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Constrained Extended Kalman Filter based on Kullback-Leibler (KL) Divergence*

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Abstract— **Extended Kalman Filter (EKF) is one of the most extensively used state estimator for nonlinear systems. As this technique cannot handle constraints, it might result in physically meaningless state estimates. Therefore, in this work, we focus on imposing inequality constraints in the state estimation problem to obtain physically meaningful state estimates as well as improve the estimation accuracy. For this purpose, we project the unconstrained EKF solution into the constrained region by minimizing the Kullback-Leibler (KL) divergence. The proposed constrained EKF framework updates the values of the states and error covariances by solving the convex optimization problem involving conic constraints. The efficacies of the proposed algorithm are demonstrated in a batch reaction system, and the performance of the proposed approach is found to outperform the recursive nonlinear dynamic data reconciliation solution.**

I. INTRODUCTION

State estimation plays an important role in achieving good performance of control, optimization, and process monitoring. Over the years, various filtering algorithms have been proposed for state estimation, among which the famous Kalman filter (KF) is an optimal filter for linear systems in the presence of Gaussian noise. Extended Kalman Filter (EKF) is a straightforward extension of the KF to nonlinear systems [1]. This is based on approximating the nonlinear dynamics of the model with its first-order linearized version to obtain the state estimates. However, the estimated states from this technique might result in physically meaningless values of the states because the physical constraints such as non-negative values of pressure and concentrations are not incorporated in the state estimation procedure [2]. Hence, to obtain a physically meaningful estimate, the clipping strategy has been used but it results in poor state estimation. Therefore, the focus of this work is to develop a constrained state estimation in the EKF framework such that the resulting states can be accurately estimated in a recursive fashion.

There exists very limited literature in the constrained state estimation using Kalman filter and Extended Kalman filter. Two distinct methods to handle inequality constraints using both KF and EKF approaches have been proposed [3]. The first method attempts to project the violated posterior estimate back into the constrained space by solving a quadratic programming problem. The second method focuses on restricting the Kalman gain, which produces an updated estimate that lies within the constrained region. Furthermore, a maximum a *posteriori* (MAP) solution to deal with equality constraints in the constrained EKF framework has been presented [4]. Also, an iterative algorithm was proposed to handle inequality constraints.

The most common strategy to handle constraints in state estimation is Moving Horizon Estimation (MHE) filter [5]. MHE can naturally handle constraints on sates by solving an optimization problem over a finite horizon with constraints easily enforced. In this regard, a moving horizon strategy that uses a fixed set of measurements to limit the size of the optimization problem being solved at each estimation step was proposed [6]. Later, [7] presented the MHE procedure for constrained state estimation of discrete-time system. In this study, the moving horizon window requires one to use the approximated arrival cost to account for the past data that are not included in the estimation. However, the choice of the approximation function must ensure that the estimator does not diverge. Despite this, the heavy computation load of the optimization problem and non-recursive nature of the MHE poses difficulties for online applications.

In order to retain the recursive nature of EKF and higher accuracy of non-linear dynamic data reconciliation results that are obtained by incorporating constraints, [8] proposed the Recursive Nonlinear Dynamic Data Reconciliation (RNDDR) approach. The RNDDR attempts to solve an optimization problem by imposing constraints while obtaining the updated state estimates. This is accomplished by embedding the optimization problem into the EKF to form a predictor-corrector framework. However, this approach cannot handle the nonlinearities while calculating the error covariance matrix. Therefore, using the idea of unscented transformation, an Unscented RNDDR (URNDDR) estimation algorithm was proposed [9]. This approach integrates the information of constraints into the selection of sigma points and their corresponding weights, so that the resulting covariance calculation is within the constrained region. Recently, the RNDDR method is applied in the particle based filters, the ensemble Kalman filter (EnKF) and the particle filter (PF). Prakash et al. [10] proposed a constrained EnKF with the RNDDR applied on each individual particle to render it constrained. A truncation method is also used for drawing the particles from the prior distribution. Alternatively, constrained EnKF to deal with inequality constraints, with the RNDDR applied on the posterior mean value was proposed [11]. The particles are then shifted by the same distance as the moving distance from constrained mean to the unconstrained mean. For the

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PF, the most straightforward existing constraining method is the acceptance/rejection approach, which simply removes the particles that violate the constraints. Several optimization formulations for the constrained PF have been proposed, in which the RNDDR is applied on the prior, posterior particle and posterior mean respectively [12].

The disadvantage of constrained EKF based on RNDDR is that it does not update the error covariance matrices according to constraints, leaving the unconstrained covariance matrix being used in subsequent steps, hence causing inaccurate estimation results. Therefore, several researchers studied particle filter (PF) with RNDDR applied on individual particles. However, it requires solving an optimization problem for each particle, leading to heavy computation load as the number of the particles increases.

In this paper, we propose a KL divergence based method to cope with constraints, which targets constraining both mean and covariance at every time step of estimation. This approach can handle inequality constraints for any recursive Bayesian estimator, with the state distribution approximated by Gaussian distribution, i.e. the statistical information of the state space can be described with only mean and covariance. In this work, we only consider the EKF as the application of our approach. The estimation performance of the KL based EKF is compared with the original RNDDR based EKF to show the merits of our approach.

The remainder of this paper is organized as follows: Section 2 briefly reviews the EKF for nonlinear state estimation. Section 3 reviews the original RNDDR approach to include constraints on the EKF framework. Section 4 presents the proposed constrained state estimation framework by formulating a tractable convex optimization problem based on KL divergence. Section 5 presents the simulation results of our proposed method on a two-state batch reaction system.

II. Extended Kalman filter

In this section, the details of the EKF approach for nonlinear state estimation are briefly reviewed. Consider a nonlinear discrete time system given by

$$\begin{aligned} x_k &= f(x_{k-1}, u_{k-1}) + v_k \\ y_k &= h(x_k) + w_k \end{aligned} \tag{1}$$

where v_k is the Gaussian process noise with zero mean and covariance Q, and w_k is Gaussian measurement noise with zero mean and covariance R.

Assume at time step k, the posterior state distribution is given by $x \sim N(x; \hat{x}_{k|k}, P_{k|k})$. At the next time step $k+1$, the EKF first linearizes the nonlinear model f around $\hat{x}_{k|k}$ to obtain the linear operator A_k of the process model.

$$A_k = \frac{\partial f(x_k, u_k)}{\partial x}\Big|_{\hat{x}_{k|k}, u_k}$$

However, this linearized model is used only in approximating the estimation error covariance ($P_{k+1|k}$), whereas, the nonlinear model is used for predicting the states. Now, the predictor - correction steps of the EKF filter are presented as follows:

Prediction:

At the prediction step, the predicted mean and covariance are calculated as follows.

$$\hat{x}_{k+1|k} = f(\hat{x}_{k|k}, u_k) \tag{2}$$

$$P_{k+1|k} = A_k P_{k|k} A_k^T + Q_k \tag{3}$$

Update:

The linear measurement operator is calculated as

$$H_{k+1} = \frac{\partial h(x_k)}{\partial x}\Big|_{\hat{x}_{k+1|k}}$$

The Kalman gain is calculated as

$$K = P_{k+1|k} H_{k+1} (H_{k+1} P_{k+1|k} H_{k+1}^T + R_k)^{-1} \tag{4}$$

The final Kalman update of mean and covariance at time step $k+1$ is given by

$$\hat{x}_{k+1|k+1} = \hat{x}_{k+1|k} + K(y_{k+1} - h(\hat{x}_{k+1|k})) \tag{5}$$

$$P_{k+1|k+1} = (I - KH_{k+1}) P_{k+1|k} \tag{6}$$

It is important to note that the updated state estimation obtained using (5) - (6) cannot handle constraints. Therefore, the resulting state estimation might yield physically meaningless estimates. Further, [2] has shown that the EKF can fail when the multiple states satisfy the steady state measurements and the poor initial guess of the state is used in the estimator.

III. Recursive nonlinear dynamic data reconciliation

In this section, we briefly review the Recursive Nonlinear Dynamic Data Reconciliation (RNDDR) approach used in constrained state estimation of nonlinear systems [8]. The basic idea of RNDDR method is to replace the Kalman update step (5) of the EKF algorithm by solving an optimization problem such that the posterior estimates, $\hat{x}_{k+1|k+1}$, are within the constrained region. Given the state constraints of the form, $x_{lb} \le x \le x_{ub}$, the constrained state update step requires one to solve the following optimization problem:

$$\begin{aligned} \hat{x}^c_{k+1|k+1} = \underset{x}{\operatorname{argmin}} & (x - \hat{x}_{k+1|k})^T P^{-1}_{k+1|k} (x - \hat{x}_{k+1|k}) \\ & + (y - h(x))^T R^{-1} (y - h(x)) \\ s.t. \quad & x_{lb} \le x \le x_{ub} \end{aligned} \tag{7}$$

where $P_{k+1|k}$ is the predicted covariance at time step $k+1$, obtained using (3). The above optimization problem provides a better constrained estimate as it penalizes the deviation of both the state vector and the measurement vector. The resulting state estimate will be inside the constrained region in this case. Without the state constraints, the unconstrained optimization problem will reduce to the EKF solution. It is important to note that states are the only decision variables in the optimization problem, and the estimation error covariance matrix is obtained as in the conventional EKF using (4) - (6). Therefore, the estimation error covariance might not lie inside the constrained region. In other words, the RNDDR only updates the mean value and the constraint information is not accounted while updating the covariance matrix. Thus, the unconstrained covariance is propagated into subsequent iterations, leading to inaccurate estimation. Other variants of RNNDR approach have been proposed using unscented transformation, and interested readers can refer to the works of [13], [9] and [14].

IV. Proposed KL divergence based approach

As mentioned previously, the RNDDR approach cares only about constraining the mean value, leaving the covariance an unaccounted factor in the constraining step. The motivation of our proposed method is to embrace the constraints in updating both the states and estimation error covariance matrix. Recall that the update equations of unconstrained EKF, (5) - (6), represent the ellipsoidal uncertain region around the state estimate ($\hat{x}_{k+1|k+1}$). This signifies the multivariate Gaussian distribution with mean $\hat{x}_{k+1|k+1}$, and covariance $P_{k+1|k+1}$. The main idea of our approach is to project the unconstrained solution into the constrained region such that both the state and its estimation error lie within the constrained space. Since Kullback-Leibler (KL) divergence is known to be a measure of similarity between two density functions, we seek to determine the multivariate Gaussian density function in the constrained region that is close and similar to the unconstrained multivariate Gaussian density function obtained from EKF approach. The KL divergence of f(x) from g(x) is defined as [15]:

$$D(f||g) = \int f(x) log \frac{f(x)}{g(x)} dx \tag{8}$$

If f(x) and g(x) are of both Gaussian distributions, the KL divergence has a closed form which can be expressed as,

$$\begin{aligned} D(f||g) = \frac{1}{2}[log\frac{|\Sigma_g|}{|\Sigma_f|} + Tr(\Sigma_g^{-1}\Sigma_f) - d \\ + (\mu_f - \mu_g)^T \Sigma_g^{-1}(\mu_f - \mu_g)] \end{aligned} \tag{9}$$

where $f(x) = N(x;\mu_f,\Sigma_f)$, $g(x) = N(x;\mu_g,\Sigma_g)$, the symbol $|M|$ denotes the determinant of the covariance matrix M, and d is the dimension of x.

Let us denote the constrained distribution $f(x) = N(x;\hat{x}^c_{k+1|k+1}, P^c_{k+1|k+1})$ obtained by projecting the unconstrained distribution $g(x) = N(x;\hat{x}_{k+1|k+1}, P_{k+1|k+1})$. Recall that $\hat{x}_{k+1|k+1}$ and $P_{k+1|k+1}$ are the solution of the unconstrained Kalman update (5) -(6). Since we are considering the complete distribution information of the unconstrained EKF solution to be projected into the constrained region, we seek the state covariance to be completely inside the constrained region. It is important to note that the state covariance $P_{k+1|k+1}$ obtained from the EKF signifies the ellipsoid representation around the state estimates. Therefore, to constrain the state covariance, we utilize the following expression of ellipsoid,

$$\mathscr{E} = \{\hat{x}_{k+1|k+1} + \alpha S_{k+1} z \mid \|z\|_2 \leq 1\} \tag{10}$$

where S_{k+1} is the positive square root of $P_{k+1|k+1}$ and α depends on the confidence limit and it is prescribed by the user (e.g., $\alpha = 2$ signifies a confidence limit of 95%). In order to bound the state covariances, we enforce the following constraints:

$$\mathscr{E} = \{(x_{lb} \leq \hat{x}_{k+1|k+1} + \alpha S_{k+1} z \leq x_{ub}) \mid \|z\|_2 \leq 1\} \tag{11}$$

or equivalently, the above constraint can rewritten as

$$\tilde{x} := \hat{x}_{k+1|k+1} + \alpha S_{k+1} z \mid \|z\|_2 \leq 1 \tag{12}$$

$$h_i^T \tilde{x} + t_i \leq 0; i = 1, \ldots, m \tag{13}$$

where h_i is the i^{th} row of the matrix $H = [I;-I]$ and t_i is the i^{th} element of vector $t = [x_{ub}; -x_{lb}]$. Now, the optimization formulation that can simultaneously determine the state updates and state covariances of the constrained filtering problem can be formulated as follows:

$$\min_{\hat{x}^c_{k+1|k+1}, P^c_{k+1|k+1}} D(f||g) \tag{14}$$

$$\text{s.t.} \quad x_{lb} \leq \hat{x}^c_{k+1|k+1} \leq x_{ub} \tag{15}$$

$$S_{k+1} = {P^c}^{1/2}_{k+1|k+1} \tag{16}$$

$$\tilde{x} := \hat{x^c}_{k+1|k+1} + \alpha S_{k+1} z \mid \|z\|_2 \leq 1 \tag{17}$$

$$h_i^T \tilde{x} + t_i \leq 0; i = 1, \ldots, m \tag{18}$$

The above optimization problem is a semi-infinite optimization problem and it is not computationally tractable owing to the nonlinear matrix constraint (16) and infinite dimensional constraints (17).

A. Convex reformulations

In this subsection, we present the convex optimization techniques to reformulate the above infinite dimensional optimization problem such that it can be solved efficiently. First, let us consider the objective function of the proposed optimization problem to be expressed as,

$$\begin{aligned} D(f||g) = \frac{1}{2}[log\frac{|P_{k+1|k+1}|}{|P^c_{k+1|k+1}|} + Tr(P^{-1}_{k+1|k+1} P^c_{k+1|k+1}) - d \\ + (\hat{x}^c_{k+1|k+1} - \hat{x}_{k+1|k+1})^T P^{-1}_{k+1|k+1} (\hat{x}^c_{k+1|k+1} - \hat{x}_{k+1|k+1})] \end{aligned} \tag{19}$$

Recalling ${P^c}_{k+1|k+1} = S_{k+1} S^T_{k+1}$ and using the properties of determinants and trace invariance under cyclic permutations, the objective function can be rewritten as:

$$\begin{aligned} D(f||g) = \frac{1}{2}[log\mathbf{det}(P_{k+1|k+1}) - d - 2log\mathbf{det}(S_{k+1}) \\ + Tr(S^T_{k+1} P^{-1}_{k+1|k+1} S_{k+1}) \\ + (\hat{x}^c_{k+1|k+1} - \hat{x}_{k+1|k+1})^T P^{-1}_{k+1|k+1} (\hat{x}^c_{k+1|k+1} - \hat{x}_{k+1|k+1})] \end{aligned} \tag{20}$$

The first two terms in the above expression is constant, the negative log term is convex. However, the trace term is non convex because the decision variables are expressed in quadratic form of unknown matrices. To alleviate the computational difficulty arising due to the trace term in the objective function, we use the definition of epigraph of a function and Schur complement of matrix $Y = S^T_{k+1} P^{-1}_{k+1|k+1} S_{k+1}$. For

TABLE I

CONSTRAINED EKF ALGORITHM BASED ON KL DIVERGENCE

1	Given the initial values for $x_{0\|0}$ and $P_{0\|0}$
2	At time step k, obtain the unconstrained EKF solution, $\hat{x}_{k+1\|k+1}$ and $P_{k+1\|k+1}$, using (5) and (6), respectively
3	Solve the optimization problem [(24) to (28)] using CVX to obtain the constrained EKF solution, $\hat{x}^c_{k+1\|k+1}$ and $P^c_{k+1\|k+1}$.
4	Use the constrained EKF solution obtained in Step 3 to do prediction at time step $k+1$ using (2) - (3), and then proceed to Step 2.

more details on the definitions, the reader is referred to [16]. These convex optimization tricks enable one to replace the trace term, $Tr(S_{k+1}^T P_{k+1|k+1}^{-1} S_{k+1})$, with a linear term, q, in the objective function along with an upper bound for the trace term, and an LMI constraint. The corresponding constraints can be expressed as

$$Tr(Y) \leq q \tag{21}$$

$$\begin{bmatrix} Y & S_{k+1} \\ S_{k+1}^T & P_{k+1|k+1} \end{bmatrix} \succeq 0 \tag{22}$$

where Y is an additional matrix variable defined as a result of convex relaxation using Schur complement of a matrix, and q is an additional scalar variable defined using the definition of epigraph of a function. Now, let us consider reformulating the infinite dimensional constraints (17) - (18). This constraints can be rewritten in terms of the following second order cone constraints [16],

$$\alpha||S_{k+1}h_i|| + h_i^T \hat{x}_{k+1|k+1} \leq t_i \tag{23}$$

The resulting optimization problem for updating the state estimates and its covariances is presented below:

$$\min_{\hat{x}^c_{k+1|k+1}, S_{k+1}} \frac{1}{2}[log\mathbf{det}(P_{k+1|k+1}) - d - 2log\mathbf{det}(S_{k+1}) + q$$
$$+ (\hat{x}^c_{k+1|k+1} - \hat{x}_{k+1|k+1})^T P_{k+1|k+1}^{-1}$$
$$(\hat{x}^c_{k+1|k+1} - \hat{x}_{k+1|k+1})] \tag{24}$$
$$\text{s.t.} \quad x_{lb} \leq \hat{x}^c_{k+1|k+1} \leq x_{ub} \tag{25}$$
$$Tr(Y) \leq q \tag{26}$$
$$\begin{bmatrix} Y & S_{k+1} \\ S_{k+1}^T & P_{k+1|k+1} \end{bmatrix} \succeq 0 \tag{27}$$
$$\alpha||S_{k+1}h_i|| + h_i^T \hat{x}_{k+1|k+1} \leq t_i \tag{28}$$

In the above formulation, the decision variables are $\hat{x}^c_{k+1|k+1}$, S_{k+1}, q, and Y. The solution to this optimization problem directly yields the state updates, $\hat{x}^c_{k+1|k+1}$, whereas the error covariance of the states ($P^c_{k+1|k+1}$) can be updated from S_{k+1} as:

$$P^c_{k+1|k+1} = S_{k+1}S_{k+1}^T \tag{29}$$

After acquiring the constrained estimate $\hat{x}^c_{k+1|k+1}$ and $P^c_{k+1|k+1}$, pass them to the next time step as prior estimates. The proposed constrained EKF algorithm is presented in Table I. It should be noted that the proposed optimization problem is convex and hence, it can be solved for global optimality using available convex optimization tool, CVX, which is a MATLAB based software for solving convex optimization problems [17].

V. CASE STUDY: A TWO-STATE BATCH REACTION SYSTEM

To demonstrate our proposed approach, we consider the batch reaction system studied by [10], [12] and [4]. Consider a gas phase reaction given by

$$2A \rightarrow B \quad k = 0.16 \tag{30}$$

Let the states of the process be partial pressures of A and B, $x = [P_A, P_B]$, and the total pressure $P = P_A + P_B$ is measured. Assuming the reaction occurs in a well-mixed isothermal batch reactor, the state space model can be written as:

$$\dot{x} = f(x) = \begin{bmatrix} -2 \\ 1 \end{bmatrix} kP_A^2, \quad y = \begin{bmatrix} 1 & 1 \end{bmatrix} x \tag{31}$$

The model is discretized at an interval of 0.1 s and simulated from an initial value of $x_0 = [3, 1]$. The process and measurement noises are both assumed to be Gaussian with zero mean. Their respective covariances are $Q = diag(0.001^2, 0.001^2)$ and $R = 0.1^2$. A poor initial guess is given to the state estimator with $\bar{x}_0 = [0.1, 4.5]$ and a large covariance matrix $P_0 = diag(6^2, 6^2)$ is used.

First, the EKF without any constraint is applied on the model to estimate the states $[P_A, P_B]$. It can be seen from Fig. 1 that the estimation results using the unconstrained EKF diverge from the true values. This poor estimation performance is caused because of the intentionally chosen large initial error. Then, the constrained estimation with EKF is performed with the following inequality constraints imposed on state variables,

$$\begin{bmatrix} 0 \\ 0 \end{bmatrix} \leq \begin{bmatrix} P_A \\ P_B \end{bmatrix} \leq \begin{bmatrix} 5 \\ 5 \end{bmatrix}$$

Fig. 2 shows the comparison of constrained estimation results using the RNDDR method and our proposed KL divergence based method. Both the methods yield convergent estimation results because of the incorporation of constraints, and they both perform well in the light of satisfying constraints. The reason for the superior performance of KL based method is that RNDDR only enforces the mean value to be inside the constraints and does not constrain the state error covariance matrix, whereas, the KL based method adjusts both the mean and error covariance by incorporating constraints. The modified covariance is directly propagated on to the calculation of Kalman gain in the next iteration, providing a faster impact on the estimation from the constraints compared to the RNDDR solution.

In Fig. 3, we present the state estimate and its error covariance at first and second time steps to show that the constrained error covariance is obtained using KL method. The ellipses represent the two-dimensional projection of the state PDF on xy plane and the rectangular region denotes the constrained space. It should be noted that, at first time step, the RNDDR does not deviate much from the

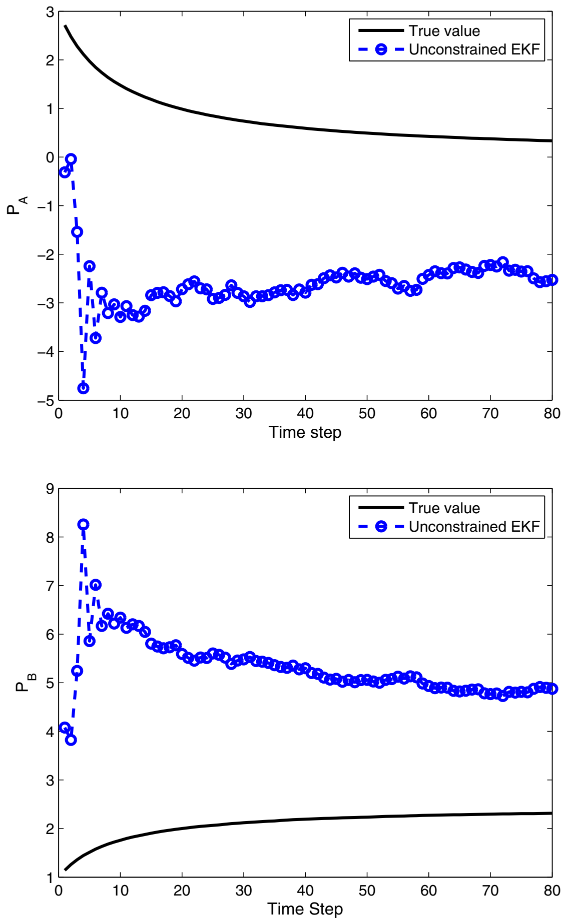

Fig. 1. State estimates using unconstrained EKF approach

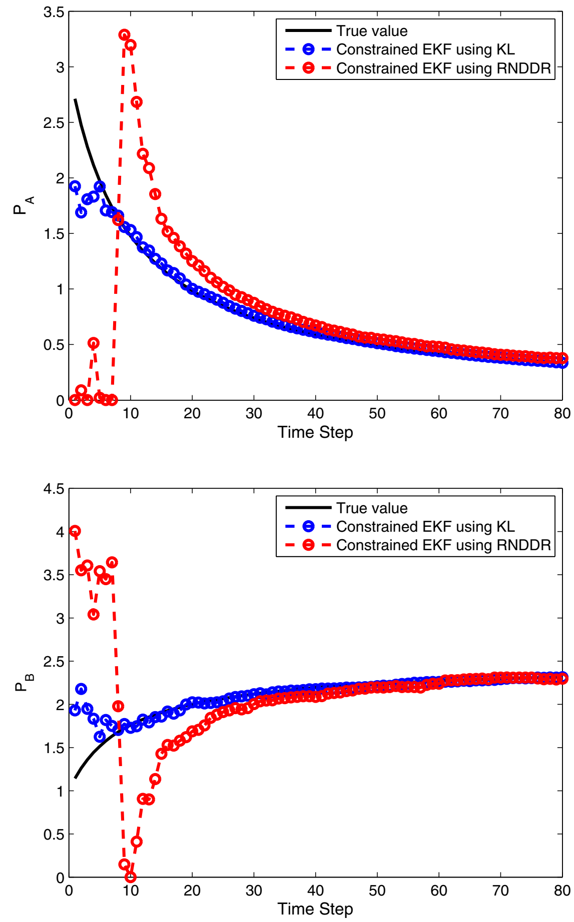

Fig. 2. Comparison of state estimates obtained using the proposed KL approach with the RNDDR approach

unconstrained result because it only projects the violated mean $\hat{x} = [-0.16 \quad 4.23]$ to the boundary (i.e., the RNDDR estimate is $\hat{x} = [0.001 \quad 4.25]$), whereas, the KL method shrinks the original distribution by a large portion to fit inside the constrained region. At second time step, the estimation error covariance obtained using the KL method shrinks even further into the constrained region, whereas, the RNDDR still yields a large error covariance.

Fig. 4 shows the evolution of variance of P_A for first 20 time steps. P_B also produces a very similar result. The KL method provides a much smaller variance from the beginning, while the RNDDR is stuck at a large error for several time steps. The smaller covariance obtained from the KL method remedies the large error covariance exerted on the initial state distribution since the prediction part of the Kalman update produces more reliable results with smaller covariance. The KL based method has a faster convergence rate, and also results in smaller estimation error. Table II presents the root mean square error (RMSE) of estimated states, P_A and P_B, and average computation time per estimation step using the RNDDR method and our proposed KL based method, respectively. The higher computational time of the KL method can be attributed to the increased number of decision variables while solving the conic optimization problems in the update step of the proposed state estimation procedure, whereas, the RNDDR solves a nonlinear optimization problem to update the states.

TABLE II

PERFORMANCE COMPARISON OF RNDDR AND KL METHODS

		RNDDR	KL
RMSE	P_A	0.7220	0.1417
	P_B	0.7422	0.1613
CPU (s / step)		0.1938	2.4663

VI. CONCLUSIONS

In this paper, a KL divergence based approach is proposed to replace the popular RNDDR method to handle inequality constraints. The RNDDR formulates a quadratic programming optimization problem based on the estimated mean value. The KL method attempts to take both of the decision parameters of the Gaussian state distribution, namely mean and covariance, into consideration when dealing with the constraints. It formulates a convex optimization problem to penalize the deviation of whole distribution instead of just the mean in the RNDDR, with both mean and the covariance

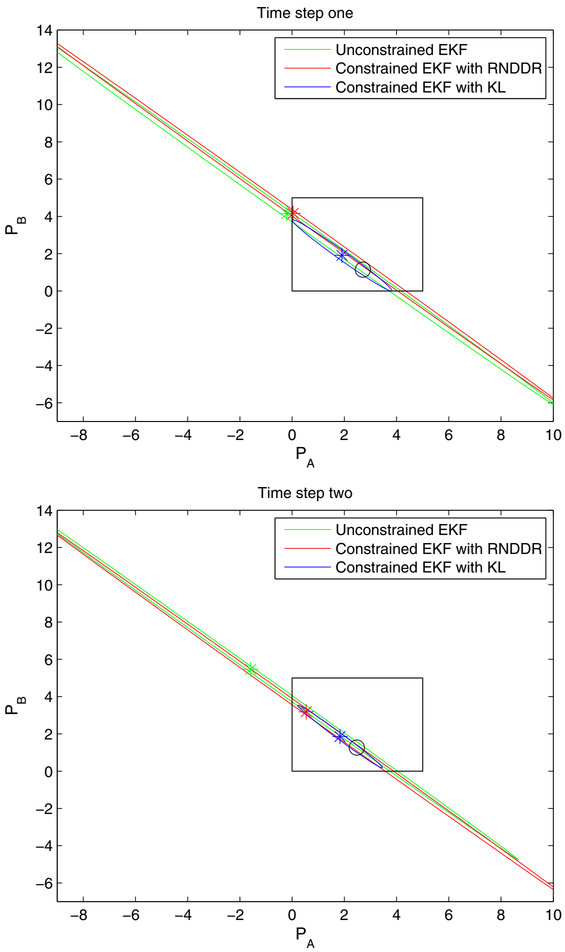

Fig. 3. State space showing the state estimates and error covariance obtained using Unconstrained EKF, RNDDR, and KL methods (a) at first time step; (b) at second time step. True value of the states is marked by a black circle. The markers shown in the center of ellipse denotes the state estimates obtained using respective methods

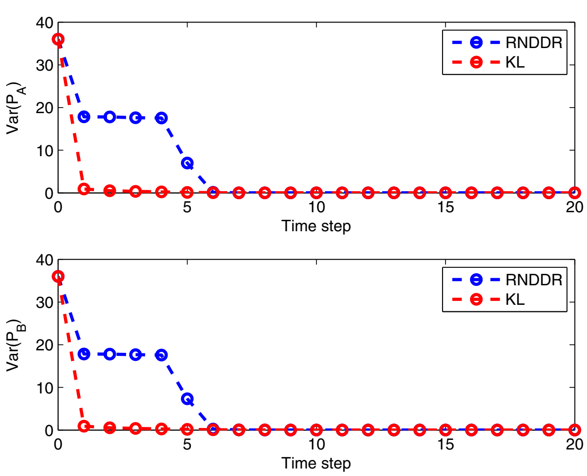

Fig. 4. Evolution of error variances of P_A and P_B

as the decision variables. Thus, the KL method is shown to have faster convergence rate. As the KL method requires only the mean and covariance of distribution before and after the constraining step, this approach can be integrated into other filtering methods, such as UKF and EnKF, in which the state distribution is approximated by a Gaussian distribution.

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