$

where $\mathbf{x} \in \mathbb{R}^n$ represents differential state variables, $\mathbf{z} \in \mathbb{R}^a$ represents algebraic state variables, $\mathbf{m} \in \mathbb{R}^m$ represents manipulated inputs, $\boldsymbol{\theta} \in \mathbb{R}^p$ represents slowly varying model parameters / unmeasured disturbances, $\mathbf{d} \in \mathbb{R}^d$ represents true measured disturbances and $\mathbf{y}_T \in \mathbb{R}^r$ represents true measured variables.

The following modelling assumptions have been made for simulating the process plant and carrying out predictions in estimation:

- **Assumption 1:** Measurements ($\mathbf{y}$) from plant simulation are available at a regular sampling interval h *i.e.,*
$$\mathbf{y}_k = \mathbf{C} \begin{bmatrix} \mathbf{x}_k \\ \mathbf{z}_k \end{bmatrix} + \mathbf{v}_k \tag{4}$$
where, $\mathbf{C} = [\mathbf{C}_x \;\; \mathbf{C}_z]$ and $\mathbf{v}_k \in \mathbb{R}^r$, represents the measurement noise, which is modeled as zero mean Gaussian white noise process with covariance matrix $\mathbf{R}$ i.e., $\mathbf{v}_k \sim \mathcal{N}(\bar{\mathbf{0}}, \mathbf{R})$.
- **Assumption 2:** Manipulated inputs ($\mathbf{m}$) are held as piecewise constant over a sampling interval (h) and the true values of the manipulated inputs ($\mathbf{m}$) are related to the known/computed manipulated inputs ($\mathbf{u}$) by :
$$\mathbf{m}_k = \mathbf{u}_k + \mathbf{w}_{\mathbf{u},k}$$
where, $\mathbf{w}_{\mathbf{u},k} \in \mathbb{R}^m$, is an unknown disturbance in manipulated inputs such that, $\mathbf{w}_{\mathbf{u},k} \sim \mathcal{N}(\bar{\mathbf{0}}, \mathbf{Q}_u)$.
- **Assumption 3:** Sampling time is chosen small enough such that the variation of true measured disturbances, $\mathbf{d}$, can be adequately represented as a piecewise constant over a sampling interval (h). Further, true measured disturbances ($\mathbf{d}$) are related to measured disturbances ($\mathbf{d}_{m,k}$) by :
$$\mathbf{d}_{m,k} = \mathbf{d}_k + \mathbf{v}_{\mathbf{d},k} \tag{5}$$
where, $\mathbf{v}_{\mathbf{d},k} \in \mathbb{R}^d$, represents the measurement noise, such that, $\mathbf{v}_{\mathbf{d},k} \sim \mathcal{N}(\bar{\mathbf{0}}, \mathbf{R}_{\mathbf{d}})$.

Under the above assumptions, the true system dynamics of DAEs given by equations (1) -(2) are represented in discrete form as follows :

$$\mathbf{x}_{k+1} = \mathbf{x}_k + \int_{kh}^{(k+1)h} \mathbf{f}(\mathbf{x}(\tau), \mathbf{z}(\tau), \mathbf{m}_k, \boldsymbol{\theta}, \mathbf{d}_k) d\tau \tag{6}$$

$$\bar{\mathbf{0}} = \mathbf{G}(\mathbf{x}(\tau), \mathbf{z}(\tau)), \quad \boldsymbol{\tau} \in [kh, (k+1)h] \tag{7}$$

For further simplicity of notation the integration step can be represented as

$$\mathbf{x}_{k+1} = \mathbf{F}[\mathbf{x}_k, \mathbf{z}_k, \mathbf{m}_k, \boldsymbol{\theta}, \mathbf{d}_k] \tag{8}$$

$$\bar{\mathbf{0}} = \mathbf{G}[\mathbf{x}_{k+1}, \mathbf{z}_{k+1}] \tag{9}$$

This discrete DAE model is used for nonlinear plant simulation by using a suitable DAE solver.

- **Assumption 4 :** It is assumed that the variation of parameters/unmeasured disturbances ($\boldsymbol{\theta}$) occur at a significantly slower rate than the rates at which states and measured disturbances change over a time window, $[k-N,\, k]$, in the recent past.

Two different models are proposed under Assumption 4.

- **Model A:** It is assumed that the model parameters remain constant over the time window, $[k-N,\, k]$. To emphasize this, we use $\bar{\boldsymbol{\theta}}$ to represent the parameter