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Constrained State Estimation Using Particle Filters

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Abstract: Recursive estimation of constrained nonlinear dynamical systems has attracted the attention of many researchers in recent years. For nonlinear/non-Gaussian state estimation problems, particle filters have been widely used. As pointed out by Daum (2005), particle filters require a proposal distribution and the choice of proposal distribution is the key design issue. In this paper, a novel approach for generating the proposal distribution based on a Constrained Unscented Kalman filter is proposed. The efficacy of the proposed constrained state estimation algorithm using a particle filter (CUPF) is illustrated via a successful implementation on a simulated gas-phase reactor.

Keywords: Particle Filter, Constrained State Estimation, Unscented Particle Filter.

1. INTRODUCTION

State estimation of dynamic systems is an important prerequisite for safe and economical process operations. The state estimation problem in a stochastic linear system is solved by the well-known Kalman filter. For linear systems, the Kalman filters generate optimal estimates of state variables from observations. The Kalman filter as a state estimator has become useful even for complicated real-time applications and has attracted widespread attention from the engineering community because of the relatively simple recursive nature of its computational scheme. The Extended Kalman filter (EKF) is a natural extension of the linear filter to the nonlinear domain through local linearization. The Extended Kalman filter is probably the most widely used nonlinear filter. While EKF formulations have been successful in solving many industrial problems, its implementation is not always simple as the state error covariance prediction step requires analytical computation of Jacobians at each time step. This can prove to be prohibitively complex and computationally demanding for high dimensional systems. Moreover, this also implies that nonlinear function vectors appearing in system equations should be smooth and at least once differentiable. Recently, the unscented Kalman filter (UKF) has been proposed as an alternative to the Extended Kalman filter where the above limitation has been overcome using the concept of sample statistics (Julier and Uhlmann, 2004). The UKF uses a deterministic sampling technique to select a minimal set of sample points (called sigma points) around the mean. These sigma points are then propagated through the nonlinear functions and the covariance of the estimate is then recovered.

In most physical systems, states/parameters are bounded, which introduces constraints on the state/parameter estimates. One major limitation of the EKF and UKF is that these formulations cannot handle such bounds or constraints systematically. Furthermore both the EKF and UKF require that the noise processes that affect the process be Gaussian. Nonlinear dynamic data reconciliation (NDDR) (Liebman et al. 1992) and Moving horizon estimation (MHE) formulations provide systematic approaches to handling of bounds on states/parameters or any other algebraic constraints. The MHE problem is formulated as a constrained nonlinear optimization problem defined over a moving time window in the past. While MHE alleviates difficulties associated with constraint handling, it requires a large dimensional nonlinear optimization problem to be solved at each time step and is not suitable for on-line implementation. Recently, Vachhani et al. (2005) have proposed a recursive constrained formulation called recursive nonlinear dynamic data Reconciliation (RNDDR). This approach combines computational advantages of recursive estimation while handling constraints on the states. The state and covariance propagation steps and the updated covariance computation in RNNDR are identical to that of EKF. The updated state estimates are obtained by solving a constrained optimization problem formulated only over one sampling interval, which significantly reduces the computational burden compared with MHE or NDDR formulations. Vachhani et al. (2006) later developed a constrained version of the UKF (unscented recursive nonlinear dynamic data reconciliation or URNDDR) for state estimation and parameter estimation in nonlinear systems. This approach combines the advantages of the UKF and the RNDDR formulations.

The EK and UK filters can be used for nonlinear systems in which second order moments are sufficient to characterize the underlying probability density functions of state estimation errors. Thus, results obtained using these filters are satisfactory when state error probability density functions can be approximated as Gaussian distributions. In general, the distribution of {**w**(k)} and {**v**(k)} can be multi-modal and non-Gaussian. Thus, in many situations Gaussian approximation may not suffice. A new class of filtering technique, called particle filtering, can deal with state estimation problems arising from such multimodal and non-Gaussian distributions (Arulampalam et al., 2002, Bakshi and Rawlings, 2006). A particle filter (PF) approximates multi-dimensional integration involved in the propagation and update steps using Monte Carlo sampling. The selection of a suitable form of importance function to represent the true posterior density is a crucial step in the particle filter (Arulampalam et al., 2002). In general, it is difficult to design such proposal distributions and its choice is highly problem dependent. As pointed out by Daum (2005), in almost all successful implementations of PF, the proposal density is a Gaussian density obtained from an EKF or UKF as proposal. Thus, at each sampling step, the EKF or UKF is used to compute the mean and covariance of the importance distribution for each propagated particle.

If it is desired to apply particle filtering for state estimation when states are bounded, then EKF and UKF cannot be used for generating proposal densities. The main difficulty arises from the fact that EKF and UKF formulations are unconstrained state estimators and, therefore, are not suited for handling bounds and algebraic constraints. To deal with bounds and constraints in particle filtering framework, we have to address two issues:

- Generate samples (particles) that are consistent with bounds and constraints
- Generate proposal distributions that can explicitly account for bounds on states

In this work, we develop a novel particle filtering based scheme that can handle bounds on states and/or parameters. Two salient features of the proposed constrained particle filtering scheme are as follows: (a) we propose to use URNDDR (or constrained UKF) formulation to generate the truncated proposal distributions required in particle filtering. (b) In order to deal with the requirement of generating particles consistent with the bounds, we draw samples from a truncated multivariate normal distribution. Suitable combinations of these two steps are used to handle constraints in the particle filtering framework. While the URNDDR formulation can deal with the constraints, one limitation of the URNDDR algorithm is that it inherits the assumption of Gaussianity implicit in the UKF formulation. In other words, the URNDDR formulation cannot handle state and measurement noise with multi-modal distributions. The proposed constrained PF formulation will overcome these limitations when state and measurement noise distributions are known **accurately**. It may be noted that, most other available state estimation approaches, cannot deal with this scenario even when the distributions are exactly known. The efficacy of the proposed approach is demonstrated using a simulated gas-phase reactor benchmark problem (Rawlings and Bakshi, 2006).

The organization of the paper is as follows. Section 2 discusses the particle filter with proposal distribution. The choice of importance distributions for constrained state estimation is presented in Section 3. The simulation results are presented in Section 4 followed by main conclusions reached through analysis of these results in Section 5.

2. PARTICLE FILTER

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

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

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

In the above process model, $\mathbf{x}(k)$ is the system state vector $(\mathbf{x} \in R^n)$, u(k) is known system input $(\mathbf{u} \in R^m)$, $\mathbf{d}(k) \in R^p$ is the unknown system input, $\mathbf{w}(k)$ 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 noise and measurement noise may have arbitrary (but known) distributions. Also, they can influence the system dynamics and measurement map in a non-additive manner.

2.1 Recursive Bayesian Estimation

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

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

The update stage involves the application of Bayes' rule:

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

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

Combining equations 3, 4 and 5 gives

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

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).

2.2 Approximate Solution through Monte Carlo Sampling

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. While dealing with nonlinear systems, it becomes necessary to develop approximate and computationally tractable sub-optimal solutions to the above sequential Bayesian estimation problem. The particle filter is a numerical method for implementing an optimal recursive Bayesian filter through Monte-Carlo simulation. Classical particle filters approximate the distribution $p\left[\mathbf{x}(k)\mid\mathbf{Y}^{k}\right]$, using a set of random samples $\{\mathbf{x}^{(i)}(k): i=1.....N\}$ together with associated weights $\{\omega_i(k): i=1.....N\}$:

$$p\left[\mathbf{x}(k)\mid\mathbf{Y}^{k}\right]\approx\sum_{i=1}^{N}\omega_i(k)\delta\left[\mathbf{x}(k)-\mathbf{x}^{(i)}(k)\right] \quad (7)$$

where $\delta\left[\mathbf{x}(k)-\mathbf{x}^{(i)}(k)\right]$ denotes the Dirac delta function. The weights $\{\omega_i(k)\}$ can be viewed as approximations to the relative posterior probabilities of the particles. It should be noted that the posterior density ($p\left[\mathbf{x}(k)\mid\mathbf{Y}^{k}\right]$) is seldom known. Therefore, it is not possible to draw samples from this distribution. For this reason, $q\left[\mathbf{x}^{(i)}(k)\mid\mathbf{x}^{(i)}(k-1),\mathbf{Y}^{k}\right]$, a proposal density or importance density, is used. At each sampling instant, a sample is drawn from the proposal distribution generated around each particle. To compensate for the difference between the proposal density and the true posterior density, the weights are then computed as follows:

$$\tilde{\omega}_i(k)=\frac{p\left[\mathbf{x}^{(i)}(1:k)\mid\mathbf{Y}^{k}\right]}{q\left[\mathbf{x}^{(i)}(1:k)\mid\mathbf{Y}^{k}\right]} = \frac{p\left[\mathbf{y}(k)\mid\mathbf{x}^{(i)}(k)\right]p\left[\mathbf{x}^{(i)}(k)\mid\mathbf{x}^{(i)}(k-1)\right]}{q\left[\mathbf{x}^{(i)}(k)\mid\mathbf{x}^{(i)}(k-1),\mathbf{Y}^{k}\right]}\tilde{\omega}_i(k-1) \quad (8)$$

$$\omega_i(k)=\frac{\tilde{\omega}_i(k)}{\sum_{j=1}^{N}\tilde{\omega}_j(k)} \quad (9)$$

The above equation provides a mechanism to sequentially update the weights. The updated state estimates $\hat{x}(k\mid k)$ at the k^{th} sampling instant are given by

$$E\left[\mathbf{x}(k)\mid\mathbf{Y}^{k}\right)\right]=\sum_{i=1}^{N}\omega_i(k)\mathbf{x}^{(i)}(k) \quad (10)$$

2.3 Selection of Proposal Distributions for Unconstrained State Estimation

The selection of a suitable form of importance function to represent the true posterior density is a crucial step in the particle filter (Arulampalam et al., 2002, Rawlings and Bakshi, 2006). In general, it is difficult to design such a proposal and the choice of proposal distribution is highly problem dependent. EKF and UKF are popular choices for proposal distribution in particle filters (EKF-PF and UPF). The computational steps involved are as follows Arulampalam et al. (2002):

Initialization: At k = 0, M samples are drawn from $N(\bar{0},Q)$ as follows:

$$\hat{x}^{(i)}(0\mid 0)=\hat{x}(0\mid 0)+Q^{1/2}\Upsilon^{(i)}$$
$$\Upsilon^{(i)}\sim N(0,I)$$

and associated weights are initialized as $\omega_i=1/M$.

Importance sampling: At the k'th time step, after obtaining measurement **y**(k), M observers (EKF or UKF) are used in parallel to compute means and covariances of the proposal distributions, i.e. $\left\{\bar{\mathbf{x}}^{(i)}(k\mid k),P^{(i)}(k\mid k)\right\}$ for each propagated particle $\hat{\mathbf{x}}^{(i)}(k-1\mid k-1)$ .The importance density is then approximated as

$q\left[\mathbf{x}(k)\mid\mathbf{Y}^{(k)}\right]=\mathbf{N}\left[\bar{\mathbf{x}}^{(i)}(k\mid k),P^{(i)}(k\mid k)\right]$ and used to draw a sample around each particle as follows:

$$\hat{\mathbf{x}}^{(i)}(k\mid k)=\bar{\mathbf{x}}^{(i)}(k\mid k)+\left[P^{(i)}(k\mid k)\right]^{1/2}\Upsilon^{(i)}$$
$$\Upsilon^{(i)}\sim N(0,I)$$

Computation of weights: The weights associated with each particle are now computed as follows

$$\tilde{\omega}_i(k)=\frac{p\left[\mathbf{y}(k)\mid\mathbf{x}^{(i)}(k)\right]p\left[\mathbf{x}^{(i)}(k)\mid\mathbf{x}^{(i)}(k-1)\right]}{N\left[\bar{\mathbf{x}}^{i}(k\mid k),P^{(i)}(k\mid k)\right]}\left(\frac{1}{M}\right) \quad (11)$$

It may be noted that, at the end of the re-sampling step, all samples are assigned equal weights, i.e. $\tilde{\omega}_i(k-1) = 1/M$. These $\tilde{\omega}_i(k)$ weights are then normalized to obtain $\{\omega_i(k)\}$ as given by equation (9). In the special case when state and measurement noise signals are zero mean Gaussian white noise, the numerator can be computed as follows

$$p\left[\mathbf{y}(k) \mid \mathbf{x}^{(i)}(k)\right] p\left[\mathbf{x}^{(i)}(k) \mid \mathbf{x}^{(i)}(k-1)\right] = N\left[H\left[\hat{\mathbf{x}}^{i}(k)\right], R\right] N\left[\bar{\mathbf{x}}^{i}(k \mid k-1), Q\right]$$

Re-sampling: This step involves discarding samples that have low importance and reassigning weights to the remaining particles. Various approaches have been suggested in the literature for carrying out this step. Arulampalam et al. (2002) have recommended the use of residual systematic re-sampling algorithm (RSR). At the end of this step, the sample set typically contains multiple replicas of important samples, thereby effectively increasing weight of these samples in the ensemble. The updated state estimate is next constructed as $E\left[\mathbf{x}(k) \mid \mathbf{Y}^{k}\right] = \frac{1}{M}\sum_{i=1}^{M} \mathbf{x}^{(i)}(k)$. When compared to the conventional particle filter that uses $q\left[\mathbf{x}^{(i)}(k) \mid \mathbf{x}^{(i)}(k-1), \mathbf{Y}^{k}\right] \approx p\left[\mathbf{x}^{(i)}(k) \mid \mathbf{x}^{(i)}(k-1)\right]$ the use of proposal density can significantly reduce the number of particles required for generating accurate estimates.

3. CONSTRAINED STATE ESTIMATION USING A PARTICLE 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 particle filtering for state estimation when states are bounded, then it becomes necessary to modify the above algorithm. The selection of suitable form of importance function to approximate the true posterior density is a crucial step in the particle filter formulation for handling constraints. As discussed in the introduction, the EKF and the UKF formulations are unconstrained state estimators and, therefore, are not suited for handling bounds and algebraic constraints. In this section, we discuss how the URNDDR algorithm can be used to generate truncated proposal distributions that are consistent with bounds on the state variables.

3.1 Unscented Recursive Nonlinear Dynamic Data Reconciliation

The RNDDR approach combines computational advantages of recursive estimation while handling constraints on the states. The updated state estimates are obtained by solving a constrained optimization problem formulated over one sampling interval. When the RNDDR formulation is used to generate means and covariances of proposal distributions, the following optimization problem is solved for each particle

$$\min_{\hat{\mathbf{x}}(k \mid k)} \left[\xi(k)^{T} P^{(i)}(k \mid k-1)^{-1} \xi(k) + \mathbf{e}(k)^{T} R^{-1} \mathbf{e}(k)\right] \quad (12)$$

$$\xi(k) = \hat{\mathbf{x}}(k \mid k-1) - \hat{\mathbf{x}}(k \mid k) \quad \mathbf{e}(k) = \mathbf{y}(k) - H\left[\hat{\mathbf{x}}(k \mid k)\right]$$

subject to: Dynamic Model Equation (1)-(2)

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

The state and covariance propagation steps and the updated covariance computation in RNNDR are identical to that of EKF (See Vachhani et al, 2005 for details). The covariance propagation does not account for bounds systematically at propagation stage.

Vachhani et al. (2006) later developed a constrained version of the UKF (unscented recursive nonlinear dynamic data reconciliation or URNDDR) for state and parameter estimation in nonlinear system. This approach combines advantages of the UKF (derivative free covariance update) and the RNDDR formulation (constraint handling ability). Unlike the conventional UKF where the sigma points are chosen symmetrically, the sigma points $\{\hat{\mathbf{x}}^{(i,j)}(k-1 \mid k-1) : j = 0,1,..2n\}$ are located asymmetrically around $\{\hat{\mathbf{x}}(k-1 \mid k-1)\}$ to better approximate covariance information in the presence of bounds in the state. The corresponding weights $\{\gamma_i : i = 0,1,...,2n\}$ associated with sigma points are also computed by taking into account the asymmetric nature of the sigma point (Ref. Vachhani et al, 2006 for details). These sigma points are then propagated through the system dynamics to compute a cloud of transformed points

$$\bar{\mathbf{x}}^{(i,j)}(k \mid k-1) = \sum_{j=0}^{2L} \gamma_j \chi^{(i,j)}(k \mid k-1) \quad (13)$$

$$\bar{\mathbf{y}}^{(i,j)}(k \mid k-1) = \sum_{j=0}^{2n} \gamma_j H\left[\chi^{(i,j)}(k \mid k-1)\right] \quad (14)$$

$$P^{(i)}(k \mid k-1) = \sum_{j=0}^{2n} \gamma(j)\left[\boldsymbol{\varepsilon}^{(i,j)}(k)\right]\left[\boldsymbol{\varepsilon}^{(i,j)}(k)\right]^{T} + Q \quad (15)$$

Here, γ_j represents fixed weights associated with sigma points, which are chosen such that their sum equals unity. The weights are functions of N and a tuning parameter (κ). The tuning parameter can be used for adjusting the spread of the sigma points around the mean. The updated state estimates are obtained by solving a constrained optimization problem formulated over one sampling interval as follows

$$\min_{\hat{\mathbf{x}}^{(i)}(k \mid k)} \left[\xi^{(i)}(k)^{T} P(k \mid k-1)^{-1} \xi^{(i)}(k) + \mathbf{e}(k)^{T} R^{-1} \mathbf{e}(k)\right] \quad (16)$$

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

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

subject to: $\mathbf{x}_L \le \hat{\mathbf{x}}(k \mid k) \le \mathbf{x}_U$

The update state estimate and posterior covariance are computed as

$$\hat{\mathbf{x}}(k \mid k) = \sum_{i=0}^{2L} \omega_i \hat{\mathbf{x}}^{(i)}(k \mid k) \quad (17)$$

$$P(k \mid k) = \sum_{i=0}^{2N} \omega(i)\left[\hat{\mathbf{x}}^{(i)}(k \mid k) - \hat{\mathbf{x}}(k \mid k)\right]\left[\hat{\mathbf{x}}^{(i)}(k \mid k) - \hat{\mathbf{x}}(k \mid k)\right]^{T} \quad (18)$$

Depending on the nature of problem at hand, either of the above two recursive constrained state estimation approaches can be used to generate proposal distributions for constrained particle filtering.

3.2 Generation of Truncated Proposal Distributions

When states have bounds, it becomes necessary to generate proposal distributions 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

$$f\left[\zeta \mid a<\zeta\le b\right]=\frac{f(\zeta)}{\Phi(b)-\Phi(a)} \tag{19}$$

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

$$N\left[\zeta,\sigma \mid a<\zeta\le b\right]=\frac{\frac{1}{\sigma\sqrt{2\pi}}\exp\left(-\frac{\left(\zeta-\bar{\zeta}\right)^2}{2\sigma^2}\right)}{\Phi\left(\frac{b-\bar{\zeta}}{2\sigma^2}\right)-\Phi\left(\frac{a-\bar{\zeta}}{2\sigma^2}\right)} \tag{20}$$

Now, if RNDDR/URNDDR is used for generating importance distributions for constrained state estimation, then $q\left[\mathbf{x}^{(i)}(k)\mid\mathbf{x}^{(i)}(k-1),\mathbf{Y}^k\right]$ has to be a truncated distribution in order to be consistent with the bounds on the states. In this work, we draw samples from the truncated multivariable normal distribution $\mathbf{N}\left[\bar{\mathbf{x}}^{(i)}(k\mid k),P^{(i)}(k\mid k)\right]$ defined over $(\mathbf{x}_L,\mathbf{x}_H)$. Since $P^{(i)}(k\mid k)$ is a symmetric and positive definite matrix, Cholesky factorization on $P^{(i)}(k\mid k)$ will lead to

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

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

$$\mathbf{x}^{(i)}(k\mid k)=\bar{\mathbf{x}}^{(i)}(k\mid k)+\sqrt{P^{(i)}(k\mid k)}\,\mathbf{u}^{(i)}(k) \tag{21}$$

such that

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

(or)

$$\begin{bmatrix}u_{L,1}^{(i)}(k)\\ u_{L,2}^{(i)}(k)\\ .\\ u_{L,n}^{(i)}(k)\end{bmatrix}\prec\begin{bmatrix}u_1^{(i)}(k)\\ u_2^{(i)}(k)\\ .\\ u_n^{(i)}(k)\end{bmatrix}\prec\begin{bmatrix}u_{H,1}^{(i)}(k)\\ u_{H,2}^{(i)}(k)\\ .\\ u_{H,n}^{(i)}(k)\end{bmatrix} \tag{22}$$

The above transformation requires that we draw samples recursively. Thus, we first draw $u_1^{(i)}(k)$ from $N\left[0,1\mid\frac{\mathbf{x}_{L,1}-\bar{\mathbf{x}}_1^{(i)}(k\mid k)}{S_{11}^{(i)}},\frac{\mathbf{x}_{H,1}-\bar{\mathbf{x}}_1^{(i)}(k\mid k)}{S_{11}^{(i)}}\right]$, then $u_2^{(i)}(k)$ from $N\left[0,1\mid\frac{\mathbf{x}_{L,2}-\bar{\mathbf{x}}_2^{(i)}(k\mid k)-S_{21}^{(i)}u_1(k)}{S_{22}^{(i)}},\frac{\mathbf{x}_{H,2}-\bar{\mathbf{x}}_2^{(i)}(k\mid k)-S_{21}^{(i)}u_1(k)}{S_{22}^{(i)}}\right]$ and so on. Now, we can define n-truncated uni-variate normal distributions $N^{(j)}\left[0,1\mid u_{L,j}^{(i)}(k)<u_j^{(i)}(k)\le u_{H,j}^{(i)}(k)\right]$, 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:

$$\hat{x}^{(i)}(k\mid k)=\bar{x}^{(i)}(k\mid k)+\sqrt{P^{(i)}(k\mid k)}\,\Upsilon^{(i)} \tag{23}$$

$$\Upsilon_j^{(i)}\sim N^{(j)}\left[0,1\mid u_{L,j}^{(i)}(k)<u_j^{(i)}(k)\le u_{H,j}^{(i)}(k)\right] \tag{24}$$

Thus, in the proposed constrained PF formulation, the importance sampling step is carried out as described above. Also, the samples generated in the initialization step have to be drawn from truncated normal distributions following the procedure outlined above. The computation of weights and re-sampling steps are identical to that of the unconstrained PF algorithm described in Section 2.

4. SIMULATION STUDIES

4.1 *Gas-Phase Reactor* (Rawlings and Bakshi, 2006)

Consider the gas-phase irreversible reaction in a well mixed, constant volume, isothermal batch reactor $2A\rightarrow B$ $k_1=0.6$. The governing equation for the isothermal batch reactor is as follows:

$$\frac{dp_A}{dt}=-2k_1p_A^2 \tag{25}$$

$$\frac{dp_B}{dt}=k_1p_A^2 \tag{26}$$

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

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

$$Q=\begin{bmatrix}(0.001)^2 & 0\\ 0 & (0.001)^2\end{bmatrix}\quad\text{and}\quad R=\left[(0.1)^2\right].$$

The sampling time has been chosen as 0.1. The initial state error covariance matrix has been chosen as $P(0\mid0)=\begin{bmatrix}36 & 0\\ 0 & 36\end{bmatrix}$. The initial state for the process and the state estimator are chosen as $\mathbf{x}(0\mid0)=\begin{bmatrix}3 & 1\end{bmatrix}$ and $\hat{\mathbf{x}}(0\mid0)=\begin{bmatrix}0.1 & 4.5\end{bmatrix}$ respectively. The problem at hand is to generate non-negative estimates of partial pressures starting from given initial estimates. 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.

4.2 Performances of Constrained and Unconstrained UKF as proposals:

The performance of the particle filters with constrained UKF as proposal (CUPF) and UKF as proposal (UPF) in the presence of deliberately introduced large initial plant model mismatch are shown in figures 1 and 2 respectively. From figures 1 and 2 it can be concluded that estimates of the partial pressures of A and B obtained using constrained UKF as proposal (CUPF) are fairly accurate, whereas, the estimated partial pressures A and B are found to be significantly biased in the case of UKF as proposal(UPF) for the number of particles 25 and 10 respectively. In the case of UPF the estimated value of the partial pressure of A has been found to be negative. On the other hand, constraints never get violated when the proposed CUPF as proposal is employed for state estimation.

5. CONCLUSION

In this paper, a PF with constrained UKF for generating distribution to obtain state estimates without violating state constraints has been proposed. The preliminary investigations demonstrate that the performance of the proposed CUPF is superior to that of UPF.

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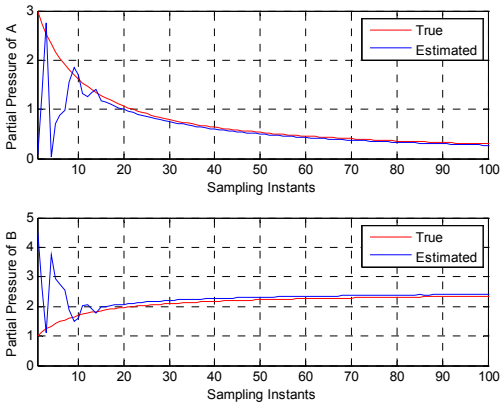

Figure 1: Evolution of true and estimated states of partial pressures in Gas-phase reactor (CUPF) (a) Partial Pressure of A (b) Partial Pressure of B.

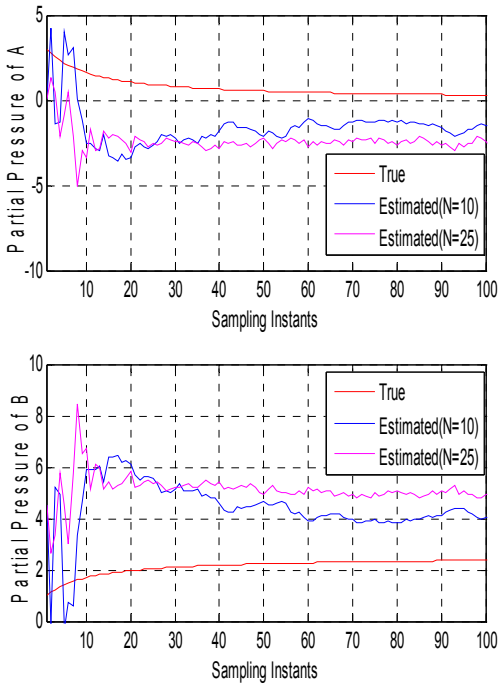

Figure 2: Evolution of true and estimated states of partial pressures in Gas-phase reactor (UPF) (a) Partial Pressure of A (b) Partial Pressure of B