ROBUST CONSTRAINED ESTIMATION VIA UNSCENTED TRANSFORMATION

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Abstract: The task of improving the quality of the data so that it is consistent with material and energy balances is called reconciliation. Since chemical processes often operate dynamically in nonlinear regimes, techniques like Extended Kalman Filter (EKF) and Nonlinear Dynamic Data Reconciliation (NDDR) have been developed. There are various issues that arise with the use of either of these techniques: EKF cannot handle inequality or equality constraints, while the NDDR has high computational cost.
In this paper, first, a recursive nonlinear dynamic data reconciliation (RNDDR) formulation is discussed. The RNDDR formulation extends the capability of the EKF by allowing for incorporation of algebraic constraints and bounds during correction. The covariance calculations arising in the RNDDR are same as EKF, i.e., both, nonlinearity and constraints are neglected during covariance propagation and calculation of uncertainty in filtered estimates. The use of Unscented Transformation with the RNDDR gives the Unscented Recursive Nonlinear Dynamic Data Reconciliation (URNDDR) formulation, which addresses all the aspects of nonlinearity and constraints in a recursive estimation framework, thus proving to be an efficient tool for real-time estimation.

Keywords: State and Parameter Estimation, Nonlinearity, Algebraic Constraints

1. INTRODUCTION

The quality of process data in a chemical process significantly affects the performance and benefits gained from activities like performance monitoring, online optimization and control. Processes are invariably subject to random disturbances and process measurement is corrupt with random errors. In order to ameliorate the effect of these random errors, estimation methods can be used to obtain accurate estimates of the process states and parameters.

Several different estimation methods have been proposed in the literature depending on the assumptions made. For linear dynamic systems, the Kalman Filter (KF) gives optimal estimates in presence of measurement and state uncertainties (Gelb, 1988). For nonlinear systems, Extended Kalman Filters (EKF) have been developed, which are based on linearising the nonlinear equations and applying the Kalman filter update equations to the linearised system. The advantages of the KF, the EKF and their variants lie in their predictive-corrective form and the recursive nature of estimation. The recursive form of these estimation methods allows for rapid estimation in real-time, which is extremely important for online deployment. A major disadvantage of the KF and all its variants is that they cannot take into account bounds on process variables or other algebraic constraints.

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In this paper, first, a Recursive Nonlinear Dynamic Data Reconciliation (RNDDR) formulation is presented. The RNDDR formulation extends the capability of EKF by allowing for incorporation of algebraic constraints and bounds. The covariance calculations arising in the RNDDR formulation are similar to the EKF, which is, linearized model based covariance propagation and the calculation of uncertainty in filtered estimates by using the Kalman gain i.e. by assuming an unconstrained correction. This formulation has been extended with the aid of Unscented Transformation (Julier and Uhlmann, 1997), to give the Unscented Recursive Nonlinear Dynamic Data Reconciliation (URNDDR) formulation which addresses nonlinearity and constraints arising in both the propagation and correction steps.

2. RECURSIVE NONLINEAR DYNAMIC DATA RECONCILIATION (RNDDR)

In Kalman filter and its variants, the estimation procedure at each sampling instant can be regarded as composed of two steps (as described in Vachhani *et al.* (2003)). In the first step, the state estimates from the previous time instant are propagated through the process dynamic equations (along with its error covariance matrix), while in the second step, the predicted estimates are corrected using the measurements available at the current time instant. It is known that the optimal updated estimates for KF (as also its variants) are obtained by solving an unconstrained optimization problem for which the objective function is given in Equation A.5. In the absence of any constraints, the solution of this optimization problem is given by the standard Kalman filter update equation for the state estimates given in Equations A.6 - A.7. The Kalman filter can be extended to obtain simultaneous state and parameter estimates, by treating the parameters to be estimated as augmented states (Jazwinski, 1970).

If algebraic constraints or bound constraints have to be imposed on the state estimates, these can be conveniently included in this optimization problem. In this case, the solution of the optimization problem has to be obtained numerically. This forms the basis for the RNDDR method.

$$\begin{aligned} x_{k+1} &= x_k + \int_{k\Delta t}^{(k+1)\Delta t} f(x(\tau), u_k, p) d\tau + w_k \\ y_{k+1} &= g(x_{k+1}) + v_{k+1} \end{aligned} \tag{1}$$

Consider the system given by Equation 1 with bounds and algebraic constraints imposed on the states and parameters. Let $\hat{x}_{k|k}$, $\hat{p}_{k|k}$, and $P_{k|k,a}$ (a in the subscript here refers to the augmented system) be given at time instant 'k'. The predicted state estimates $\hat{x}_{k+1|k}$ is determined by integration for the given parameter estimate $\hat{p}_{k|k}$ (same as $\hat{p}_{k+1|k}$) and the variance of uncertainty in the predicted estimates is calculated by covariance propagation as with EKF.

For covariance propagation, the nonlinear state space model is linearized around $[\hat{x}_{k|k}, \hat{p}_{k|k}]$,

$$\begin{bmatrix} \dot{x} \\ \dot{p} \end{bmatrix} = \underbrace{\begin{bmatrix} A_k & \Gamma_{pk} \\ 0 & 0 \end{bmatrix}}_{A_{k,a}} \begin{bmatrix} x \\ p \end{bmatrix}$$

and the state transition matrix is approximated assuming an equivalent LTI system, $\bar{A}_{k,a} = exp(A_{k,a}\Delta t)$. Using this linearized approximation, the covariance matrix of estimation errors is propagated as

$$P_{k+1|k,a} = \left[\, \bar{A}_{k,a} \,\right] P_{k|k,a} \left[\, \bar{A}_{k,a} \,\right]^T + \begin{bmatrix} Q_k & 0 \\ 0 & Q_{pk} \end{bmatrix} \tag{2}$$

In order to obtain the updated state estimates, the following optimization problem is solved.

$$\begin{aligned} \min_{x_{k+1}, p_{k+1}} \quad & (y_{k+1} - g(x_{k+1}))^T R_{k+1}^{-1} (y_{k+1} - g(x_{k+1})) + \\ & \left(\begin{bmatrix} x_{k+1} \\ p_{k+1} \end{bmatrix} - \begin{bmatrix} \hat{x}_{k+1|k} \\ \hat{p}_{k+1|k} \end{bmatrix} \right)^T (P_{k+1|k,a})^{-1} \left(\begin{bmatrix} x_{k+1} \\ p_{k+1} \end{bmatrix} - \begin{bmatrix} \hat{x}_{k+1|k} \\ \hat{p}_{k+1|k} \end{bmatrix} \right) \end{aligned}$$

subject to the following constraints,

$$\begin{aligned} x_L \leq x_{k+1} &\leq x_U \\ p_L \leq p_{k+1} &\leq p_U \\ h(x_{k+1}, p_{k+1}) &\leq 0 \\ e(x_{k+1}, p_{k+1}) &= 0 \end{aligned}$$

The optimal solution to this problem (x^*_{k+1}, p^*_{k+1}) provides the corrected state and parameter estimates. The solution obtained using EKF is used as an initial guess for solving the above optimization problem. It should be noted that if the measurement model is linear, and none of the inequality constraints are active in the optimal solution, then the solution for the updated state estimates obtained will be the same as the one computed using Equation A.6. The covariance matrix of the error in the updated state and parameter estimates is computed using Equations (A.7 and A.8). It should also be noted that while equations (A.6, A.7 and A.8) are for state estimation, the Kalman filter can be used for simultaneous state and parameter estimation by augmenting the system with parameters as additional state variables and applying the Kalman filter equations to the augmented system. By using these equations, the effect of the constraints on the covariance matrix of estimation errors is neglected. This limitation is addressed in the proposed URNDDR formulation.

3. UNSCENTED TRANSFORMATION

The use of unscented transformation in estimation theory was first studied by Julier and Co-workers (Julier and Uhlmann, 1997; Julier *et al.*, 2000). Traditionally, the covariance calculation in the Extended Kalman filter for nonlinear systems have used linearized approximation of the process for propagation, see Equation 2. This approximation has two drawbacks:
(i) The linearized model may prove to be coarse, and
(ii) The analytical expression for the Jacobian matrix

may not be easy for large systems, requiring the use of finite difference methods. This would involve further computational errors.

The motivation for the unscented transformation is that *it is easier to approximate a probability distribution than it is to approximate an arbitrary nonlinear function or transformation* (Julier and Uhlmann, 1997). In the unscented transformation a set of weighed points are chosen to parameterize the mean and covariance of the probability distribution. The set of points undergo the nonlinear transformation at hand, and the statistical property of the result is calculated from the transformed data set. The exact procedure of the unscented transformation is presented below.

A n-dimensional random variable $\mathbf{x}$ with mean $\bar{\mathbf{x}}$ and covariance $\mathbf{P_{xx}}$ is approximated by $2n+1$ weighed points around the mean of distribution. The set of points $\mathscr{X}$ is also referred to as the sigma set. The first point chosen is the mean of the distribution,

$$\mathscr{X}_0 = \bar{\mathbf{x}} \quad W_0 = \frac{\kappa}{n+\kappa}$$

The rest of the $2n$ translated sigma points are chosen symmetrically around the mean as,

$$\mathscr{X}_i = \bar{\mathbf{x}} + (\sqrt{(n+\kappa)\mathbf{P_{xx}}})_i \quad W_i = \frac{1}{2(n+\kappa)}$$

and

$$\mathscr{X}_{i+n} = \bar{\mathbf{x}} - (\sqrt{(n+\kappa)\mathbf{P_{xx}}})_i \quad W_{i+n} = \frac{1}{2(n+\kappa)}$$

where $(\sqrt{(n+\kappa)\mathbf{P_{xx}}})_i$ is the ith column of the matrix square root of $((n+\kappa)\mathbf{P_{xx}})$ and W_i is the weight associated with the corresponding point. Here κ is a tuning parameter and the heuristic $\kappa + n = 3$ has been suggested for normal distribution (Julier and Uhlmann, 1997).

The transformed set of sigma points are evaluated by $\mathscr{Y}_i = g(\mathscr{X}_i)$ and the predicted mean is computed as

$$\bar{\mathbf{y}} = \sum_{i=0}^{2n} W_i \mathscr{Y}_i \tag{3}$$

The predicted covariance is calculated from the transformed set and the predicted mean

$$\mathbf{P_{yy}} = \sum_{i=0}^{2n} W_i [\mathscr{Y}_i - \bar{\mathbf{y}}][\mathscr{Y}_i - \bar{\mathbf{y}}]^T \tag{4}$$

Thus, the unscented transformation can be used to better model the changes in the statistical properties of a random variable through a nonlinear transformation. In the unscented transformation for more than three dimensional variables, κ can take a negative value and in such a case there is a possibility that the predicted covariance becomes non-positive semi-definite. In this situation, it is possible to modify the prediction algorithm (Julier and Uhlmann, 1997).

Inequality constraints like bounds, for example $x \leq x_U$, take the following form

$$\text{if } \mathscr{X}_i > x_U, \quad \text{then } \mathscr{X}_i = x_U$$

This briefly describes the unscented transformation. Detailed discussion on Unscented Kalman Filter can be found in Wan and van der Merwe (2000). In the next section, the use of unscented transformation is proposed towards addressing constrained nonlinear transformations arising in the RNDDR formulation.

4. UNSCENTED RECURSIVE NONLINEAR DYNAMIC DATA RECONCILIATION (URNDDR)

In the previous section, the unscented transformation was explained. The advantage of the unscented transformation is that it can handle nonlinearity and constraints in the transformation. Here, the algorithmic implementation of the unscented recursive nonlinear dynamic data reconciliation formulation is presented.

Consider the system given by Equation 1 with bounds and algebraic constraints imposed on the states and parameters. Let $\hat{x}_{k|k}$, $\hat{p}_{k|k}$, and $\mathbf{P_{k|k,a}}$ be given at time instant 'k'. In the first step of prediction, the unscented transformation is used to determine the mean and covariance of uncertainty in the propagated states. A set of sigma points are selected for propagation, involving uncertain states and uncertainty in the equations (Wan and van der Merwe, 2000). The selection follows the approach outlined in the section on unscented transformation (section 3). Bounds are imposed on the above set of points.

The constrained sigma points are propagated through the nonlinear differential equations governing the process to arrive at the set of translated sigma points. The bounds are imposed on the set of translated sigma points, to compute the propagated sigma points. Once the propagated set of data has been determined, the mean $\hat{x}_{k+1|k,a}$ and the variance $\mathbf{P_{k+1|k,a}}$ are calculated using the unscented transformation. Notice that in the propagation step, the equality and inequality constraints are not taken into account. These constraints are conveniently handled in the correction step which is solved as an optimization problem. Further, imposing bounds and constraints on the sigma points (in the correction and propagation steps), might not preserve the original properties of the unscented transformation. This has not been addressed in this paper.

In the correction step of the URNDDR, there is an uncertainty associated with the n_a (number of states + number of parameters) propagated states $\hat{x}_{k+1|k,a}$ ($\mathbf{P_{k+1|k,a}}$). Therefore, $2(n_a)+1$ sigma points are used for the correction step. The selection of the sigma points is,

$$\left[\hat{\mathscr{X}}_{0,k+1|k,a}\right] = \left[\hat{x}_{k+1|k,a}\right], W_0 = \frac{\kappa}{(n_a+\kappa)}$$

$$\left[\hat{\mathscr{X}}_{i,k+1|k,a}\right] = \left[\,\hat{x}_{k+1|k,a}\,\right] + \left(\sqrt{(n_a+\kappa)\left[\,\mathbf{P_{k+1|k,a}}\,\right]}\right)_i$$

$$W_i = \frac{1}{2(n_a+\kappa)}$$

$$\left[\hat{\mathscr{X}}_{i+n_a,k+1|k,a}\right] = \left[\hat{x}_{k+1|k,a}\right] - \left(\sqrt{(n_a+\kappa)\left[\,\mathbf{P_{k+1|k,a}}\,\right]}\right)_i$$

$$W_{i+n_a} = \frac{1}{2(n_a+\kappa)}$$

and $2(n_a)+1$ optimization problems are solved.

$$\min_{\mathscr{X}_{j,k+1,a}} \left(y_{k+1} - g(\mathscr{X}_{j,k+1})\right)^T \mathbf{R_{k+1}^{-1}} \left(y_{k+1} - g(\mathscr{X}_{j,k+1})\right) + \left(\mathscr{X}_{j,k+1,a} - \hat{\mathscr{X}}_{j,k+1|k,a}\right)^T (\mathbf{P_{k+1|k,a}})^{-1} \left(\mathscr{X}_{j,k+1,a} - \hat{\mathscr{X}}_{j,k+1|k,a}\right)$$

subject to the following constraints,

$$x_L \leq \mathscr{X}_{j,k+1} \leq x_U$$

$$p_L \leq \mathscr{P}_{j,k+1} \leq p_U$$

$$h(\mathscr{X}_{j,k+1}, \mathscr{P}_{j,k+1}) \leq 0$$

$$e(\mathscr{X}_{j,k+1}, \mathscr{P}_{j,k+1}) = 0$$

The optimal solutions to the $2(n_a)+1$ optimization problems are the corrected sigma point set of $\hat{\mathscr{X}}_{j,k+1|k+1,a}$. The mean $\hat{x}_{k+1|k+1,a}$ and the covariance $\mathbf{P_{k+1|k+1,a}}$ of the corrected estimates are calculated using the unscented transformation.

For comparison purposes, the Unscented Kalman filter (UKF) is also implemented in a similar fashion, with the Kalman gain being used in the correction step and constraints are not applied on the translated sigma points during propagation.

5. STATE ESTIMATION PROBLEM

The first case study selected for the URNDDR is the state estimation in a gas phase reversible reaction in an isothermal batch reactor (Haseltine and Rawlings, 2003)

$$2A \xrightarrow{\bar{k}} B \quad \bar{k} = 0.16$$

where reaction rate $r = \bar{k}P_A^2$. The partial pressures are the state variables and the total pressure is measured.

$$x = \begin{bmatrix} P_A \\ P_B \end{bmatrix}, \quad y_k = [1 \;\; 1]x_k$$

The initial state is $x_0 = [3 \;\; 1]^T$. For state estimation problem, the following parameters have been used:

$$\Delta t = 0.1,\; P_0 = \begin{bmatrix} 36 & 0 \\ 0 & 36 \end{bmatrix},\; Q = \begin{bmatrix} 10^{-6} & 0 \\ 0 & 10^{-6} \end{bmatrix}$$

$$R = 0.01, \hat{x}_0 = [0.1 \;\; 4.5]^T,\; x_L = [0 \;\; 0]^T,$$
$$x_U = [100 \;\; 100]^T$$

First the EKF result is presented in Figure 1 for the above initialization scheme. As it can be seen without the information about the constraints the EKF could not converge to the actual dynamics and gives unrealistic estimates for partial pressure of component 'A'. The same was the case with UKF. With the added information of constraints the RNDDR result is presented in Figure 2.

The RNDDR did converge to the actual dynamics of the reaction system but it was stuck at the lower bound for few sample instants before it could respond. This can be explained by the fact that the covariance calculation did not take into account the presence of constraint and the correction step relies on the reliability of the covariance calculation. In case of the URNDDR, which takes the effects of constraints as well as process nonlinearity during covariance calculation, it would be expected that it tracks the actual dynamics better than RNDDR. This is verified by the results presented in Figure 3 for the URNDDR. The

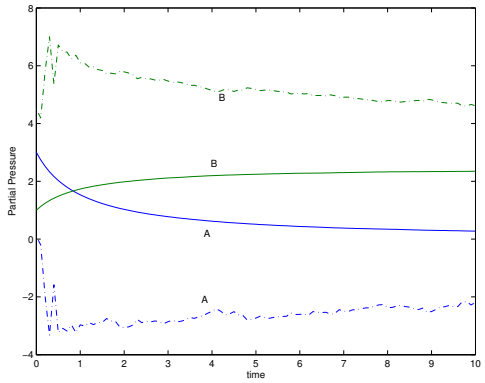

Fig. 1. EKF Case 1 State Estimates. Line: Actual, Dash-Dot: Estimated

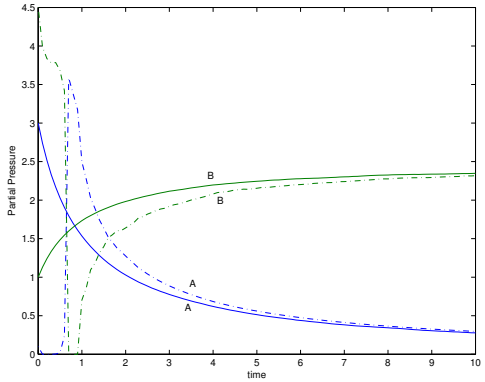

Fig. 2. RNDDR Case 1 State Estimates. Line: Actual, Dash-Dot: Estimated

URNDDR converged to the actual dynamics within a few sample instants. This result is comparable with the MHE results presented by Haseltine and Rawlings (Haseltine and Rawlings, 2003) which is computationally a more expensive procedure.

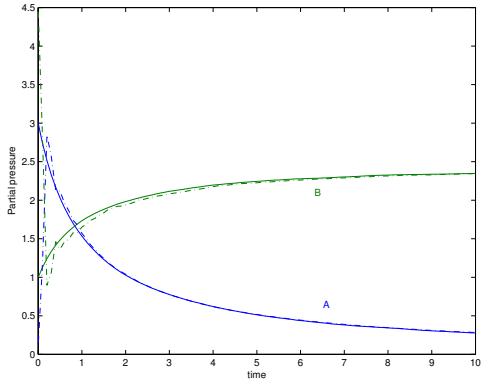

Fig. 3. URNDDR Case 1 State Estimates. Line: Actual, Dash-Dot: Estimated

6. CSTR CASE STUDY

In the previous section, a state estimation example was chosen to show the efficacy of the proposed approach. In this section, the proposed URNDDR formulation is rigorously compared against the EKF, Unscented Kalman Filter (UKF) and the RNDDR formulations

for simultaneous state and parameter estimation in a Continuous Stirred Tank Reactor (CSTR). The simulation result presented is the case when the catalyst activity undergoes a change, and it is required to simultaneously estimate the states and the catalyst activity parameter. The implementation details of the case study can be found in Vachhani *et al.* (2003).

Three different step changes in catalyst activity of 1 to 0.7, 1 to 0.8 and 1 to 0.9 at sampling instant of 20 are introduced. The process is simulated for 100 sampling instants with sampling time of 0.05 hour, and the four estimators namely: EKF, RNDDR, UKF and URNDDR are implemented. The Root Mean Square (RMS) errors in the measurements (difference between measured and true values) and the RMS errors in the estimates (difference between estimated and true values) of both measured variables and parameters are computed and averaged over the three simulation runs for each of the methods, the results of which are presented in Table 1. As it can be seen the performance of the URNDDR is better than RNDDR in terms of accuracy of results. The RMS errors in the UKF result are marginally better than the URNDDR result but at the trade-off of unrealistic estimates of catalyst activity greater than one, as shown in Figure 4. Hence, UKF is not a valid estimator for this problem. A comparison of RMS errors reflects the accuracy of the URNDDR formulation. It can be seen that the URNDDR performs relatively better than the RNDDR formulation. The computational cost for this problem correspondingly increases approximately from 0.2 seconds for RNDDR to 5 seconds for URNDDR formulation. The RMS errors in the UKF result are similar to URNDDR formulation, but at the trade-off of unrealistic estimates of catalyst activity greater than one, as shown in Figure 4. Hence, UKF is not a valid estimator for this problem.

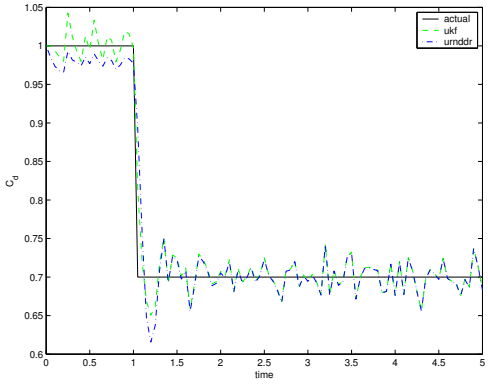

Fig. 4. Catalyst activity estimate - UKF and URNDDR

In Figure 5, the results for all the discussed formulations are presented for a ramp change in the catalyst activity. On comparing the URNDDR with the RNDDR result, it can be seen that with the use of the unscented transformation, realistic estimates which are consistently away from the constraints are achieved. The result of the URNDDR is same as the UKF if the constraints are not activated, this can be seen in Figure 5 when catalyst activity has decreased to less than one.

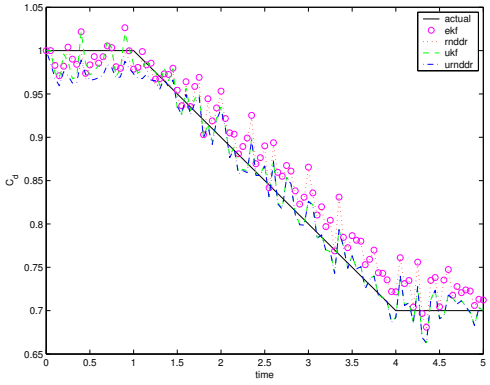

Fig. 5. Catalyst activity estimate - EKF, RNDDR, UKF and URNDDR

7. CONCLUSIONS

The Unscented RNDDR is motivated by the limitation of the RNDDR in taking into account effect of nonlinearity and algebraic constraints on the covariance matrix of estimation errors. In the RNDDR, the basis of covariance propagation is on a linearized representation of the process and the covariance calculation arising in the correction step is based on an equivalent unconstrained minimization solution. With the use of the unscented transformation, the effect of nonlinearity and constraints is taken into account in both propagation and correction steps of the URNDDR formulation.

The proposed method is an extension of the unscented Kalman filter, without sacrificing the essential recursive computation advantage of the Kalman filter. The results of simulation studies indicate that the proposed method provides more accurate estimates of states and parameters, than previous approaches without significant increase in computation effort. The method can be deployed online for real time state and parameter estimation in nonlinear processes.

Appendix A. KALMAN FILTER

Let the discrete linear stochastic state-space system be of the form,

$$\begin{aligned} x_{k+1} &= \bar{A}_k x_k + w_k \\ y_{k+1} &= \bar{C}_{k+1} x_{k+1} + v_{k+1} \end{aligned} \tag{A.1}$$

where w_k and v_{k+1} are independent normally distributed random variables with covariance Q_k and R_{k+1} respectively.

Assume unbiased estimates of the state at time instant 'k' ($\hat{x}_{k|k}$) and the measurement at time instant '$k+1$' (y_{k+1}) are available. The state estimate for time

Table 1. Catalyst deactivation

RMS Errors	V	P	T	C_A	T_c	Par Est
Data	0.4892	1.9373	0.6913	0.0050	0.6553	-
EKF	0.1629	2.0122	0.4419	0.0020	0.4128	0.0297
UKF	0.1740	1.6352	0.1981	0.0006	0.1659	0.0207
RNDDR	0.1528	1.9023	0.4056	0.0018	0.3768	0.0271
URNDDR	0.1452	1.8350	0.2277	0.0010	0.1830	0.0248

instant '$k+1$' ($\hat{x}_{k+1|k+1}$) can be expressed as a linear combination of the two,

$$\hat{x}_{k+1|k+1} = K'_{k+1}\hat{x}_{k|k} + K_{k+1}y_{k+1} \tag{A.2}$$

For $\hat{x}_{k+1|k+1}$ to be an unbiased estimate of x_{k+1}, we require $K'_{k+1} = (I - K_{k+1}\bar{C}_{k+1})\bar{A}_k$. Thus the recursive estimator can be rewritten in two parts, first for prediction and the second for correction.

$$\begin{aligned}\hat{x}_{k+1|k} &= \bar{A}_k\hat{x}_{k|k} \\ \hat{x}_{k+1|k+1} &= \hat{x}_{k+1|k} + K_{k+1}\left(y_{k+1} - \bar{C}_{k+1}\hat{x}_{k+1|k}\right)\end{aligned} \tag{A.3}$$

We also assume $P_{k|k}$, defined by the covariance matrix of errors in the state estimates $\hat{x}_{k|k}$, is known. Therefore, the uncertainty in $\hat{x}_{k+1|k}$ can be calculated as,

$$P_{k+1|k} = \bar{A}_k P_{k|k}\bar{A}_k^T + Q_k \tag{A.4}$$

The Kalman gain matrix is arrived at by solving the following unconstrained optimization problem

$$\begin{aligned}\min_{x_{k+1}} \; &(y_{k+1} - \bar{C}_{k+1}x_{k+1})^T(R_{k+1})^{-1}(y_{k+1} - \bar{C}_{k+1}x_{k+1}) \\ &+(x_{k+1} - \hat{x}_{k+1|k})^T(P_{k+1|k})^{-1}(x_{k+1} - \hat{x}_{k+1|k})\end{aligned} \tag{A.5}$$

giving the filtered state estimate as,

$$\hat{x}_{k+1|k+1} = \hat{x}_{k+1|k} + K_{k+1}(y_{k+1} - \bar{C}_{k+1}\hat{x}_{k+1|k}) \tag{A.6}$$

$$K_{k+1} = P_{k+1|k}\bar{C}_{k+1}^T(R_{k+1} + \bar{C}_{k+1}P_{k+1|k}\bar{C}_{k+1}^T)^{-1} \tag{A.7}$$

The covariance matrix of errors in the filtered state estimates is given by

$$P_{k+1|k+1} = (I - K_{k+1}\bar{C}_{k+1})P_{k+1|k} \tag{A.8}$$

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