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The Reduced Rank of Ensemble Kalman Filter to Estimate the Temperature of Non Isothermal Continue Stirred Tank Reactor

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Abstract: Kalman filter is an algorithm to estimate the state variable of dynamical stochastic system. The square root ensemble Kalman filter is an modification of Kalman filter. The square root ensemble Kalman filter is proposed to keep the computational stability and reduce the computational time. In this paper we study the efficiency of the reduced rank ensemble Kalman filter. We apply this algorithm to the non isothermal continue stirred tank reactor problem. We decompose the covariance of the ensemble estimation by using the singular value decomposition (the SVD), and then we reduced the rank of the diagonal matrix of those singular values. We make a simulation by using Matlab program. We took some the number of ensemble such as 100, 200 and 500. We compared the computational time and the accuracy between the square root ensemble Kalman filter and the ensemble Kalman filter. The reduced rank ensemble Kalman filter can't be applied in this problem because the dimension of state variable is too less.

Keywords: Ensemble Kalman filter, reduced rank, stirred tank reactor.

Introduction

Kalman filter is an algorithm to estimate the state variable of the stochastic dynamical linear system. This algorithm combines the mathematical model with the measurement data (Lewis, [6]). Kalman filter has been applied in various problems such as the estimation of the water level in the river, wave of ocean and the tide. There are many modification of Kalman filter algorithm, such as the ensemble Kalman Filter (Burger *et al.* [3]), the reduced rank square root covariance filter (Verlaan [8]), the square root ensemble Kalman filter (Evensen, [4]) and the variance reduced ensemble Kalman filter (Heemink, [5]). These modifications have been done to avoid the convergence of algorithm, to reduce the computation time, to decrease the error of estimation and other. In the Ensemble Kalman filter, it is generated an ensemble value as initial estimation of state variable and an ensemble measurement data based on real measurement data (Burger *et al.*, [3]. So in the ensemble Kalman filter, we need more computational time than the Kalman filter. The square root ensemble Kalman filter is proposed to keep the computational stability and the variance reduced ensemble Kalman filter is proposed to keep the computational stability and reduce the computational time of square root ensemble Kalman filter (Heemink, [5]).

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In this paper we study the efficiency of the reduced rank ensemble Kalman filter. We apply this algorithm in non linear dynamic stochastic system such as the non isothermal continue stirred tank reactor.

Methods

The mathematical model of non isothermal continue stirred tank reactor is (Qu, [7])

$$\frac{dC_A}{dt} = \frac{F}{A}(C_{Ain} - C_A) - 2k_0 e^{-\frac{E}{RT}} C_A^2 \quad (1a)$$
$$\frac{dT}{dt} = \frac{F}{V}(T_{in} - T) - 2\frac{\Delta H}{\rho C_p} R k_0 e^{-\frac{E}{RT}} C_A^2 - \frac{UA}{V_p C_p}(T - T_j) \quad (1b)$$
$$\frac{dT_j}{dt} = \frac{F_W}{V_W}(T_{jin} - T_j) + \frac{UA}{V_w \rho_w C_{pw}}(T - T_j) \quad (1c)$$

where, $k(T) = k_0 e^{-E/RT}$, C_A is concentration of reactance, T temperature of tank reactor, T_j temperature of cooling jacket reactor, F is inlet feed flow, C_{Ain} is input concentration, V is volume of reactor, T_{in} is inlet feed temperature, F_w is inlet feed flow in cooling jacket, V_w is volume of cooling jacket, T_{jin} is cooling inlet temperature, c_p is heat capacity of reactance, c_{pw} is heat capacity of cooling jacket, ρ is reactance density and ρ_w is cooling density.

In this paper we estimate the concentration of reactance, C_A, temperature of tank reactor, T and the temperature of cooling jacket of reactor, T_j if we can measure the concentration of reactance, C_A, and temperature of tank reactor, T or we just can measure temperature of tank reactor, T. Because the non isothermal continues stirred tank reactor is a non linear dynamic system, then we estimate those three parameters by using the square root Ensemble Kalman filter.

The ensemble Kalman filter and the square root ensemble Kalman filter are modified of Kalman filter. Kalman filter is an algorithm to estimate the state variable of the stochastic dynamical linear system. This algorithm combines the mathematical model with the measurement data (Lewis, [6]). Kalman filter has been applied in various problems such as the estimation of the water level in the river, wave of ocean and the tide. There are many modification of Kalman filter algorithm, such as the ensemble Kalman Filter (Evensen, [4]), the reduced rank square root covariance filter (Verlaan, [8]), the square root ensemble Kalman filter (Evensen, [4]) and the variance reduced ensemble Kalman filter (Heemink, [5]). These modifications have been done to avoid the convergence of algorithm, to reduce the computation time, to decrease the error of estimation and other. In the Ensemble Kalman filter, it is generated an ensemble value as initial estimation of state variable and an ensemble measurement data based on real measurement data (Evensen [4]). So in the ensemble Kalman filter, we need more computational time than the Kalman filter. The square root ensemble Kalman filter is proposed to keep the computational stability and the variance reduced ensemble Kalman filter is proposed to keep the computational stability and reduce the computational time of square root ensemble Kalman filter (Heemink, [5]).

At the previous research, we had applied the ensemble Kalman filter in the non isothermal continue stirred tank (Baehaqi, [2]). We compared the accuracy and efficiency between the Ensemble Kalman Filter with the Unscented Kalman filter. The ensemble Kalman filter need less computational time than the unscented Kalman filter, but the unscented Kalman filter more accuracy than the ensemble Kalman filter. We also applied the reduced rank ensemble Kalman filter in the diffusion problem (Albab, [1]). In that research, we reduced 30 rank of covariance from 100. We compare the computational time and efficiency between the ensemble Kalman filter, the square root ensemble Kalman filter and the reduced rank ensemble Kalman filter. From the simulation we obtained that the square root ensemble Kalman filter need more computational time than others, the reduced rank ensemble Kalman filter has more accurate than others but need more computational time than the ensemble Kalman filter. So in this paper, we combined those research, we estimate the variable state of non isothermal continue stirred tank by using the reduced rank ensemble Kalman filter.

The square root ensemble Kalman filter is a modification of ensemble Kalman filter algorithm. In this algorithm we write the covariance error of ensemble Kalman filter as square root matrix. The square root ensemble Kalman filter is usually more stable than the ensemble Kalman filter.

Suppose, it is given stochastic dynamic system and measurement equation

$$x_{k+1} = f(x_k, u_k) + w_k, w_k \sim N(0, Q_k) \quad (2)$$
$$z_k = Hx_k + v_k, v_k \sim N(0, R_k) \quad (3)$$

Let, we want estimate the state variable x_{k+1} based on the measurement data z_k by using the square root ensemble Kalman filter, then we use the algorithm of square root ensemble Kalman filter as follows:

Initial Estimation

Based on initial estimation x_0, where x_0 has normal Gaussian distribution with mean $\bar{x}_0$ and covariance P_0, we generated the n_e ensemble of initial estimation $\hat{x}_{0,i}$ with mean $\bar{x}_0$ and covariance P_0 ($\hat{x}_{0,i} \sim N(\bar{x}_0, P_0)$)

Prediction Step

We predict the state $\hat{x}_{k,i}^-$ based on the previous state $\hat{x}_{k-1,i}^-$ and mathematical model of system (non isothermal continuous stirred tank reactor). Substitute the n_e ensemble of estimation $\hat{x}_{k-1,i}^-$ into eq. (2)

$$\hat{x}_{k,i}^- = f\left(\hat{x}_{k-1,i}^-, u_{k-1}\right) + w_{k,i}; i = 1,2, \dots, n_e \quad (4)$$

Mean of ensemble estimation: $\bar{x}_k^- = mean(\hat{x}_{k,i}^-)$
Error of ensemble $\tilde{x}_{k,i}^- = \hat{x}_{k,i}^- - \bar{x}_k^-, i = 1,2, \dots, n_e$

Correction Step

We use measurement data z_k to make correction on the prediction state $\hat{x}_{k,i}^-$.
Generated the n_e ensemble measurement data from eq. (3): $z_{k,i} = z_k + v_{k,i}; i = 1,2, \dots, n_e$
Define $S_k = H\tilde{x}_{k,i}^-$; $E_k = v_{k,i}$; and $C_k = S_k S_k^T + E_k E_k^T$
Matrix S_k is a square root of covariance matrix P_k.
$P_k = S_k S_k^T$.

The ensemble correction estimation

$$\bar{x}_{k,i} = \hat{x}_{k,i}^- + \tilde{x}_{k,i}^- S^T C_k^- (z_{k,i} - H\hat{x}_{k,i}^-)$$

We decomposed the matrix C_k by using the singular value decomposition: $[U, D, V] = \mathrm{svd}(C_k)$
Define matrix $M_k = DU^T S_k$, then decompose matrix M_k, $[U_1, D_1, V_1] = \mathrm{svd}(M_k)$. The errors of ensemble estimations are $\tilde{x}_{k,i} = \tilde{x}_{k,i}^- V_1 (I - D_1^T D_1)^{1/2}$

The ensembles of estimations are

$$\hat{x}_{k,i} = \tilde{x}_{k,i} + \bar{x}_{k,i} \qquad (5)$$

Estimation state variable is mean of the ensemble estimation

$$\hat{x}_k = \frac{1}{n_e - 1}\sum_{i=1}^{n_e} \hat{x}_{k,i} \qquad (6)$$

Finally, we substitute Eq. (5) into Eq. (4) in the prediction step and continue with the correction step such that we get the state estimation $\hat{x}_k$, in time step k.

Result and Discussion

Here, we make a simulation using Matlab program. We took some the number of ensemble such as 100, 200 and 500. We compare the computational time and the accuracy between the reduced rank ensemble Kalman filter, the square root ensemble Kalman filter and the ensemble Kalman filter.

Before we applied the reduced rank ensemble Kalman filter, we rewrite Eq. (1) as a discrete time non linear dynamic stochastic system

$$\begin{bmatrix} C_A \\ T \\ T_j \end{bmatrix}_{k+1} = w_k + \begin{bmatrix} \frac{F\Delta t}{A} C_{Ain} + \left[1 - \frac{F\Delta t}{A}\right] C_A - 2\Delta t k_0 e^{-\frac{E}{RT}} C_A^2 \\ \frac{F\Delta t}{V} T_{in} + \left[1 - \frac{F\Delta t}{V} - \frac{UA\Delta t}{V_p C_p}\right] T - 2\frac{\Delta t \Delta H}{\rho C_p} R k_0 e^{-\frac{E}{RT}} C_A^2 - \frac{\Delta t UA}{V_p C_p} T_j \\ \frac{F_w \Delta t}{V_w} T_{jin} + \left[1 - \frac{F_w \Delta t}{V_w} - \frac{UA\Delta t}{V_w \rho_w C_{pw}}\right] T_j + \frac{\Delta t UA}{V_w \rho_w C_{pw}} T \end{bmatrix}$$

Define $x_k = \left[C_A\ T\ T_j\right]^T$ and the eq. (5) has a same form as eq. (2). To make a correlation between the measurement data and the state variable which we will estimate, we define the measurement equation as stated in Eq. (3), where $x_k = \left[C_A\ T\ T_j\right]^T$, the state variable, $w_k \sim N(0, Q_k)$ is a system noise. Matrix H represented the number of variable which can be measured. Suppose we can measure the concentration of reactance, then we take $H = [1\ \ 0\ \ 0]$. If we can measure the temperature of tank T, we take $H = [0\ \ 1\ \ 0]$. If we can measure the concentration C_A and the temperature of tank, T, then we take $H = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \end{bmatrix}$, and so on.

Because the model, Eq.(5) is a non linear system, we estimate state variable $x_k = \left[C_A\ T\ T_j\right]^T$ by using the ensemble Kalman filter, the square root ensemble Kalman filter and the reduced rank ensemble Kalman filter.

In the reduced rank ensemble Kalman filter, the rank reducing is applied in the square root inverse diagonal matrix D in Eq. (4) has same dimension with the dimension of state variable $x_k = \left[C_A\ T\ T_j\right]^T$, that is three. Therefore, we can't apply the reduced rank ensemble Kalman filter in this non isothermal stirred tank problem.

Here we take the ensemble estimation are 100, 200 and 500. Figure 1a, 1b. Figure 2a, 2b. represented the estimation result by taking ensemble 100, matrix measurement $H = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \end{bmatrix}$, that means, based on the data of C_A concentration, and the tank temperature T , we estimate the concentration, the temperature of tank and the temperature of cooling jacket. Figure 1a, 1b. represent the Ensemble Kalman Filter (EnKF) and Figure 2a, 2b. represent the Square root Ensemble Kalman Filter (SQRT EnKF). The absolute error of C_A is 0.0969, T is 0.0002 and T_j is 0.002 for the square root ensemble Kalman filter, otherwise C_A is 0.0414, T is 0.0001 and T_j is 0.0008 for the ensemble Kalman filter. The computational time is 0.5781 sec and 0.56 sec for the square root ensemble Kalman filter and the ensemble Kalman filter respectively (Table 1). The others result of simulation is represented in Table 2.

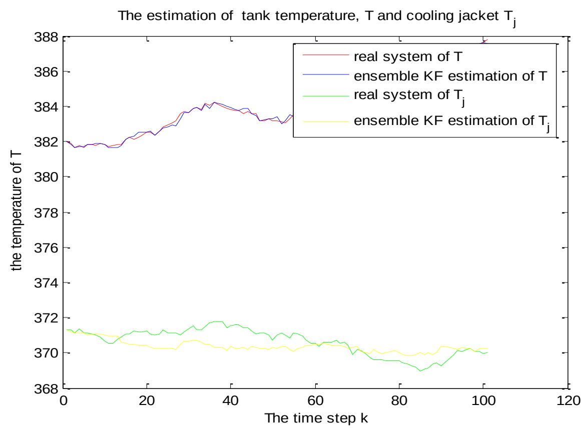

Figure 1a. The EnKF estimation of temperature for Ne=100, H=[1 0 0;0 1 0]

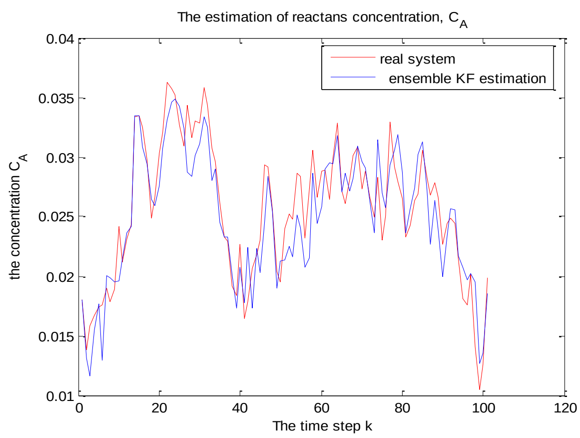

Figure 1b. The EnKF estimation of concentration for Ne=100, H=[1 0 0;0 1 0]

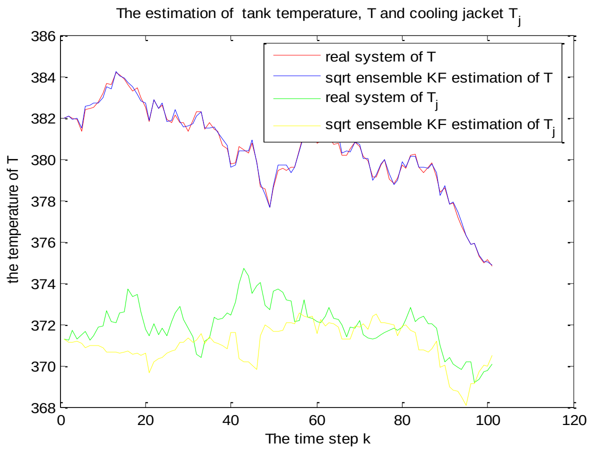

Figure 2a. The SQRT EnKF estimation of temperature for Ne=100, H=[1 0 0;0 1 0].

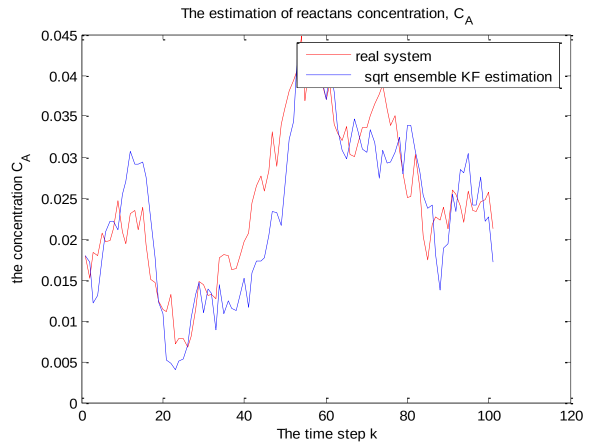

Figure 2b. The SQRT EnKF estimation of concentration for Ne=100, H=[1 0 0;0 1 0]

Table 1 shows the SQRT EnKF need more computational time than the EnKF and the SQRT EnKF is not more accurate than the EnKF. From our simulation, we found that the data of temperature cooling jacket T_j can't use to estimate the concentration and the temperature. In general cases, the number of ensemble influence the accuracy of estimation result, that means more the number of ensemble give more accurate the estimation, but in this problem the number of ensemble is not influence the accuracy of estimation. In SQRT EnKF, for $H=\begin{bmatrix}1&0&0\\0&1&0\end{bmatrix}$, the variable T has same error

Table 1. The absolute error and the computational time

H	# Ensem-ble	Time k	Varia-ble	Error SQRT-EnKF	Error EnKF	Compu-tation Time SRQRT -EnKF	Compu-tation Time EnKF
[1 0 0; 0 1 0]	500	100	C_A	0.1194	0.0325	10.9375	1.2109
			T	0.0002	0.0002		
			T_j	0.0046	0.0007		
	200	100	C_A	0.2040	0.0662	2.0078	0.8203
			T	0.0002	0.0001		
			T_j	0.0030	0.0023		
	100	100	C_A	0.0969	0.0414	0.5781	0.5600
			T	0.0002	0.0001		
			T_j	0.0020	0.0008		
[1 0 0]	200	100	C_A	0.1644	0.0556	1.9375	0.7969
			T	0.0046	0.0006		
			T_j	0.0020	0.0011		
	100	100	C_A	0.0860	0.0044	0.7109	0.3281
			T	0.0058	0.0008		
			T_j	0.0027	0.0021		
[0 1 0]	200	100	C_A	0.4577	0.3005	1.9297	0.5547
			T	0.0002	0.0002		
			T_j	0.0042	0.0019		
	100	100	C_A	0.6932	0.26	0.7109	0.3359
			T	0.0002	0.0001		
			T_j	0.0025	0.001		

for number ensemble 100, 200 and 500, the variable C_A, T_j have the smallest error in number ensemble 100, and give the difference result for $H=[1\ 0\ 0]$ and $H=[0\ 1\ 0]$. In EnKF, the smallest error is happen in various variables with various number of ensembles. Of course, more the number of ensembles need more computational time.

From Table 2. We know that the variable C_A has the largest error than others The measurement matrix

H is not influence the accuracy of the estimation such as variable C_A has good estimation for $H=[1\ 0\ 0]$, variable T has good estimation for $H=\begin{bmatrix}1&0&0\\0&1&0\end{bmatrix}$, and the variable T_j has good estimation for $H=[1\ 0\ 0]$ and $H=\begin{bmatrix}1&0&0\\0&1&0\end{bmatrix}$. So, the certain measurement matrix gives different accuracy for different variables.

Finally, the EnKF and the SQRT EnKF can be applied to estimate the non isothermal stirred tank

Table 2. The error estimation with different measurement matrix H

#Ensemble	Variable	ERROR SQRT EnKF			Error EnKF		
		H=[1 0 0; 0 1 0]	H=[1 0 0]	H=[0 1 0]	H=[1 0 0; 0 1 0]	H=[1 0 0]	H=[0 1 0]
200	C_A	0.2040	0.1644	0.4577	0.0662	0.0556	0.3005
	T	0.0002	0.0046	0.0002	0.0001	0.0006	0.0002
	T_j	0.0030	0.0020	0.0042	0.0023	0.0011	0.0019
100	C_A	0.0969	0.0860	0.6932	0.0414	0.0044	0.2600
	T	0.0002	0.0058	0.0002	0.0001	0.0008	0.0001
	T_j	0.0020	0.0027	0.0025	0.0008	0.0021	0.0010

problem with small absolute error. For further research, we can extend the application of this algorithm to more complicated problem, such as the stirred tank problem with more dimensions or other non linear stochastic dynamical system to know the influence the number of ensemble and the measurement matrix respect to the accuracy of estimation result.

Conclusion

From the simulation result and the analysis we conclude that: The reduced rank ensemble Kalman filter can't be applied in the non isothermal stirred tank problem, because the dimension of state variable is too less. The ensemble Kalman filter needs less computational time than the square root ensemble Kalman filter. The square root ensemble Kalman filter is not more accurate than the ensemble Kalman filter. The number of ensemble in this case is not influence the accuracy of estimation result. The type of measurement matrix or the type of variable that can be measured is not influence the accuracy of the estimation result

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