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Inequality constrained parameter estimation using filtering approaches

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HIGHLIGHTS

- Development of inequality parameter constraints from steady state data.
- Implementation of parameter inequality constraints in recursive estimators and MHE.
- Two-stage approach to constrained parameter estimation.
- Initial unconstrained estimate followed by one-step constrained optimization.
- Improved estimation and control performance demonstrated on realistic processes.

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ABSTRACT

Parameter estimation is usually approached by augmenting parameters to the states, leading to the simultaneous estimation of states and parameters. In practice, constraints on the values of the parameters can often be generated, and the incorporation of these constraints could improve the estimation performance. In this paper, we consider the inequality constrained parameter estimation problem. A new method of constructing inequality parameter constraints from routine operating data is introduced. Then, we introduce a framework for constraint implementation, based on first solving an unconstrained estimation problem and then a constrained problem, with recursive estimators such as the unscented Kalman filter (UKF) and the ensemble Kalman filter (EnKF); we also show that the same framework is applicable for moving horizon estimation (MHE). Then, we develop a method for constraint implementation for the UKF and the EnKF that yields faster convergence than the conventional projection method. Through simulations of two chemical processes, we show that the proposed method is able to provide fast recovery of state and parameter estimates from inaccurate initial guesses, leading to better estimation and control performance.

1. Introduction

An accurate dynamic model is required to achieve good monitoring, online optimization and control performance of chemical processes. Most process models and measurements are corrupted by noise and modeling inaccuracy, leading to the need for estimation of states and parameters. Very often, the state and parameter estimation problems are solved simultaneously; this is done by specifying the parameters to be estimated as augmented states. This dual estimation problem is a nonlinear filtering problem for most chemical processes. Various estimation algorithms have been developed to sequentially estimate a nonlinear system with online measurements.

Sequential filtering algorithms such as the extended Kalman filter (EKF), the unscented Kalman filter (UKF) (Julier et al., 2000), the ensemble Kalman filter (EnKF) (Evensen, 1994) and moving horizon estimation (MHE) (Robertson et al., 1996) are powerful tools for nonlinear state estimation. The most widely used algorithm for nonlinear systems is the EKF, which employs the Jacobian to locally linearize the model so that the conventional Kalman filter (KF) algorithm can be applied. However, the performance of the EKF may suffer with highly nonlinear systems due to the error introduced by linearization. Also, the calculation of Jacobian matrices can be computationally intensive for large systems. To overcome these difficulties encountered with the EKF, Julier et al. (1995) proposed the UKF. It uses the unscented transform (UT), which employs a set of weighted points (called sigma points) to represent the estimated mean and covariance, and the sigma points are propagated through the nonlinear system dynamics. It has computational efficiency owing to its Kalman filtering structure, as well as a better approximation than the EKF for nonlinear systems. Furthermore, it eliminates the need for the calculation of the Jacobian. The superior performance of the UKF compared to the EFK is demonstrated by Wan and van der Merwe (2002),

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Romanenko and Castro (2004) and Shenoy et al. (2010), among others. The ensemble Kalman filter (EnKF), originally proposed by Evensen (1994), is another approach for nonlinear estimation. Instead of the deterministic sampling strategy used in the UKF, the EnKF employs the Monte Carlo sampling method to generate a large number of random samples to carry out the prediction and update required in Kalman filtering. The EnKF is generally acknowledged to be efficient for systems with a large number of variables. MHE, which is an optimization based method, solves a nonlinear programming (NLP) problem subject to constraints over a finite horizon. However, the computational efficiency remains an issue for a long horizon or a large number of decision variables (Lopez-Negrete et al., 2011).

In most processes, it is possible to specify constraints on parameter values; these may be equality or inequality constraints. For example, the surface area of a reactor should be positive (and fall within a reasonable range). In most cases, it is easier to obtain accurate inequality constraints, which provide bounds on the parameter to be estimated, compared to equality constraints (Zhu and Huang, 2011). Walker (2006) proposed unstable fixed points as additional constraints in the parameter estimation process. In this paper, we introduce an approach to constructing inequality parameter constraints from steady-state measurement data corrupted with moderate noise. Inequality constraints are naturally handled by moving horizon estimation (MHE) due to its optimization based algorithm. However, MHE requires a heavy on-line computational load, and the exact arrival cost is hard to determine for the constrained estimation. Due to this, some researchers have explored the implementation of constraints within the framework of recursive estimation. Vachhani et al. (2005a) proposed the recursive nonlinear dynamic data reconciliation (RNDDR) method, in which the constraints are taken into consideration and the nonlinear state and covariance propagation are based on the EKF algorithm. Vachhani et al. (2006) later proposed the unscented recursive nonlinear dynamic data reconciliation (URNDDR) method as a combination of the UKF and RNDDR, which provided more accurate and efficient nonlinear constrained estimation. Recently, Prakash et al. proposed constrained ensemble Kalman filtering (C-EnKF) (Prakash et al., 2010) and constrained particle filtering (C-PF) (Prakash et al., 2011) with the use of constrained Monte Carlo samples and probability density function (PDF) truncation for nonlinear estimation. In this paper, we propose a new constraint handling method with the UKF and the EnKF specifically for the inequality constrained parameter estimation problem, and show that it provides improved estimation performance.

Therefore, the main contributions of this paper are (i) the formulation of inequality constraints on parameters using routine steady-state operating data, (ii) the development of a framework for constraint handling in recursive estimation with the UKF and the EnKF involving solving for the unconstrained estimate followed by the solution of a constrained optimization problem, and (iii) the development of new constraint-handling methods that avoid inconsistency between state and parameter estimates. The rest of the paper is organized as follows. Section 2 addresses the parameter estimation problem as a nonlinear estimation problem by augmenting unknown parameters as states. The proposed approach to constructing inequality parameter constraints from routine operating data is introduced in Section 3. Then, in Section 4, we propose a constrained parameter estimation scheme with inequality constraints, as well as constraint implementation methods with the UKF and the EnKF that provide better performance than the conventional projection method. We also discuss the use of this constraint implementation method with the MHE. Section 5 presents open and closed-loop simulations of a CSTR and a PMMA polymerization reactor system to demonstrate the performance of the proposed method for improved estimation and control performance.

2. Problem formulation

In this work, we consider the following continuous-discrete nonlinear stochastic process model:

$$\dot{x} = f(x, u, \theta) + w \tag{1a}$$

$$y_k = h(x_k) + v_k \tag{1b}$$

where $x, x_k \in \mathbb{R}^n$ denote the vector of states, $u \in \mathbb{R}^q$ denotes the vector of known manipulated variables and $y_k \in \mathbb{R}^m$ denotes the vector of available measurements. $f: \mathbb{R}^n \to \mathbb{R}^n$ is the state function with parameters $\theta \in \mathbb{R}^p$ and $h: \mathbb{R}^n \to \mathbb{R}^m$ is the measurement function. $w \in \mathbb{R}^n$ and $v_k \in \mathbb{R}^m$ are process and measurement noise respectively, with independent distributions

$$w \sim \mathcal{N}(0, Q) \tag{2}$$

$$v_k \sim \mathcal{N}(0, R) \tag{3}$$

where Q and R are covariance matrices.

The dual estimation problem arises when we have incomplete knowledge of the parameters, and we attempt to estimate states and parameters simultaneously. The most common approach for dual estimation is to combine the state and parameter vectors x and θ into an augmented state $x_a \in \mathbb{R}^{n+p}$ and carry out standard state estimation on the augmented system:

$$x_a = \begin{bmatrix} x \\ \theta \end{bmatrix} \tag{4}$$

$$\dot{x} = f(x, u, \theta) + w \tag{5a}$$

$$\dot{\theta} = 0 + w_p \tag{5b}$$

$$y_k = h(x_k) + v_k \tag{5c}$$

where Eq. (5b) is a random walk model for the parameter θ. w_p is chosen as a zero mean Gaussian noise with covariance matrix Q_p. Rewriting the model with augmented state x_a gives

$$\dot{x}_a = f(x_a, u) + w_a \tag{6a}$$

$$y_k = h(x_{ak}) + v_k \tag{6b}$$

where we redefine $f: \mathbb{R}^{n+p} \to \mathbb{R}^{n+p}$ as the nonlinear state function and $h: \mathbb{R}^{n+p} \to \mathbb{R}^m$ as the measurement function. $w_a = [\begin{smallmatrix} w \\ w_p \end{smallmatrix}]$ denotes the augmented state noise, which has the following distribution:

$$w_a \sim \mathcal{N}(0, Q_a), \quad Q_a = \begin{bmatrix} Q & 0 \\ 0 & Q_p \end{bmatrix} \tag{7}$$

State estimation techniques for this system are described later. It should be noted that we consider the true parameter values θ to be constant but unknown. Also, the measurement equation indicates that the outputs depend on the states, but not directly on the parameters.

3. Construction of inequality parameter constraints

In this section, we introduce a method to specify inequality constraints from routine steady-state operating data. We consider inequality constraints on parameters of the form

$$d^L \le c(\theta_1, \theta_2, \ldots, \theta_p) \le d^U \tag{8}$$

where $c(\cdot)$ is a function describing the parameter relationship, and d^L and d^U indicate the lower and upper bounds of the inequality constraints. In the following content, $c(\theta_1, \theta_2, \ldots, \theta_p)$ is written as $c(\theta)$ for notational simplicity.

The inequality constraints given by Eq. (8) may be obtained from some steady-state measurements, say $\{y_1, y_2, \ldots, y_N\}$. The process