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A Comparison of Moving Horizon and Bayesian State Estimators with an Application to a pH Process

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Abstract: The moving horizon estimator (MHE) formulation utilizes a window of measurements to compute the estimates of the states in that particular window. This approach leads to smoothing of the state estimates included in the window, since future information is used to compute the same. However, the effect of smoothing, in the MHE algorithm, on the state estimates has not been studied in the literature. In this work the performance of the MHE is compared with recursive Bayesian state estimators (such as UKF, EnKF) to study the effect of the moving window of the past data on the quality of state estimates, via an application on a benchmark pH simulation case study. The simulations are carried out for two scenarios– the ideal case and the case with a parametric model-plant mismatch. The results obtained indicate that the use of MHE results in improved state estimates when compared to the recursive Bayesian state estimators, but does not help compensate for model-plant-mismatch.

1. INTRODUCTION

Bayesian state estimation, using nonlinear dynamic mechanistic models, is an important tool in various applications of systems engineering to obtain the estimates of the unmeasured or infrequently measured process states and parameters. The Bayesian approach attempts to reconstruct the posterior distribution of the states, using Bayes' rule, based on the entire data available in the past. It is, however, well-known that the Bayesian expressions for the posterior probability density function (*pdf*) of the states are, in general, analytically intractable. Hence, various filtering techniques have been developed which yield an approximate and computationally tractable suboptimal solution to the Bayesian estimation problem.

Bayesian state estimation algorithms can be broadly divided into two categories– a) Those which obtain an approximation of the conditional *pdf* of the posterior of the states and b) those which assume a suitable form for the *pdf* of the prior and convert the state estimation problem directly into an optimisation problem (Patwardhan et al., 2012). The approximation of the conditional *pdf* of the states can be obtained through various methods, such as Taylor series approximation (Sorenson, 1985), statistical linearisation (Gelb, 1974) or through Monte Carlo methods (Gordon et al., 1993; Evensen, 2007). On the other hand, optimisation based formulations have been specifically developed for estimation of states in the presence of constraints or bounds (Patwardhan et al., 2012). The moving horizon estimator (MHE) (Rao et al., 2001) is an optimisation-based approach to compute the state estimates using a moving window of the past data. Other examples are the constrained EKF (Vachhani et al., 2005), constrained UKF (Vachhani et al., 2006) and the constrained EnKF (Prakash et al., 2010), in which the measurement update step is formulated as a constrained optimisation problem in order to obtain state estimates that are consistent with the constraints. The main difference is that the MHE computes the state estimates for a window of time, whereas the other constrained estimators compute the state estimates only at the current sampling instant. Thus, the moving window formulation enables the MHE to use future measurements to compute the state estimates at the beginning of the window.

1.1 Comparison of Bayesian state estimators and MHE

A brief description about the properties of recursive Bayesian state estimators and the MHE is given in this section. Particularly the contrasting features of both types of state estimators are described. The unscented Kalman filter (UKF) (Julier and Uhlmann, 2004) belongs to a class of filters based on statistical linearisation for approximating the nonlinear state and measurement equations. These filters are based on the observation that the moments of the distribution can be better approximated using samples, rather than Taylor series approximation of the nonlinear function (Patwardhan et al., 2012). The UKF uses deterministically drawn samples, known as 'sigma points', to approximate the distribution of the states as a Gaussian distribution. On the other hand, the ensemble Kalman filter (EnKF) (Evensen, 2007) is a Monte Carlo sampling based state estimator, which is based on the premise that the statistical properties of the states can be sufficiently described using their first two moments, the mean and covariance, which are obtained as sample statistics. The

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main difference between the UKF and EnKF is that while the UKF assumes that the *pdf* of the posterior of the states can be adequately approximated as a Gaussian distribution, the EnKF does not make any assumption about the nature of the *pdf* of the posterior of the states.

On the other hand, the MHE formulates a constrained optimisation problem over a fixed-size window of past sampling instants to compute the state estimates in that window. Hence, the MHE not only yields the state estimates for the current sampling instant, but also for the previous sampling instants upto the length of the moving window. One of the principle advantages of the MHE formulation is that it systematically incorporates algebraic constraints and bounds on the states. The constrained optimisation problem is formulated using the information of the states available at the beginning of the moving window, termed as the 'arrival cost'. The arrival cost can be interpreted as the conditional *pdf* of the states obtained using the data available upto the beginning of the moving window. However, the computation of the arrival cost is an open problem in the literature. For general nonlinear systems, an analytical approach to compute the arrival cost is not available. Therefore, one approach suggested is to ignore the effect of the arrival cost by assuming it to be a constant. This, however, leads to incorrect propagation of the *pdf* of the states and hence a large window is required to suppress the error introduced by this approach. The down side of this approach is that it significantly increases the computation complexity and costs involved in obtaining the state estimates. Therefore, various suboptimal approximations using Bayesian estimators, such as EKF (Rao and Rawlings, 2002), UKF (Qu and Hahn, 2009; Ungarala, 2009), C-EnKF (López-Negrete et al., 2011) and constrained particle filters (Lang et al., 2007; López-Negrete et al., 2011), have been proposed in the literature to approximate the arrival cost. Accurate computation of the arrival cost helps in significantly reducing the length of the moving window needed to generate reasonably accurate state estimates (López-Negrete et al., 2011).

In contrast to recursive Bayesian state estimators, the MHE uses a window of measurements to compute the state estimates. The MHE formulation, therefore, uses the measurements at the current sampling instant to compute the state estimates at the previous sampling instants. This results in smoothing of the states at the previous sampling instants (Rao et al., 2001), particularly of those at the beginning of the moving window. While the state estimates at the current instant are filtered estimates, they are computed using the smoothed state estimates obtained at the previous sampling instants. It has been shown that smoothing yields more accurate values of the posterior of the states because of using the future information of the process to compute the state distributions (Gelb, 1974). The disadvantage of most smoothing algorithms (Rauch et al., 1965; Sarkka, 2008) is that they cannot be used for online correction of the states based on future measurements. On the other hand, the advantage of the MHE formulation is that it can be deployed for online state estimation, as well as utilise the moving window for smoothing of the states.

The effectiveness of the MHE for state estimation of constrained and bounded systems has been widely documented in state estimation literature. However, the impact of smoothing, due to the use of a moving horizon of measurements, on the quality of state estimates has not been investigated in state estimation literature. Further, there is no work reported on the effect of the moving window of measurements on state estimates in the presence of model-plant mismatch. In this work, the performance of MHE is compared with recursive nonlinear Bayesian state estimators, specifically the UKF and EnKF. Of particular interest in this study, is the effect of smoothing as the window size changes and its impact on the quality of the state estimates in the following scenarios: a) no model-plant mismatch (MPM) and b) in presence of MPM. It is a widely reported fact in the literature that the performance of the MHE is dependent on how accurate is the computation of the arrival cost. Hence, to minimise the influence of arrival cost on the effect of smoothing, the arrival cost is approximated using either the UKF or EnKF. The performance of the state estimators is compared on the pH balancing CSTR system (Romanenko et al., 2004), which is well-known for exhibiting highly nonlinear state dynamics and a nonlinear measurement equation.

The rest of the paper is organised as follows. Section 2 describes the process model used for simulations and state estimation. The state estimation algorithms that are evaluated in this work are described in detail in Section 3. The simulation case study on which these approaches are evaluated and the results obtained are discussed in Section 4. Finally, the conclusions drawn from this study are detailed in Section 5.

2. PROCESS MODEL

The model for a continuous nonlinear process can be described by the following differential equations

$$\frac{d\mathbf{x}}{dt} = \mathbf{f}\left(\mathbf{x}, \mathbf{u}, \boldsymbol{\theta}, t\right) \tag{1}$$

$$\mathbf{y}\left(t\right) = \mathbf{h}\left(\mathbf{x}, t\right) \tag{2}$$

where, $\mathbf{x} \in \mathbb{R}^n$ represents the process states, $\mathbf{u} \in \mathbb{R}^m$ represents the manipulated inputs, $\boldsymbol{\theta} \in \mathbb{R}^p$ represents the process parameters and $\mathbf{y} \in \mathbb{R}^r$ represents the measurements. For the purpose of simulations and modelling for state estimation, a discrete-time approximation of the process is obtained as follows

$$\mathbf{x}_k = \mathbf{x}_{k-1} + \int_{(k-1)T}^{kT} \mathbf{f}\left[\mathbf{x}(\tau), \mathbf{u}(\tau)\right] d\tau + \mathbf{w}_k \tag{3}$$

$$= \mathbf{F}\left(\mathbf{x}_{k-1}, \mathbf{u}_{k-1}\right) + \mathbf{w}_{k-1} \tag{4}$$

$$\mathbf{y}_k = \mathbf{h}\left(\mathbf{x}_k\right) + \mathbf{v}_k \tag{5}$$

where, $\mathbf{w}_{k-1} \in \mathbb{R}^n$ represents the random unmeasured process disturbances modelled as additive in the process dynamics and $\mathbf{v}_k \in \mathbb{R}^r$ represents the measurement noise. The *pdf*s of these random disturbances are assumed to be known. It is also assumed that $\mathbf{w}_{k-1}$ and $\mathbf{v}_k$ are independent and mutually uncorrelated. Further, it is assumed that the measurements are sampled at regular time intervals, which are integral multiples ($k \in \mathbb{I}$) of the sampling time T. The manipulated inputs $\mathbf{u}_{k-1}$ are held piece-wise constant between two sampling intervals $(k-1) \leq t < k$.

3. STATE ESTIMATION ALGORITHMS

3.1 Recursive Bayesian state estimation

Recursive Bayesian state estimation algorithms approximate the conditional *pdf* of the posterior of the states using the measurements available upto the corresponding sampling instant. In this work, state estimation algorithms that approximate the *pdf* of the posterior based on statistical linearisation techniques are considered for state estimation. These state estimators are based on the observation that better approximations of the *pdf* of the states can be obtained using samples rather than Taylor series linearisation (Patwardhan et al., 2012). The unscented Kalman filter (UKF) (Julier and Uhlmann, 2004) and the ensemble Kalman filter (EnKF) (Evensen, 2007) are the two widely used filters, based on statistical linearisation. A brief and compact description of the UKF and EnKF algorithms is provided in this section.

N_p samples of the states, process disturbances and measurement noise are drawn at the $(k-1)^{th}$ sampling instant as follows

$$X_{k-1} = \left\{ \hat{\mathbf{x}}^{(1)}_{k-1|k-1}, \hat{\mathbf{x}}^{(2)}_{k-1|k-1}, \ldots, \hat{\mathbf{x}}^{(N_p)}_{k-1|k-1} \right\} \tag{6}$$

$$W_{k-1} = \left\{ \mathbf{w}^{(1)}_{k-1}, \mathbf{w}^{(2)}_{k-1}, \ldots, \mathbf{w}^{(N_p)}_{k-1} \right\} \tag{7}$$

$$V_k = \left\{ \mathbf{v}^{(1)}_{k}, \mathbf{v}^{(2)}_{k}, \ldots, \mathbf{v}^{(N_p)}_{k} \right\} \tag{8}$$

These samples can either be drawn deterministically, as in the UKF algorithm or by drawing them randomly from their given *pdf*, as in the EnKF algorithm. Every particle, $(i = 1, 2, \ldots, N_p)$, is propagated through the state dynamics and measurement equations

$$\hat{\mathbf{x}}^{(i)}_{k|k-1} = \mathbf{F}\left(\hat{\mathbf{x}}^{(i)}_{k-1|k-1}, \mathbf{u}_{k-1} \right) + \mathbf{w}^{(i)}_{k-1} \tag{9}$$

$$\hat{\mathbf{y}}^{(i)}_{k|k-1} = \mathbf{h}\left(\hat{\mathbf{x}}^{(i)}_{k|k-1} \right) + \mathbf{v}^{(i)}_{k} \tag{10}$$

The weighted mean of the predicted states and measurement particles is obtained as follows

$$\bar{\mathbf{x}}_{k|k-1} = \sum_{i=1}^{N_p} \omega_i \hat{\mathbf{x}}^{(i)}_{k|k-1} \tag{11}$$

$$\bar{\mathbf{y}}_{k|k-1} = \sum_{i=1}^{N_p} \omega_i \hat{\mathbf{y}}^{(i)}_{k|k-1} \tag{12}$$

where, ω_i are suitable weights such that $\sum_{i=1}^{N_p} \omega_i = 1$. The UKF assigns a higher weight to the mean, compared to the rest of the sigma points

$$\omega_1 = \frac{\kappa}{n+\kappa}; \quad \omega_i = \frac{1}{2(n+\kappa)} \; i = 2, \ldots, N_p \tag{13}$$

where, ω_1 is the weight assigned to the mean, while ω_i is the weight assigned to the rest of the sigma points. The number of sigma points are fixed at $N_p = 2(2n+r)+1$. Thus, since N_p is fixed, κ is a tuning parameter that governs the spread of the sigma points around the mean and the weights associated with the sigma points. On the other hand, the EnKF assigns an equal weight to all particles, $\omega_i = \frac{1}{N_p}$ $(\forall\, i = 1, 2, \ldots, N_p)$. Thus, N_p is a tuning parameter for the EnKF.

The cross-covariance of states and measurement errors and innovations covariance is obtained as follows

$$\boldsymbol{\varepsilon}^{(i)}_{k|k-1} = \hat{\mathbf{x}}^{(i)}_{k|k-1} - \bar{\mathbf{x}}_{k|k-1} \tag{14}$$

$$\mathbf{e}^{(i)}_{k} = \hat{\mathbf{y}}^{(i)}_{k|k-1} - \bar{\mathbf{y}}_{k|k-1} \tag{15}$$

$$\mathbf{P}_{xe,k} = \sum_{i=1}^{N_p} \omega_i \left[\boldsymbol{\varepsilon}^{(i)}_{k|k-1} \right] \left[\mathbf{e}^{(i)}_{k} \right]^T \tag{16}$$

$$\mathbf{P}_{ee,k} = \sum_{i=1}^{N_p} \omega_i \left[\mathbf{e}^{(i)}_{k} \right] \left[\mathbf{e}^{(i)}_{k} \right]^T \tag{17}$$

For the update step, the Kalman gain and the updated particles of the states are computed as follows

$$\mathbf{K}_k = \mathbf{P}_{xe,k} \mathbf{P}^{-1}_{ee,k} \tag{18}$$

$$\hat{\mathbf{x}}^{(i)}_{k|k} = \hat{\mathbf{x}}^{(i)}_{k|k-1} + \mathbf{K}_k \left[\mathbf{y}_k - \mathbf{h}\left(\hat{\mathbf{x}}^{(i)}_{k|k-1} \right) \right] \tag{19}$$

The updated estimate of the states is obtained as a weighted mean of the updated particles

$$\bar{\mathbf{x}}_{k|k} = \sum_{i=1}^{N_p} \omega_i \hat{\mathbf{x}}^{(i)}_{k|k} \tag{20}$$

It may be noted that in the UKF algorithm, samples of the states are drawn from their posterior at every sampling instant using their filtered mean and the corresponding covariance. However, in the EnKF algorithm, the filtered particles are propagated to the next sampling instant without any re-sampling.

3.2 Moving Horizon Estimator

The moving horizon estimator (MHE) obtains the state estimates as a solution to the optimisation problem that maximises the following *pdf* of the past trajectory of the states over a fixed window of measurements

$$p\left(\mathbf{X}^{k-1}_{k-N_h} \,\middle|\, \mathbf{Y}^{k}_{0} \right) \tag{21}$$

where, $\mathbf{X}^{k-1}_{k-N_h} = \{\mathbf{x}_{k-N_h}, \ldots, \mathbf{x}_{k-1}\}$ and N_h denotes the length of the window. Under the assumptions that the states follow a first order Markov process and the modelling assumptions described in Sec. 2, the MHE is formulated to solve the following problem

$$\left\{ \hat{\mathbf{x}}_{j|k} \right\}^{k}_{j=k-N_h} = \arg \min_{\mathbf{X}^{k-1}_{k-N_h}} \; \mathcal{P}_{k-N_h} + \sum_{l=k-N_h}^{k-1} \| \mathbf{w}_l \|^2_{\mathbf{Q}^{-1}} + \sum_{l=k-N_h+1}^{k} \| \mathbf{e}_l \|^2_{\mathbf{R}^{-1}} \tag{22}$$

s.t.

$$\mathbf{x}_{l+1} = \mathbf{F}(\mathbf{x}_l, \mathbf{u}_l) + \mathbf{w}_l \tag{23}$$

$$\mathbf{e}_l = \mathbf{y}_l - \mathbf{h}(\mathbf{x}_l) \tag{24}$$

$$\mathbf{x}_L \le \mathbf{x}_l \le \mathbf{x}_H \tag{25}$$

The term $\mathcal{P}_{k-N_h}$ is the 'arrival cost' , which sums up the effect of past observations on the state $\mathbf{x}_{k-N_h}$ (Rao and Rawlings, 2002) and is given by

$$\mathcal{P}_{k-N_h} = -\log\left[p\left(\mathbf{x}_{k-N_h} \middle| \mathbf{Y}_{0:k-N_h} \right) \right] \tag{26}$$

For the general class of nonlinear systems it is difficult to obtain the negative of the log–likelihood function of the states. Hence, the arrival cost is approximated as the square of the weighted two–norm of the estimation error at the beginning of the window (López-Negrete et al., 2011)

$$\mathcal{P}_{k-N_h} \approx \left\|\mathbf{x}_{k-N_h} - \hat{\mathbf{x}}_{k-N_h|k-N_h}\right\|^2_{\mathbf{P}^{-1}_{k-N_h|k-N_h}} \tag{27}$$

The above approximation can be obtained using recursive Bayesian state estimators such as the EKF, UKF or EnKF, which yield the first two moments of the posterior distribution used in Eq. 27. It may be noted that the above formulation of the MHE utilises the moments of the posterior of the states distributions to approximate the arrival cost. This, consequently yields the filtered estimates of the states at the current time instant. In this work it is proposed to use the UKF and EnKF to approximate the arrival cost in the MHE formulation.

4. THE pH PROBLEM

The pH system Romanenko et al. (2004) consists of a CSTR in which a neutralisation reaction between a strong acid (HA) and strong base (BOH) occurs in the presence of a buffer agent (BX). The process is described by the following equations

$$\frac{dx_1}{dt} = \frac{q_A}{V}\left(x_{1,in} - x_1\right) - \frac{1}{V}x_1 q_B \tag{28}$$

$$\frac{dx_2}{dt} = -\frac{q_A}{V}x_2 + \frac{1}{V}\left(x_{2,in} - x_2\right) q_B \tag{29}$$

$$\frac{dx_3}{dt} = -\frac{q_A}{V}x_3 + \frac{1}{V}\left(x_{3,in} - x_3\right) q_B \tag{30}$$

$$\xi^3 + \left(\frac{K_w}{K_x} + x_3 + x_2 - x_1\right)\xi^2 + \left(x_2 - x_1 - K_x\right)\frac{K_w}{K_x}\xi - \frac{K_w^2}{K_x} = 0 \tag{31}$$

where x_1, x_2, x_3 refer to the concentrations of acid (A), base (B) and buffer agent (X) respectively. q_A is acid flow rate and q_B is the base flow rate. K_x and K_w are the dissociation constants of the buffer and water respectively and $\xi = 10^{-pH}$. The value of the pH, which is the measured variable, is derived as follows

$$a = 1; \quad b = \frac{K_w}{K_x} + x_3 + x_2 - x_1; \quad g = -\frac{3b}{a}$$

$$c = \left(x_2 - x_1 - K_x\right)\frac{K_w}{K_x}; \quad z = \frac{c}{3a}$$

$$d = -\frac{K_w^2}{K_x}; \quad q = g^3 + \frac{bc - 3ad}{6a^2}$$

$$pH = -\log_{10}\left\{\left[q + \sqrt{q^2 + \left(z - g^2\right)^3}\right]^{1/3} + \left[q - \sqrt{q^2 + \left(z - g^2\right)^3}\right]^{1/3} + g\right\} \tag{32}$$

The process parameters taken from the work by Romanenko et al. (2004) are given in Table 1. The operating conditions are chosen such that the system exhibits a highly nonlinear behaviour in the given region. Random disturbances in the process were simulated by adding a zero-mean Gaussian white noise signal in the state dynamics. To simulate the effect of measurement noise, a zero-mean Gaussian white noise was added to the pH measurement signal. The values of the noise covariance matrices and operating conditions are given in Table 2. A sampling time of $T = 5\ s$ was chosen for the process.

Table 1. pH process: process and model parameters

Parameter	Process	Model (MPM)
$C_{A,i}$	1.2×10^{-3}	1.2×10^{-3}
$C_{B,i}$	2.0×10^{-3}	2.0×10^{-3}
$C_{X,i}$	1.2×10^{-3}	1.2×10^{-3}
V	2.5	2.5
K_w	1.0×10^{-14}	1.0×10^{-14}
K_x	1.0×10^{-7}	*2.0×10^{-7}*

Table 2. pH process: operating conditions

Variable	Operating Value	Unit
$\mathbf{u}$	$\begin{bmatrix}1 & 0.265\end{bmatrix}$	l/min
$\mathbf{x}_0$	$10^{-4} \times \begin{bmatrix}9.30 & 5.40 & 4.30\end{bmatrix}$	mol/l
$\hat{\mathbf{x}}_0$	$10^{-4} \times \begin{bmatrix}9.76 & 5.67 & 4.52\end{bmatrix}$	mol/l
pH (true)	5	–
$\mathbf{Q}$	$10^{-11} \times \begin{bmatrix}2 & 2 & 2\end{bmatrix}$	mol^2/l^2
$\mathbf{R}$	1×10^{-4}	–

4.1 Results

The comparison of the state estimators was carried out for two scenarios: a) state estimation with no model-plant mismatch (MPM) and b) state estimation with a parametric MPM. For each scenario, the simulations were carried out for 3000 s (600 sampling instants). The system was excited by subjecting the acid (q_A) and base (q_B) flow rates to a pseudo random binary sequence (PRBS) of inputs. The amplitude of the input in q_A was 0.1 l/min with switching frequency $[0 \quad 0.09\ \omega_N]$, where ω_N is the Nyquist frequency of the process. Similarly, the amplitude of the input in q_B was 0.026 l/min with switching frequency $[0 \quad 0.13\ \omega_N]$. The root mean square error (RMSE) of the state estimates is used as a criterion for comparing the performance of the state estimators

$$RMSE = \sqrt{\frac{1}{N}\sum_{j=1}^{N}\left(\mathbf{x}_{i,j} - \bar{\mathbf{x}}_{i,j|j}\right)^2} \tag{33}$$

where, N is the number of samples of the data and the subscript i refers to the i^{th} element of the state vector. An average value of the RMSE obtained through 25 Monte Carlo simulations of the process, with every state estimator, is reported in the results. For each of the runs, the initial conditions of the process and the state estimator along with the input changes are identical, while the realizations of the process and measurement noise are different.

The performance of the state estimators, namely the UKF, EnKF and the MHE are first compared for the scenario with no MPM. The process parameters are given in Table 1, with the model parameters being identical to those of the process. First, the performances of the

UKF and EnKF are evaluated for different values of their respective tuning parameters. This is done with a twofold objective. At first, it compares the performance of the two recursive Bayesian state estimators. Second, this exercise helps in obtaining the tuning parameters of the UKF and EnKF that provide reasonably good performance in terms of the RMSE values of the state estimates (Eq. 33), which can be further used in the MHE algorithm for approximating the arrival cost.

For the UKF, κ is a tuning parameter (Eq. 13). The performance of the UKF was evaluated for different values of κ and the results are presented in Table 3. From the table, it can be seen that there is very little change in the RMSE of the state estimates for different values of κ. This indicates that for this particular example, the value of κ does not have a significant effect on the performance of the UKF. For the EnKF algorithm, the number of particles (N_p) used to approximate the distributions is a tuning parameter. The RMSE values obtained for various values of N_p are reported in Table 3. As expected, the performance of the EnKF improves as N_p is increased. This is because a larger number of particles helps in better approximation of the *pdf* of the posterior. But, an increase in N_p results in a corresponding increase in computational time and costs and beyond $N_p = 150$, there is not much noticeable improvement in the performance of the EnKF, when compared to a corresponding increase in computational time. The comparison of the two recursive Bayesian state estimators shows that the RMSE of the state estimates obtained using the UKF are lower by at least 5.5 % than those obtained using the EnKF. Thus, for the pH simulation problem, the UKF performs better than the EnKF. State estimation with the MHE was first carried out by using the UKF (MHE-UKF) for approximating the arrival cost and then using the EnKF (MHE-EnKF) for the same. The simulation results using the UKF for state estimation indicate that the tuning parameter κ does not have a significant impact on the performance of the state estimator. Hence, while any value of κ can be used, a value of $\kappa = 3$ was chosen for the MHE-UKF. For the EnKF, there is an improvement in the performance of the estimator as N_p increases. Hence, $N_p = 150$ was chosen for the MHE-EnKF as there is no significant improvement in the EnKF performance for $N_p > 150$ compared to the increase in computation time. The RMSE of the state estimates using the MHE-UKF and the MHE-EnKF were obtained for different lengths of the moving horizon (N_h). The RMSE values of the state estimates obtained using the MHE-UKF and MHE-EnKF for various values of N_h are reported in Table 3. The performance of the MHE is compared against that of the state estimator used to approximate the arrival cost. Thus, the performance of the MHE-UKF is compared against that of the UKF and the performance of the MHE-EnKF is compared against the EnKF. In both cases the RMSE values of the state estimates reduce as the length of the window is increased. For $N_h = 8$, the RMSE of the state estimates obtained using MHE-UKF are lower by approximately 4-8 % than those obtained using the UKF. Similarly, the RMSE values obtained using MHE-EnKF are lower by approximately 3-9 % than those obtained using the EnKF. The reduction in the RMSE values is principally due to the use of the moving window of measurements. The moving window of measurements improves the approximation of the posterior of the states, thereby reducing the error in the state estimates.

Table 3. RMSE of state estimates: Comparison of state estimator performance for no MPM case

Parameter	$x_1 \times 10^4$	$x_2 \times 10^4$	$x_3 \times 10^4$
κ	UKF		
2	0.1459	0.1365	0.1505
3	0.1407	0.1357	0.1428
4	0.1423	0.1317	0.1511
5	0.1371	0.1368	0.1537
N_h	MHE-UKF ($\kappa = 3$)		
2	0.1409	0.1341	0.1411
4	0.1380	0.1321	0.1344
8	0.1374	0.1294	0.1285
N_p	EnKF		
30	0.1760	0.1650	0.1771
50	0.1691	0.1567	0.1703
80	0.1685	0.1607	0.1638
150	0.1583	0.1450	0.1601
200	0.1560	0.1445	0.1544
N_h	MHE-EnKF ($N_p = 150$)		
2	0.1494	0.1486	0.1602
4	0.1465	0.1451	0.1575
8	0.1436	0.1445	0.1550

A parametric mismatch in the value of the buffer dissociation constant (K_x) was introduced to create the scenario of model-plant mismatch (MPM). The model parameters for this scenario are given in Table 1. The simulations that were carried out for the no-MPM case were repeated for this scenario, with identical initial conditions of the estimators and the process (Table 2). The input excitation used was also the same as that used previously. The average RMSE values of the state estimates are obtained for each state estimator through 25 Monte Carlo simulations of the process. The RMSE values of the state estimates, obtained for various values of the tuning parameters of each state estimator are given in Table 4. Simulation results obtained using the UKF and EnKF confirm the fact that the performance of the state estimators is dependent on the accuracy of the model used. When compared to the RMSE values of the states in Table 3, it can be seen that due to MPM, the performance of the UKF is worse by approximately 8-30 %, while that of the EnKF is worse by approximately 10-18 %. As in the ideal case, the simulations for the MHE are repeated using the UKF and EnKF for approximating the arrival cost. The RMSE values of the state estimates obtained for the MHE-UKF and MHE-EnKF for different lengths of the moving window are given in Table 4. From the table it can be seen that the RMSE values obtained using the MHE-UKF are lower by approximately 4-7 % than those obtained using the UKF and those of the MHE-EnKF are lower by approximately 4-8 % than those obtained using the EnKF. From Tables 3 and 4 it can be seen that the RMSE values of the state estimates obtained using the MHE-UKF and MHE-EnKF are higher if there is a MPM. These results indicate that while the use of the MHE improves the approximation of the posterior of the states, it does not help in compensating for the errors introduced due to MPM.

Table 4. RMSE of state estimates: Comparison of state estimator performance for MPM case

Parameter	$x_1 \times 10^4$	$x_2 \times 10^4$	$x_3 \times 10^4$
κ	UKF		
2	0.2187	0.1785	0.1634
3	0.2165	0.1862	0.1658
4	0.2154	0.1723	0.1745
5	0.2167	0.1675	0.1664
N_h	MHE-UKF ($\kappa = 3$)		
2	0.2073	0.1836	0.1614
4	0.2119	0.1812	0.1531
8	0.2105	0.1778	0.1490
N_p	EnKF		
30	0.2550	0.1893	0.1961
50	0.2326	0.1934	0.1748
80	0.2185	0.1802	0.1766
150	0.2276	0.1772	0.1784
200	0.2230	0.1765	0.1778
N_h	MHE-EnKF ($N_p = 150$)		
2	0.2143	0.1811	0.1779
4	0.2087	0.1774	0.1757
8	0.2058	0.1762	0.1732

5. CONCLUSIONS

The objective of this work was to ascertain the effect of using a moving horizon of past data on the quality of the state estimates for the following two scenarios: ideal case where plant and model are exact and the case where there is a MPM, when compared to those obtained using recursive Bayesian state estimators. The benchmark pH simulation case study was used to study this effect. The arrival cost in the MHE was approximated with two recursive Bayesian state estimators: the UKF and the EnKF. In both cases (no-MPM and MPM), the results demonstrate that the MHE-UKF performs better than the UKF and the same for the MHE-EnKF over the EnKF. These results indicate that the moving horizon of past measurements results in the use of smoothed state estimates to compute the current estimates of the states. The smoothing operation reduces the error caused by approximation of the posterior of the states, which is the major reason for the improvement in performance. Further, as expected, the performance improves with increase in the length of the moving horizon. But, beyond a certain length, the percentage reduction achieved in the RMSE values is not commensurate with the increase in the associated computation time. However, the improvement in the performance achieved with the MHE is associated with an increase in the computation time required for the simulations. This is due to the time required to solve the nonlinear optimisation problem (Eq. 22-25) to obtain the state estimates.

In the scenario of a model-plant mismatch, as expected, the results show that the performance of the state estimators deteriorates in comparison to the ideal case. In presence of a MPM too, the use of the MHE results in lower RMSE values of the state estimates when compared to those obtained using the UKF and EnKF. The results, therefore, indicate that while the use of a moving horizon of data results in improving the approximation of the posterior distribution of the states it does not help in compensating for the error introduced due to model-plant mismatch.

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