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Constrained State Estimation Using the Ensemble Kalman Filter

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Abstract—**Recursive estimation of constrained nonlinear dynamical systems has attracted the attention of many researchers in recent years. In this work, we propose a constrained recursive formulation of the ensemble Kalman filter (CEnKF) that retains the advantages of unconstrained Ensemble Kalman Filter while systematically dealing with bounds on the estimated states. The efficacy of the proposed constrained state estimation algorithm using the EnKF is illustrated by application on a simulated gas-phase reactor problem.**

I. INTRODUCTION

The area of nonlinear state estimation is very rich and has been very well researched over the last four decades. The methods available for state estimation can be broadly categorized as nonlinear estimators developed under a deterministic framework and nonlinear estimators developed under the Bayesian framework. Approaches such as the Extended Kalman filter (EKF), unscented Kalman filter (UKF), moving horizon estimation (MHE) belong to the later category. These are employed for state estimation in nonlinear systems subject to unmeasured stochastic inputs. The Extended Kalman Filter (EKF) has long been the de-facto standard for state estimation of nonlinear systems. It may be noted that the covariance propagation step in the EKF requires linearization of nonlinear system dynamics around the mean of a Gaussian distribution. When the system dimension is large, computing derivatives of nonlinear state transition functions and measurement functions at each time step can prove to be a computationally demanding exercise.

Alleviating difficulties arising out of Jacobian computation has been the main motivation behind a new class of derivative free Kalman filters that have appeared recently in the literature. Prominent among these is the unscented Kalman filter (UKF) proposed by Uhlmann and Julier (2004), divided difference filter (DDF) proposed by Norgaard et al. (2000), and the central difference and Gauss-Hermite filters proposed by Ito and Xiong (2000). These approaches employ results from approximation theory (polynomial interpolation or matrix factorization) for calculating the statistics of a random variable, which undergoes a nonlinear transformation. A deterministic sampling technique is employed to select a minimal set of sample points around the mean. These sample points are then propagated through the nonlinear functions and used to approximate the covariance of the state estimate. The sample points straddle the discontinuity and, hence, can approximate the effect of discontinuity (Julier and Uhlmann, 2004). Thus, when compared to the EKF, the derivative free filters can be used for state estimation in a much wider class of nonlinear systems. Uhlmann and Julier (2004) have shown that the UKF results in an approximation that are accurate to the third-order for Gaussian inputs for all nonlinearities. For non-Gaussian inputs, approximations are accurate to at least the second-order, with the accuracy of third and higher order moments determined by the choice of tuning parameters.

More recently, a new class of filtering technique, called particle filtering, has attracted the attention of many researchers. The particle filter is a numerical method for implementing an optimal recursive Bayesian filter by Monte-Carlo simulation. Furthermore, a particle filter, can deal with state estimation problems arising from multimodal and non-Gaussian distributions (Arulampalam et al., 2002, Bakshi and Rawlings, 2006). These filters can also be classified as derivative free nonlinear filters. The Ensemble Kalman filter (EnKF), originally proposed by Evensen (Burger et al., 1998), belongs to the class of particle filters. In the EnKF formulation, similar to the deterministic derivative free filters, the observer gain is computed using second order moments of state error and innovations. However, the main difference is that the covariance information is generated using Monte Carlo sampling without making any assumption on the nature of underlying distributions of state estimation error. In addition, the EnKF formulation can also deal with state and measurement noise with non-Gaussian and multimodal distributions.

In most physical systems, states and/or parameters are bounded, which introduces constraints on their estimates. While the EnKF formulation appears to be a promising approach for dealing with a wide class of nonlinear state estimation problems, it cannot handle bounds on state and or the parameters that are being estimated. Nonlinear dynamic data reconciliation (NDDR) (Liebman et al. 1992) and Moving horizon estimation (MHE) (Rao and Rawlings, 2002) formulations proposed in the literature ensure that the state and parameter estimates satisfy bounds. However, the MHE and NDDR techniques are non-recursive and computationally intensive. Recursive Nonlinear Dynamic

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Data Reconciliation (RNDDR) has been recently developed to take into account the constraints on the state estimates (Vachhani et al. (2005)). This approach combines computational advantages of recursive estimation while handling constraints on the states. The state and covariance propagation steps and the step for updating the covariance in RNDDR formulation are identical to that of the Extended Kalman filter. Like the EKF, the RNDDR also requires computing derivatives of nonlinear state transition functions and nonlinear measurement functions and is accurate to the first order. Most recently, Vachhani et al. (2006) have proposed unscented recursive nonlinear dynamic data reconciliation (URNDDR) to estimate the states and parameters of the nonlinear system in real-time by combining the advantages of the unscented Kalman filter and the recursive nonlinear dynamic data reconciliation. The URNDDR formulation, however, inherits all limitations of the UKF arising from assumptions regarding distributions of estimation error, state noise and measurement noise.

In this work, we propose a constrained recursive formulation of the ensemble Kalman filter (CEnKF) that retains the advantages of unconstrained EnKF while systematically dealing with bounds on estimated states. To generate initial samples (particles), it becomes necessary to generate samples from the truncated distribution of the initial state. In the update step of the EnKF, a constrained optimization problem is formulated over one sampling interval for each particle to compute the updated state estimates for each particle. The updated state estimate is then computed using the ensemble mean of these constrained state estimates. It may be noted that, unlike the URNDDR formulation, the proposed CEnKF formulation can handle state and measurement noise with multi-modal distribution.

The organization of the paper is as follows. Section I discusses recursive Bayesian state estimation and the unconstrained EnKF formulation. Details of the proposed constrained state estimation formulation based on the Ensemble Kalman filter are presented in Section II. Simulation results are presented in Section III followed by main conclusions drawn through the analysis of these results as discussed in Section IV.

I. ENSEMBLE KALMAN FILTER

Consider a nonlinear system represented by the following nonlinear state space equations:

$$\mathbf{x}(k) = \mathbf{x}(k-1) + \int_{kT}^{(k+1)T} F[\mathbf{x}(t), \mathbf{u}(k-1), \mathbf{d}(k-1), \mathbf{w}(k-1)]\,dt \qquad -(1)$$

$$\mathbf{y}(k) = H[\mathbf{x}(k), \mathbf{v}(k)] \qquad -(2)$$

In the above process model, $\mathbf{x}(k)$ is the system state vector ($\mathbf{x} \in R^n$), $u(k)$ is known system input ($\mathbf{u} \in R^m$), $\mathbf{w}(k)$ is the state noise ($\mathbf{w} \in R^p$) with known distribution, $\mathbf{y}(k)$ is the measured state variable ($\mathbf{y} \in R^r$) and $\mathbf{v}(k)$ is the measurement noise ($\mathbf{v}(k) \in R^r$) with known distribution. The parameter k represents the sampling instant, $F[.]$ and $H[.]$ are the nonlinear process model and nonlinear measurement model respectively. The random state noises can be either due to random fluctuations in the input variables or the inaccuracies in the system model. It may be noted that we are interested in the most general case whereby state and measurement noise may have arbitrary (but known) distributions. Also, they can influence the system dynamics and measurement map in a non-additive manner.

A. Recursive Bayesian Estimation

The objective of the recursive Bayesian state estimation problem is to find the mean and variance of random variable $x(k)$ using the conditional probability density function $p\left[\mathbf{x}(k)|\mathbf{Y}^{(k)}\right]$ under following assumptions:

(i) the states follow a first-order Markov process and
(ii) the observation are independent of given states.

Here, $\mathbf{Y}^{(k)}$ denotes the set of all the available measurements, i.e. $\mathbf{Y}^{(k)} \triangleq \{\mathbf{y}(k), \mathbf{y}(k-1), ...\}$. The posterior density $p\left[\mathbf{x}(k) \mid \mathbf{Y}^{k}\right]$ is estimated in two stages: prediction, which is computed before obtaining an observation, and, update, which is computed after obtaining an observation (Arulampalam et al., 2002). In the prediction step, the posterior density $p(\mathbf{x}(k-1) \mid \mathbf{Y}^{k-1})$ at the previous time step is propagated into the next time step through the transition density $\{ p\left[\mathbf{x}(k) \mid \mathbf{x}(k-1)\right] \}$ as follows:

$$p\left[\mathbf{x}(k) \mid \mathbf{Y}^{k-1}\right] = \int p\left[\mathbf{x}(k) \mid \mathbf{x}(k-1)\right] p\left[\mathbf{x}(k-1) \mid \mathbf{Y}^{k-1}\right] d\mathbf{x}(k-1) \qquad (3)$$

The update stage involves the application of Bayes' rule:

$$p\left[\mathbf{x}(k) \mid \mathbf{Y}^{k}\right] = \frac{p\left[\mathbf{y}(k) \mid \mathbf{x}(k)\right]}{p\left[\mathbf{y}(k) \mid \mathbf{Y}^{k-1}\right]} \times p\left[\mathbf{x}(k) \mid \mathbf{Y}^{k-1}\right] \qquad (4)$$

where,

$$p\left[\mathbf{y}(k) \mid \mathbf{Y}^{k-1}\right] = \iint p\left[\mathbf{y}(k) \mid \mathbf{x}(k)\right] p\left[\mathbf{x}(k) \mid \mathbf{Y}^{k-1}\right] d\mathbf{x}(k-1)\, d\mathbf{x}(k) \quad (5)$$

Combining 3, 4 and 5 gives

$$p\left[\mathbf{x}(k) \mid \mathbf{Y}^{k}\right] = \frac{p\left[\mathbf{y}(k) \mid \mathbf{x}(k)\right] \times \int p\left[\mathbf{x}(k) \mid \mathbf{x}(k-1)\right] p\left[\mathbf{x}(k-1) \mid \mathbf{Y}^{k-1}\right] d\mathbf{x}(k-1)}{\iint p\left[\mathbf{y}(k) \mid \mathbf{x}(k)\right] p\left[\mathbf{x}(k) \mid \mathbf{Y}^{k-1}\right] d\mathbf{x}(k-1)\, d\mathbf{x}(k)} \qquad (6)$$

Equation (6) describes how the conditional posterior density function propagates from $p\left[\mathbf{x}(k) \mid \mathbf{Y}^{k-1}\right]$ to $p\left[\mathbf{x}(k) \mid \mathbf{Y}^{k}\right]$. It should be noted that the properties of the state transition equation (1) are accounted through the transition density function $p\left[\mathbf{x}(k) \mid \mathbf{x}(k-1)\right]$ while $p\left[\mathbf{y}(k) \mid \mathbf{x}(k)\right]$ accounts for the nonlinear measurement model (2). The prediction and update strategy provides an optimal solution to the state estimation problem, which, unfortunately, involves high-dimensional integration. The solution is extremely general and aspects such as multimodality, asymmetries and discontinuities can be incorporated (Julier and Uhlmann, 2004). The exact analytical solution to the recursive propagation of the posterior density is difficult to obtain. However, when the process model is linear and noise sequences are zero mean Gaussian white noise sequences, the Kalman filter describes the optimal recursive solution to the sequential state estimation problem. (Soderstrom, 2002).

B. Unconstrained State Estimation using Ensemble Kalman Filter

In this section we describe the most general form of the EnKF as available in the literature (Gillijns et al. (2006). The filter is initialized by drawing N particles $\{\mathbf{x}^{(j)}(0\,|\,0)\}$ from a suitable distribution. At each time step, N samples $\{\mathbf{w}^{(j)}(k-1), \mathbf{v}^{(j)}(k) : j = 0,1,..N\}$ for $\{\mathbf{w}(k)\}$ and $\{\mathbf{v}(k)\}$ are drawn randomly using the distributions of state and measurement noises. These sample points together with particles $\{\hat{\mathbf{x}}^{(j)}(k-1\,|\,k-1) : j = 0,1,..N\}$ are then propagated through the system dynamics to compute a cloud of transformed sample points (particles) as follows:

$$\hat{\mathbf{x}}^{(i)}(k\,|\,k-1) = \hat{\mathbf{x}}^{(i)}(k-1\,|\,k-1) + \int_{(k-1)T}^{kT} F\left[\mathbf{x}(\tau), \mathbf{u}(k-1), \mathbf{d}(k-1) + \mathbf{w}^{(i)}(k-1)\right] d\tau \tag{7}$$

$$i = 1, 2, ...N$$

These particles are then used to estimate sample mean and covariance as follows:

$$\overline{\mathbf{x}}^{(i)}(k\,|\,k-1) = \frac{1}{N}\sum_{i=1}^{N} \hat{\mathbf{x}}^{(i)}(k\,|\,k-1) \tag{8}$$

$$\overline{\mathbf{y}}^{(i)}(k\,|\,k-1) = \frac{1}{N}\sum_{i=1}^{N} H\left[\hat{\mathbf{x}}^{(i)}(k\,|\,k-1), \mathbf{v}^{(i)}(k)\right] \tag{9}$$

$$P_{\boldsymbol{\varepsilon},\mathbf{e}}(k) = \frac{1}{N-1}\sum_{i=1}^{N} \left[\boldsymbol{\varepsilon}^{(i)}(k)\right]\left[\mathbf{e}^{(i)}(k)\right]^T \tag{10}$$

$$P_{\mathbf{e},\mathbf{e}}(k) = \frac{1}{N-1}\sum_{i=1}^{N} \left[\mathbf{e}^{(i)}(k)\right]\left[\mathbf{e}^{(i)}(k)\right]^T \tag{11}$$

Where,

$$\boldsymbol{\varepsilon}^{(i)}(k) = \hat{\mathbf{x}}^{(i)}(k\,|\,k-1) - \overline{\mathbf{x}}^{(i)}(k\,|\,k-1) \tag{12}$$

$$\mathbf{e}^{(i)}(k) = H\left[\hat{\mathbf{x}}^{(i)}(k\,|\,k-1), \mathbf{v}^{(i)}(k)\right] - \overline{\mathbf{y}}^{(i)}(k\,|\,k-1) \tag{13}$$

The Kalman gain and cloud of updated samples (particles) are then computed as follows:

$$L(k) = P_{\boldsymbol{\varepsilon},\mathbf{e}}(k)\left[P_{\mathbf{e},\mathbf{e}}(k)\right]^{-1} \tag{14}$$

$$\Upsilon^{(i)}(k\,|\,k-1) = \left\{\mathbf{y}(k) - H\left[\hat{\mathbf{x}}^{(i)}(k\,|\,k-1), \mathbf{v}^{(i)}(k)\right]\right\} \tag{15}$$

$$\hat{\mathbf{x}}^{(i)}(k\,|\,k) = \hat{\mathbf{x}}^{(i)}(k\,|\,k-1) + L\,(k)\Upsilon^{(i)}(k\,|\,k-1) \tag{16}$$

$$\Upsilon^{(i)}(k\,|\,k) = \left\{\mathbf{y}(k) - H\left[\hat{\mathbf{x}}^{(i)}(k\,|\,k), \mathbf{v}^{(i)}(k)\right]\right\} \tag{17}$$

The updated state estimate is computed as the mean of the updated particles cloud, i.e.

$$\hat{\mathbf{x}}(k\,|\,k) = \frac{1}{N}\sum_{i=1}^{N} \hat{\mathbf{x}}^{(i)}(k\,|\,k) \tag{18}$$

C. Comparison with Conventional approaches

At this point, we would like to juxtapose the EnKF formulation described above with the EKF and UKF formulations. The following observations can be made by comparing these formulations:

The main limitations of EKF formulations is that the propagation step is equivalent to approximating the expected value of a nonlinear function of a random variable by propagating the mean of the random variable through the nonlinear function, i.e. $E\left[g(x)\right] \approx g\left[E(x)\right]$ (Daum, 2005). The predicted mean of the estimate is defined as follows:

$$\hat{\mathbf{x}}(k\,|\,k-1) = \hat{\mathbf{x}}(k-1\,|\,k-1) + E\left[\int_{t_{k-1}}^{t_k} F\left[\mathbf{x}(\tau), \mathbf{u}(k-1), \overline{\mathbf{d}} + \mathbf{w}(k-1), \boldsymbol{\theta}\right] d\tau\right] \tag{19}$$

In the EKF formulation, this is approximated by propagating only the previous mean as follows:

$$\hat{\mathbf{x}}(k\,|\,k-1) \approx \hat{\mathbf{x}}(k-1\,|\,k-1) + \int_{t_{k-1}}^{t_k} F\left[\mathbf{x}(\tau), \mathbf{u}(k-1), \overline{\mathbf{d}}, \boldsymbol{\theta}\right] d\tau \tag{20}$$

$$\mathbf{x}(t_{k-1}) = \hat{\mathbf{x}}(k-1\,|\,k-1)$$

On the other hand, in the EnKF formulation the predicted mean is computed as follows:

$$\overline{\mathbf{x}}^{(i)}(k\,|\,k-1) \approx \frac{1}{N}\sum_{i=1}^{N} \hat{\mathbf{x}}^{(i)}(k\,|\,k-1) \tag{21}$$

In addition, state covariance propagation is carried out using Taylor series expansion of nonlinear state transition operator and neglecting terms higher than second order. This step requires analytical computation of Jacobians at each time step. The EnKF approach, on the other hand, provides a derivative free method for estimation of predicted covariances required in the update step. Moreover, this also implies that nonlinear function vectors F[.] and H[.] need not be smooth and are at least once differentiable. Thus, a major advantage of the EnKF is that it can be applied for state estimation in systems with discontinuous nonlinear transformations. The particles straddle the discontinuity and, hence, can approximate the effect of discontinuity while estimating the covariances.

The main difference between UKF and EnKF is that the EnKF formulation can deal with state and measurement noise with arbitrary multimodal distribution. In UKF formulation, the method for drawing samples $\{\mathbf{w}^{(j)}(k-1), \mathbf{v}^{(j)}(k) : j = 0,1,..N\}$ and $\{\hat{\mathbf{x}}^{(j)}(k-1\,|\,k-1) : j = 0,1,..N\}$ has been derived based on the assumption that underlying distributions are multivariate Gaussian (Julier and Uhlmann, 2004). While it is claimed that it is possible to adjust tuning parameters to account for non-Gaussian distributions, it is far from clear how to choose these parameters when distributions are non-Gaussian. Also, in the case of UKF, the method of selecting particles (called as sigma points) is deterministic and these sample points, form a symmetric set of 2N points that lie on the $\sqrt{N}$ 'th covariance contour (Julier and Uhlmann, 2004).

Divided difference filter (DDF) formulations proposed by Norgaard et al. and Central difference and Gauss-Hermite filters proposed by Ito and Xiong (2000) are qualitatively similar to UKF. These formulations also inherit similar limitations. In the EnKF formulation, on the other hand, the particle cloud from the previous step is propagated to the next step. This step does not involve any assumptions on the nature of distribution of state estimation error.

II. CONSTRAINED STATE ESTIMATION USING THE ENSEMBLE KALMAN FILTER

In many practical problems of interest in process industry, it becomes necessary to account for bounds on states and parameters being estimated. If it is desired to apply the ensemble Kalman filter for state estimation when states are bounded, then it becomes necessary to modify the ensemble Kalman filter described in the section II. To deal with bounds in EnKF framework, we have to deal with the following issues:

- Generating initial particles $\{\mathbf{x}^{(i)}(0)\}$ that is consistent with bounds on states.
- Reformulation of the update step to account for bounds on state variables.

Based on the motivation from the URNDDR formulation, we propose a constrained version of the EnKF, which is referred to as CEnKF in the rest of the text. To begin with we describe the procedure for truncation of the distribution for a special case when, the distribution of $\mathbf{x}(0)$ is approximated by multivariate Gaussian density function. We then proceed to present the CEnKF algorithm.

A Generation of Truncated Distribution of Initial State

When states have bounds, it becomes necessary to generate particles that are consistent with these bounds. This can be achieved by using the concept of truncated distributions. A truncated distribution is a conditional distribution that is conditioned on the bounds on the random variable. For example, given probability density function $f(\zeta)$ and cumulative distribution function $\Phi(\eta)$ defined over $(-\infty,\infty)$, the truncated density function can be defined as follows

$$f\left[\zeta \mid a<\zeta\le b\right]=\frac{f(\zeta)}{\Phi(b)-\Phi(a)} \qquad (22)$$

such that

$$\int_a^b f\left[\zeta \mid a<\zeta\le b\right]=\frac{1}{\Phi(b)-\Phi(a)}\int_a^b f(\zeta)d\zeta=1$$

In particular, the truncated uni-variate normal distribution can be obtained as follows :

$$N\left[\zeta,\sigma \mid a<\zeta\le b\right]=\frac{\dfrac{1}{\sigma\sqrt{2\pi}}\exp\left(-\dfrac{\left(\zeta-\bar{\zeta}\right)^2}{2\sigma^2}\right)}{\Phi\left(\dfrac{b-\bar{\zeta}}{2\sigma^2}\right)-\Phi\left(\dfrac{a-\bar{\zeta}}{2\sigma^2}\right)} \quad (23)$$

Now, consider a situation in which the distribution of $\mathbf{x}(0)$ is approximated by truncated multivariate Gaussian density function as $\mathbf{N}\left[\bar{\mathbf{x}}(0\mid 0),P(0)\right]$ defined over $(\mathbf{x}_L,\mathbf{x}_H)$. In this work, we propose the following approach for the construction of truncated normal distribution starting from $\mathbf{N}\left[\bar{\mathbf{x}}(0\mid 0),P(0)\right]$ defined over $(\mathbf{x}_L,\mathbf{x}_H)$. Since $P(0)$ is a symmetric and positive definite matrix, Cholesky factorization on $P(0)$ will lead to

$$\sqrt{P(0)}=\begin{bmatrix} S_{11} & 0 & ... & 0 & 0\\ S_{21} & S_{22} & .. & 0 & 0\\ . & . & S_{ii} & 0 & 0\\ S_{n1} & S_{n2} & ... & S_{n1} & S_{nn}\end{bmatrix}$$

It should be noted that $\mathbf{N}\left[\bar{\mathbf{x}}(0\mid 0),P(0)\right]$ defined over $(\mathbf{x}_L,\mathbf{x}_H)$ can be rewritten as

$$\hat{\mathbf{x}}(0\mid 0)=\bar{\mathbf{x}}(0\mid 0)+\sqrt{P(0)}\,\mathbf{u}(0) \qquad (24)$$

such that

$$\begin{bmatrix} \dfrac{\mathbf{x}_{L,1}-\bar{\mathbf{x}}_1(0\mid 0)}{S_{11}}\\ \dfrac{\mathbf{x}_{L,2}-\bar{\mathbf{x}}_2(0\mid 0)-S_{21}u_1(0)}{S_{22}}\\ .\\ \dfrac{\mathbf{x}_{L,n}-\bar{\mathbf{x}}_n(0\mid 0)-\sum_{r=j-1}^{n-1}S_{nr}u_r(0)}{S_{nn}}\end{bmatrix} \prec \begin{bmatrix}u_1(0)\\ u_2(0)\\ .\\ u_n(0)\end{bmatrix} \prec \begin{bmatrix} \dfrac{\mathbf{x}_{H,1}-\bar{\mathbf{x}}_1(0\mid 0)}{S_{11}}\\ \dfrac{\mathbf{x}_{H,2}-\bar{\mathbf{x}}_2(0\mid 0)-S_{21}u_1(0)}{S_{22}}\\ .\\ \dfrac{\mathbf{x}_{H,n}-\bar{\mathbf{x}}_n(0\mid 0)-\sum_{r=j-1}^{n-1}S_{nr}u_r(0)}{S_{nn}}\end{bmatrix}$$

(OR)

$$\begin{bmatrix}u_{L,1}(0)\\ u_{L,2}(0)\\ .\\ u_{L,n}(0)\end{bmatrix} \prec \begin{bmatrix}u_1(0)\\ u_2(0)\\ .\\ u_n(0)\end{bmatrix} \prec \begin{bmatrix}u_{H,1}(0)\\ u_{H,2}(0)\\ .\\ u_{H,n}(0)\end{bmatrix} \qquad (25)$$

The above transformation requires that we draw samples recursively. Thus, we first draw $u_1(0)$ from $N\left[0,1\mid \dfrac{\mathbf{x}_{L,1}-\bar{\mathbf{x}}_1(0\mid 0)}{S_{11}},\dfrac{\mathbf{x}_{H,1}-\bar{\mathbf{x}}_1(0\mid 0)}{S_{11}}\right]$, then $u_2(0)$ from $N\left[0,1\mid \dfrac{\mathbf{x}_{L,2}-\bar{\mathbf{x}}_2(0\mid 0)-S_{21}u_1(0)}{S_{22}},\dfrac{\mathbf{x}_{H,2}-\bar{\mathbf{x}}_2(0\mid 0)-S_{21}u_1(0)}{S_{22}}\right]$ and so on.

Now, we can define n-truncated uni-variate normal distributions $N^{(j)}\left[0,1\mid u_{L,j}^{(i)}(0)<u_j^{(i)}(0)\le u_{H,j}^{(i)}(0)\right]$, for j=1,2, …n. and the sample for i'th particle can now be drawn recursively from the above n-truncated uni-variate normal distribution as follows:

$$\hat{x}^{(i)}(0\mid 0)=\bar{x}^{(i)}(0\mid 0)+\sqrt{P(0)}\Upsilon^{(i)} \qquad (26)$$

$$\Upsilon_j^{(i)}\sim N^{(j)}\left[0,1\mid u_{L,j}(0)<u_j(0)\le u_{H,j}(0)\right] \qquad (27)$$

Thus, in the proposed Constrained EnKF formulation, the above mentioned initialization steps is carried out.

B Constrained EnKF formulation

The calculation steps from equations (7) – (15) in the proposed Constrained EnKF are identical to the unconstrained formulation described in section II. The modifications necessary in the update step of the constrained formulation are as follows:

To begin with, the covariance of the predicted estimates is estimated as

$$P(k|k-1) = \frac{1}{N-1}\sum_{i=1}^{N}\left[\boldsymbol{\varepsilon}^{(i)}(k)\right]\left[\boldsymbol{\varepsilon}^{(i)}(k)\right]^{T} \quad (28)$$

The updated state estimates are then obtained by solving a constrained optimization problem formulated over one sampling interval for each particle as follows:

$$\min_{\hat{\mathbf{x}}^{(i)}(k|k)}\left[\xi^{(i)}(k)^{T}P(k|k-1)^{-1}\xi^{(i)}(k)+\mathbf{e}(k)^{T}R^{-1}\mathbf{e}(k)\right] \quad (29)$$

$$\mathbf{e}(k) = \mathbf{y}(k) - H\left[\hat{\mathbf{x}}^{(i)}(k|k), \mathbf{v}^{(i)}(k)\right]$$

$$\xi^{(i)}(k) = \hat{\mathbf{x}}^{(i)}(k|k-1) - \hat{\mathbf{x}}^{(i)}(k|k)$$

subject to:

$$\mathbf{x}_L \le \hat{\mathbf{x}}(k|k) \le \mathbf{x}_U$$

The updated state estimate is computed using equation (18).

III. SIMULATION STUDIES

A. Gas-Phase Reactor (Rawlings and Bakshi, 2006)

Consider the gas-phase irreversible reaction in a well mixed, constant volume, isothermal batch reactor

$$2A \rightarrow B \quad k_1 = 0.6$$

The governing equation for the isothermal batch reactor is as follows:

$$\frac{dp_A}{dt} = -2k_1 p_A^2 \quad (30)$$

$$\frac{dp_B}{dt} = k_1 p_A^2 \quad (31)$$

$$P = \begin{bmatrix}1 & 1\end{bmatrix}\begin{bmatrix}p_A \\ p_B\end{bmatrix}$$

Where, $\mathbf{x} = \left[P_A ; P_B\right]$ denotes the partial pressures of A and B. We have assumed that the random errors (Gaussian White noise) are present in the measurement (Total Pressure) as well as in the state variables. The covariance matrices of state noise and measurement noise are assumed as $Q = \begin{bmatrix}(0.001)^2 & 0 \\ 0 & (0.001)^2\end{bmatrix}$ and $R = \left[(0.1)^2\right]$.

The sampling time has been chosen as 0.1. The initial state error covariance matrix has been chosen as $P(0|0) = \begin{bmatrix}36 & 0 \\ 0 & 36\end{bmatrix}$. The initial state for the process and the state estimator are chosen as $\mathbf{x}(0|0) = \begin{bmatrix}3 & 1\end{bmatrix}$ and $\hat{\mathbf{x}}(0|0) = \begin{bmatrix}0.1 & 4.5\end{bmatrix}$ respectively. In all the simulation runs, the process is simulated using the nonlinear first principles model (30 and 31) and the true state variables are computed by solving the nonlinear differential equations using differential equation solver in Matlab 6.5.

B. Performances of Constrained and Unconstrained EnKF

The problem at hand is to generate non-negative estimates of partial pressures starting from given initial estimates. Thus, the lower bound and upper bound values imposed on the state variables are $\mathbf{x}_L = [0 \quad 0]^T$ and $\mathbf{x}_U = [100 \quad 100]^T$ respectively. The sample points used to estimate the statistics of the estimated state of the model in the constrained EnKF are chosen to be equal to 25 in the case of Constrained Ensemble Kalman filter. It should be noted that initial samples for the state variables ($\hat{\mathbf{x}}^{(i)}(0|0)$) are drawn from the truncated normal distribution. The performance of the constrained Ensemble Kalman filter(CEnKF) and EnKF (Unconstrained) in the presence of deliberately introduced large initial plant model mismatch are shown in figures 1 and 2 respectively. From figure 1 it can be concluded that reasonably accurate estimates of the partial pressures of A and B are obtained using the constrained Ensemble Kalman filter, whereas, the estimated partial pressures A and B are found to be significantly biased in the case of EnKF(Unconstrained) for N= 25 and 100 respectively.

IV. CONCLUSIONS

In this paper, the performances of the proposed constrained EnKF and the Unconstrained EnKF based state estimation algorithm on the benchmark example (Gas-phase reactor) have been compared. The estimated value of the partial pressure of A has been found to be negative in the case of unconstrained EnKF. On the other hand, constraints never get violated when the proposed CEnKF method is employed for state estimation. The estimates stay far from the constraint boundaries and quickly converge to the true values.

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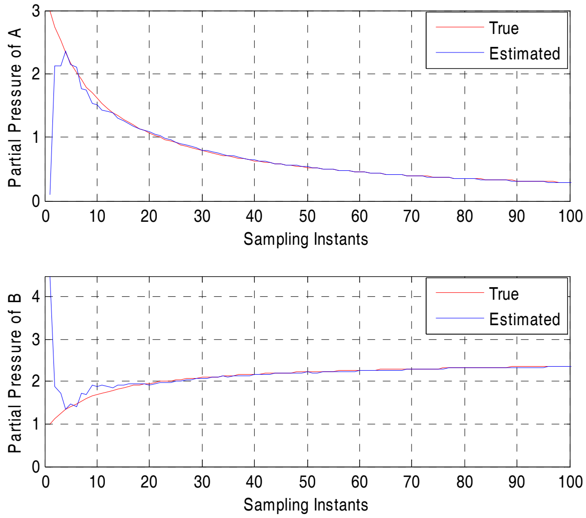

Figure 1: Evolution of true and estimated states of Partial pressures in Gas-phase reactor (CEnKF) (a) Partial Pressure of A (b) Partial Pressure of B

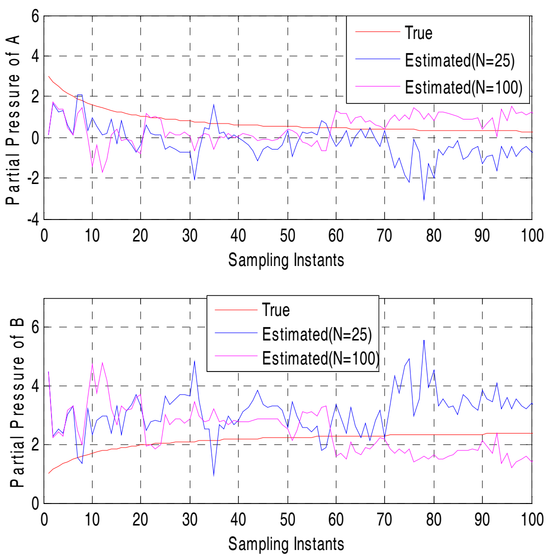

Figure 2: Evolution of true and estimated states of Partial pressures in Gas-phase reactor (Unconstrained EnKF) a) Partial Pressure of A (b) Partial Pressure of B

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