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Recursive State Estimation in Nonlinear Processes

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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, a recursive nonlinear dynamic data reconciliation (RNDDR) formulation is presented. The RNDDR formulation extends the capability of the EKF by allowing for incorporation of algebraic constraints and bounds. The RNDDR is evaluated with four case studies that have been previously studied by Haseltine and Rawlings [1]. It has been shown that the EKF fails in constructing reliable state estimates in all the four cases due to the inability in handling algebraic constraints [1]. Reliable state estimates are achieved by the RNDDR formulation in all the cases in presence of large initialization errors.

I. INTRODUCTION

The quality of process data in a chemical plant significantly affects the performance and benefits gained from activities like performance monitoring, online optimization and control. Processes are inevitably subject to random fluctuations in disturbances and the process measurements always contain 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 [2]. 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. Again several different variants of this basic strategy have been developed, which are very well described by Muske and Edgar [3]. 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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An alternative class of methods for state and parameter estimation, especially for nonlinear dynamic systems, are moving horizon optimization based techniques [4]. Liebman et al. [4] proposed the nonlinear dynamic data reconciliation (NDDR) formulation, in which the moving horizon optimization approach is extended to handle errors in measured inputs and to take into account algebraic constraints and bounds on variables. The main drawback of moving horizon based approaches is that, unlike the EKF, they can be computationally demanding due to their non-recursive form, thus raising real-time implementation concerns.

In this paper, a recursive nonlinear dynamic data reconciliation (RNDDR) solution technique is proposed that effectively combines the computational advantages of EKF, and the ability of NDDR approach to handle algebraic inequality or equality constraints. Four case studies are presented to show the efficacy of the proposed RNDDR formulation.

II. RECURSIVE NONLINEAR DYNAMIC DATA RECONCILIATION (RNDDR)

In KF and EKF, the estimation procedure at each sampling instant can be regarded as being composed of two steps (as described in Appendix A). In the first step, the state estimates from the previous time instant are propagated using the process dynamic equation (along with its error covariance matrix), while in the second step the predicted state estimates are corrected using the measurements made at the current time instant. It is shown in Appendix A that the optimal updated state estimates for KF (as also in EKF) are obtained by solving an unconstrained optimization problem for which the objective function is given in 7. 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. 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 proposed RNDDR method described below.

Consider the system given by 1 with bounds and algebraic constraints imposed on the states.

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

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Let $\hat{x}_{k|k}$ and $P_{k|k}$ be given at time instant 'k'. The predicted state estimates $\hat{x}_{k+1|k}$ is determined by integration and the variance of uncertainty in the predicted estimates is calculated by covariance propagation. For covariance propagation, the nonlinear state space model is linearized around $[\hat{x}_{k|k}]$ to give $[A_k]$, and the state transition matrix is approximated assuming the equivalent LTI system, $\bar{A}_k = exp(A_k \Delta t)$. Using this linearized approximation, the covariance matrix of estimation errors is propagated as

$$P_{k+1|k} = \left[\ \bar{A}_k\ \right] P_{k|k} \left[\ \bar{A}_k\ \right]^T + [Q_k] \qquad (2)$$

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

$$\min_{x_{k+1}} (x_{k+1} - \hat{x}_{k+1|k})^T (P_{k+1|k})^{-1} (x_{k+1} - \hat{x}_{k+1|k}) + (y_{k+1} - g(x_{k+1}))^T (R_{k+1})^{-1} (y_{k+1} - g(x_{k+1}))$$

subject to the following constraints,

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

The optimal solution to this problem (x^*_{k+1}) gives the updated state estimates $\hat{x}_{k+1|k+1}$. 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 8. The covariance matrix of the error in the updated state estimates is computed using 9 and 10. While using these equations, the effect of the constraints on the covariance matrix of estimation errors is neglected. In any case, for nonlinear systems, the covariance matrix of estimation errors represents only an approximation. Therefore, there is insufficient justification for trying to account for the effect that constraints have on the covariance propagation.

III. Results

The RNDDR has been implemented and tested with various case studies. In this paper we present results for four case studies for which the EKF fails as reported by Haseltine and Rawlings [1]. The RNDDR for the first three case studies has been implemented with the tuning parameters as proposed in Haseltine and Rawlings [1] with a lower bound of zero for the filtered state estimates.

A. Case study 1

The first example is of a gas phase reversible reaction in a well-mixed, isothermal batch reactor,

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

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

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

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

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

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

The RNDDR state estimates are presented in Fig. 1. As it can be seen, the RNDDR converges to the actual trajectory within 20 sample instants even with poor initial guess.

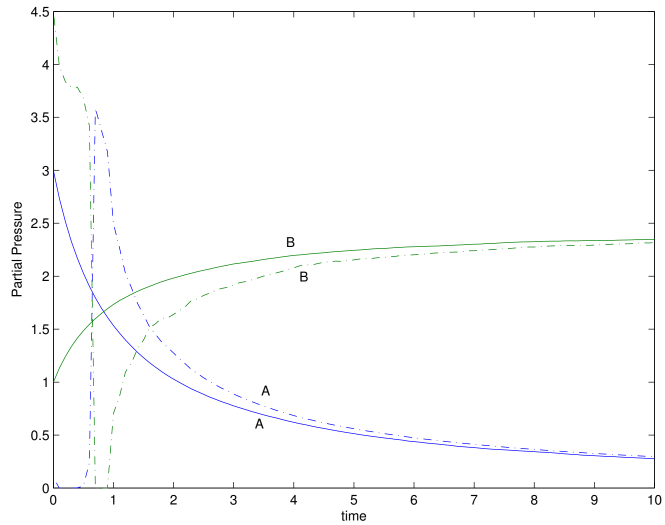

Fig. 1. RNDDR Case 1 State Estimates. Line: Actual, Dash-Dot: Estimated

B. Case study 2

The second case study involves two gas phase reversible reactions in a well-mixed isothermal batch reactor,

$$A \underset{k_2}{\overset{k_1}{\rightleftharpoons}} B + C$$

$$2B \underset{k_4}{\overset{k_3}{\rightleftharpoons}} C$$

$$k = [0.5\ 0.05\ 0.2\ 0.01]^T \ \text{ and } \ r = \begin{bmatrix} k_1 C_a - k_2 C_b C_c \\ k_3 C_b^2 - k_4 C_c \end{bmatrix}$$

with

$$x = [C_a \quad C_b \quad C_c]^T, \quad y_k = [RT \quad RT \quad RT]\, x_k$$

The initial state is $x_0 = [0.5 \quad 0.05 \quad 0]^T$. For state estimation problem, the following parameters have been used:

$$\Delta t = 0.25, \ P_0 = \begin{bmatrix} 0.25 & 0 & 0 \\ 0 & 0.25 & 0 \\ 0 & 0 & 0.25 \end{bmatrix}, \ R = 0.25^2$$

$$Q = \begin{bmatrix} 10^{-6} & 0 & 0 \\ 0 & 10^{-6} & 0 \\ 0 & 0 & 10^{-6} \end{bmatrix} \hat{x}_0 = [0 \quad 0 \quad 4]^T$$

The constraints imposed are, $x_L = [0 \quad 0 \quad 0]^T$ and $x_U = [10 \quad 10 \quad 10]^T$. The RNDDR rapidly converges, as can be seen from Fig. 2, to the correct concentration given such large initial guess error and the high certainty (low P_0) associated with the guess.

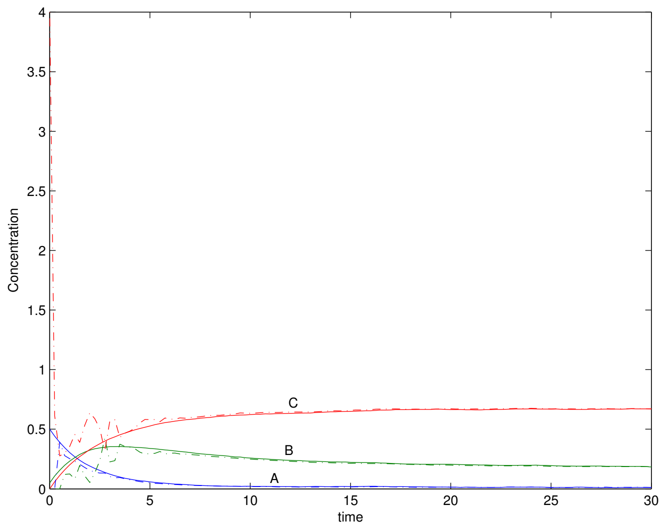

Fig. 2. RNDDR Case 2 State Estimates. Line: Actual, Dash-Dot: Estimated

C. Case study 3

This case study is of a isothermal CSTR involving the reaction system presented in Case Study 2 (Section III-B).

$$\begin{aligned}\dot{x} &= \frac{Q_f}{V_R}C_f - \frac{Q_o}{V_R}x + \nu^T r \quad \text{where} \\ C_f &= [0.5 \;\; 0.05 \;\; 0]^T, \quad Q_f = Q_o = 1 \\ x &= [C_a \;\; C_b \;\; C_c]^T \\ \nu &= \begin{bmatrix} -1 & 1 & 1 \\ 0 & -2 & 1 \end{bmatrix} \quad \text{and } x_0 = [0.5 \;\; 0.05 \;\; 0]^T\end{aligned}$$

For state estimation, the following parameters are used:

$$\Delta t = 0.25, \;\; P_0 = \begin{bmatrix} 16 & 0 & 0 \\ 0 & 16 & 0 \\ 0 & 0 & 16 \end{bmatrix}, \;\; R = 0.25^2$$

$$Q = \begin{bmatrix} 10^{-6} & 0 & 0 \\ 0 & 10^{-6} & 0 \\ 0 & 0 & 10^{-6} \end{bmatrix} \hat{x}_0 = [0 \;\; 0 \;\; 3.5]^T$$

The constraints imposed are the same as previously, $x_L = [0 \;\; 0 \;\; 0]^T$ and $x_U = [10 \;\; 10 \;\; 10]^T$. The RNDDR results for this case are presented in Fig. 3.

D. Case study 4

In the fourth case study presented by Haseltine and Rawlings [1], the batch process presented in Case study 2 is modified with new set of parameters,

$$k = [0.5 \;\; 0.4 \;\; 0.2 \;\; 0.1]^T, \quad \text{and} \quad R = 0.01$$

A fictitious measurement equation of the form,

$$y_k = [-1 \;\; 1 \;\; 1]x_k$$

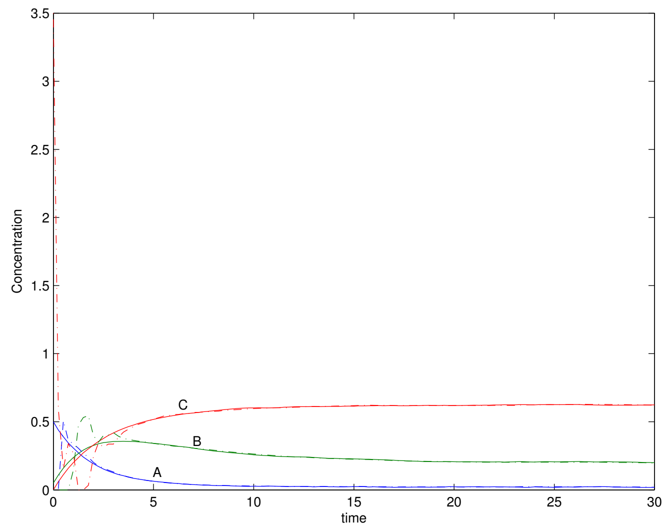

Fig. 3. RNDDR Case 3 State Estimates. Line: Actual, Dash-Dot: Estimated

is implemented. The reason for using such a measurement function is that there are multiple physically realizable steady states towards which the estimator can converge. A large initialization error in such a case would lead to an incorrectly converged solution by a recursive estimator. Therefore, an appropriate choice of a lower and upper bound on the states is necessary if the estimator has to converge to the actual scenario. This choice can be based on insight from process operation.

Another important issue in the case of unreliable initial guess is the choice of P_0. P_0 cannot be arbitrarily initialized in such cases. The choice of P_0 should be consistent with the initial guess provided. A low value of P_0 should be used only if the user is confident that the initial estimates are close to the true values. Otherwise, it is necessary to choose the elements of P_0 sufficiently high to reflect the lack of confidence in the initial estimates.

Haseltine and Rawlings [1] have used the following P_0 and $\hat{x}_0$ to show that the EKF fails to converge to the actual solution.

$$P_0 = \begin{bmatrix} 0.25 & 0 & 0 \\ 0 & 0.25 & 0 \\ 0 & 0 & 0.25 \end{bmatrix} \quad \text{with} \;\; \hat{x}_0 = [3 \;\; 0.1 \;\; 3]$$

This essentially means that the estimator is forced to give high weight to an unreliable initial guess. In such a scenario the RNDDR will not converge. If P_0 is chosen to reflect the confidence that the user has on the initial guesses, then RNDDR converges as shown below.

In the modified case study, the state estimator is initialized with $\hat{x}_0 = [4 \;\; 0 \;\; 4]^T$. Notice that we have used a $\hat{x}_0$ [1] which is more erroneous than the previous value discussed above, but we will demonstrate that with consistent initialization of P_0, the RNDDR converges. Obviously the RNDDR converges for $\hat{x}_0 = [3 \;\; 0.1 \;\; 3]^T$ also. The variance of uncertainty in the initial guess is initialized as,

$$P_0 = \begin{bmatrix} 4 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 4 \end{bmatrix}$$

while the upper and lower bounds are same as used previously in case study 2 (Section III-B). It should be noted that the choice of P_0 is different from the one used in the previous case. This choice of P_0 takes the extent of uncertainty in initial guess into account. This is necessary because without this information the estimator might incorrectly converge to another steady state solution. The RNDDR estimate for this case is presented in Fig. 4. It can be seen that with the correct initialization of the uncertainty in initial guess (P_0) which reflects the extent of error in the initial guess ($x_0 - \hat{x}_0$), the RNDDR converges to the actual trajectory.

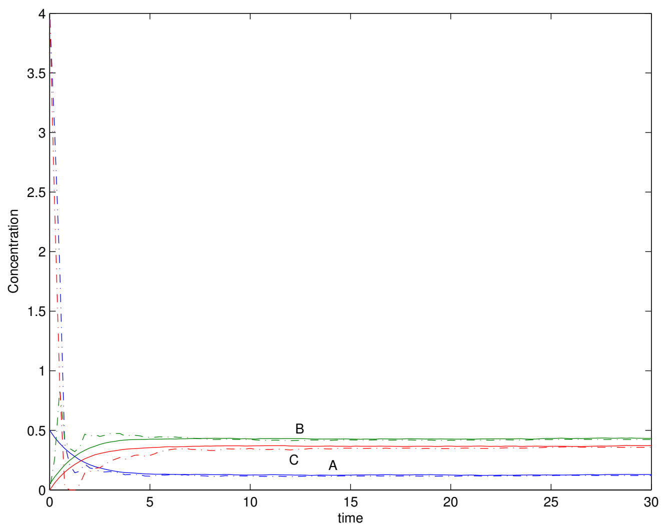

Fig. 4. RNDDR Case 4 State Estimates with modified P_0. Line: Actual, Dash-Dot: Estimated

However, if the same

$$P_0 = \begin{bmatrix} 0.25 & 0 & 0 \\ 0 & 0.25 & 0 \\ 0 & 0 & 0.25 \end{bmatrix}$$

has to be used, then a better initial guess of $\hat{x}_0 = [1.5 \quad 0.1 \quad 1.5]^T$ will make the RNDDR converge. Fig. 5 points out the convergence of RNDDR. **Note**: As it can be seen in this case, neither the upper bound nor the lower bound was activated for any of the filtering sub-problems, showing the convergence of the EKF.

E. EKF Result

The importance of giving meaningful initial guess uncertainty (P_0) measure can be duly noted with a sample EKF result based on case study 2 (Section III-B). The initial guess is changed to a non-zero $\hat{x}_0 = [0.1 \quad 0.1 \quad 4]^T$ and the

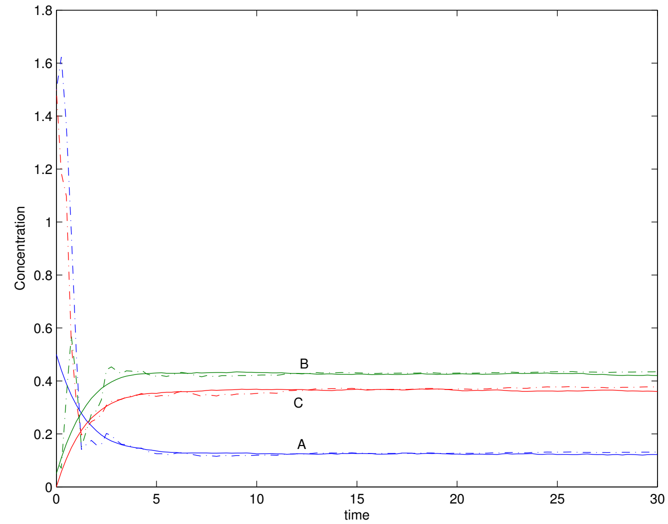

Fig. 5. RNDDR Case 4 State Estimates with modified x_0. Line: Actual, Dash-Dot: Estimated

uncertainty variance is initialized with

$$P_0 = \begin{bmatrix} 0.25 & 0 & 0 \\ 0 & 0.25 & 0 \\ 0 & 0 & 10 \end{bmatrix}$$

which is consistent with the information available about the state of the process. The EKF result, shown in Fig. 6, points out that with a systematically initialized initial state ($\hat{x}_0$) and uncertainty (P_0), the EKF can also converge without invoking the constraints.

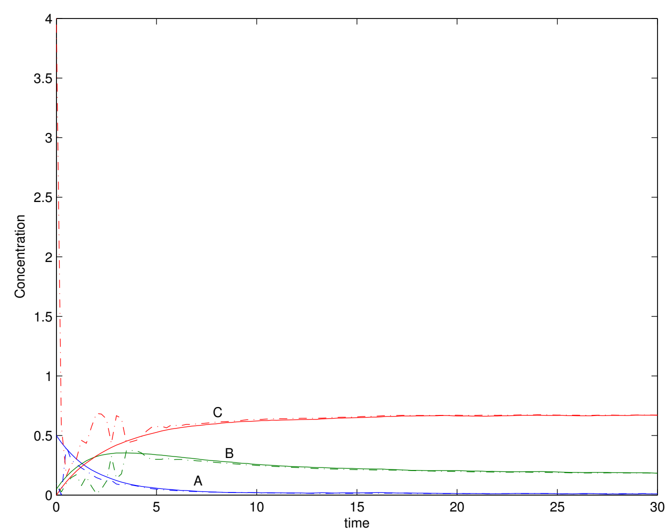

Fig. 6. EKF Case 2 State Estimates with modified $\hat{x}_0$ and P_0. Line: Actual, Dash-Dot: Estimated

IV. CONCLUSION

A Recursive Nonlinear Dynamic Data Reconciliation (RNDDR) formulation has been presented in the paper. The motivation of the RNDDR based on the recursive predictor-corrector form of the Extended Kalman Filter (EKF) has been discussed. The most important feature of the RNDDR formulation lies in the recursive nature of the estimator which also incorporates the algebraic constraints involved in the estimation problem. The RNDDR also is order of magnitude faster than traditional window based estimation approaches. The RNDDR took approximately 0.1 second to solve the estimation problem at each sample instant for the presented case studies. Therefore, the proposed formulation can be implemented on large nonlinear systems for real time dynamic data reconciliation.

Extensive simulations have been carried out with the RNDDR formulation with various cases where EKF has been known to fail in the past because of EKF's inability in handling algebraic constraints. Reliable estimates are achieved by the RNDDR formulation at only a marginal increase in the computational cost.

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APPENDIX A - KALMAN FILTER

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

$$\begin{aligned} x_{k+1} &= \bar{A}_k x_k + w_k \\ y_{k+1} &= \bar{C}_{k+1} x_{k+1} + v_{k+1} \end{aligned} \quad (3)$$

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

$$\hat{x}_{k+1|k+1} = K'_{k+1}\hat{x}_{k|k} + K_{k+1} y_{k+1} \quad (4)$$

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.

$$\begin{aligned} \hat{x}_{k+1|k} &= \bar{A}_k \hat{x}_{k|k} \\ \hat{x}_{k+1|k+1} &= \hat{x}_{k+1|k} + K_{k+1}\left(y_{k+1} - \bar{C}_{k+1}\hat{x}_{k+1|k}\right) \end{aligned} \quad (5)$$

We also assume $P_{k|k}$, the uncertainty in the state estimate $\hat{x}_{k|k}$, is known. Therefore, the uncertainty in $\hat{x}_{k+1|k}$ can be calculated as,

$$P_{k+1|k} = \bar{A}_k P_{k|k} \bar{A}_k^T + Q_k \quad (6)$$

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

$$\begin{aligned} &\min_{x_{k+1}} \\ &\quad (x_{k+1} - \hat{x}_{k+1|k})^T (P_{k+1|k})^{-1} (x_{k+1} - \hat{x}_{k+1|k}) \\ &+ (y_{k+1} - \bar{C}_{k+1} x_{k+1})^T (R_{k+1})^{-1} (y_{k+1} - \bar{C}_{k+1} x_{k+1}) \end{aligned} \quad (7)$$

giving the filtered state estimate as,

$$\hat{x}_{k+1|k+1} = \hat{x}_{k+1|k} + K_{k+1}(y_{k+1} - \bar{C}_{k+1}\hat{x}_{k+1|k}) \quad (8)$$

where the Kalman gain matrix K_{k+1} is defined as

$$K_{k+1} = (P_{k+1|k})\bar{C}_{k+1}^T (R_{k+1} + \bar{C}_{k+1} P_{k+1|k} \bar{C}_{k+1}^T)^{-1} \quad (9)$$

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

$$P_{k+1|k+1} = (I - K_{k+1}\bar{C}_{k+1}) P_{k+1|k} \quad (10)$$