Simultaneous state and parameter estimation arises from various applicational areas but presents a major computational challenge. Most available Markov chain or sequential Monte Carlo techniques are applicable to relatively low dimensional problems only. Alternative methods, such as the ensemble Kalman filter or other ensemble transform filters have, on the other hand, been successfully applied to high dimensional state estimation problems. In this paper, we propose an extension of these techniques to high dimensional state space models which depend on a few unknown parameters. More specifically, we combine the ensemble Kalman-Bucy filter for the continuous-time filtering problem with a generalized ensemble transform particle filter for intermittent parameter updates. We demonstrate the performance of this two stage update filter for a wave equation with unknown wave velocity parameter.

1 Introduction

There is a high demand across different disciplines for methods that allow for efficient and reliable state-parameter estimation for high-dimensional and nonlinear evolution equations. While the theoretical foundation of state and parameter estimation for stochastic differential equations (SDEs) is well established (see, for example, [1, 11]) and efficient computational methods for low dimensional problems are available (see, for example, [9, 12]), joint state-parameter estimation for high dimensional problems remains an area of active research. A major breakthrough in that direction has been achieved through the development of the ensemble Kalman filter (EnKF) for state estimation of discretized partial differential equation models arising, for example, from meteorology and oil reservoir exploration [10, 13, 16]. The success of the EnKF has triggered the development of a large variety of related ensemble transform filters with the aim of removing the underlying Gaussian distributional assumptions of the EnKF. Here we wish to mention in particular the work of [2, 4, 5, 17, 20] on the continuous-time filtering problem and [8, 15, 18, 19] on the intermittent filtering problem.

In this paper, we propose an extension of the ensemble transform filtering approach to the continuous-time combined state and parameter estimation problem. Instead of applying an ensemble transform filtering approach directly to the extended state-parameter phase space, we propose to exploit the particular structure of the joint conditional distribution and approximate it via a hybrid ansatz combining two different interacting particle filters; namely the ensemble Kalman-Bucy filter (EnKBF) [2] for state estimation and the ensemble transform particle filter (ETPF) [15, 16] for the parameter updates. Such an approach is advantageous provided the distribution in the states given model parameters is nearly Gaussian while the distribution in the parameters may be non-Gaussian. Furthermore, the main additional computational complexity arises from the update of the parameters through an appropriate extension of the ETPF. Here we assume that the number of unknown parameters is much smaller than the dimension of state space of the underlying SDE model.

The remainder of the paper is structured as follows. In Section 2, we will discuss the theoretical foundation of the considered Bayesian inference problem and formulate the basic algorithmic approach. Our proposed approach for a sequential update of the model parameters and the required extension of the ETPF is provided in Section 3. A summary of the overall algorithm is provided in Section 4 and numerical results for a stochastic wave equation in Section 5. Our conclusions can be found in Section 6.
2 Problem formulation and proposed ansatz

We consider the following time-continuous filtering problem: estimate a reference trajectory \( x_{ref}(t) \in \mathbb{R}^{N_x} \) and \( t \in [0, T] \) and a vector of unknown reference parameters \( \lambda_{ref} \in \mathbb{R}^{N_\lambda} \) of a SDE

\[
dx_t = f(x_t, \lambda)dt + Q^{1/2}dW_t
\]  

(1)

from continuous-time observations

\[
dy_t = h(x_t)dt + R^{1/2}dV_t.
\]

(2)

Here both \( W_t \in \mathbb{R}^{N_W} \) and \( V_t \in \mathbb{R}^{N_V} \) denote standard multi-dimensional Brownian motions. A common approach to joined parameter and state estimation is to augment the SDE (1) by the trivial dynamics

\[
d\lambda_t = 0
\]

(3)

in the parameters \( \lambda \). Then the distribution of interest is the conditional density \( \hat{\pi}_t(z) := \pi_t(z|\lambda_0, t) \) in the augmented state variable \( z = (x^T, \lambda^T)^T \in \mathbb{R}^{N_z} \). The time evolution of the conditional density \( \hat{\pi}_t \) is described by the Kushner-Stratonovich equation [1,11], which we state in the form

\[
\hat{\pi}_t(g) = \hat{\pi}_0(g) + \int_0^t \hat{\pi}_s(\mathcal{L}g)ds + \int_0^t (\hat{\pi}_s(gh) - \hat{\pi}_s(g)\bar{h}_s)\mathbf{R}^{-1}d(y_s - \bar{h}_s, ds),
\]

(4)

where \( \bar{h}_s := \hat{\pi}_s(h) \) and

\[
\mathcal{L} g := f \cdot \nabla g + \frac{1}{2} \sum_{k,i} N_W \frac{\partial^2 g}{\partial x_k \partial x_i}.
\]

Analytical solutions of (4) are generally not available and sequential Monte Carlo (SMC) methods are often employed in order to approximate the marginal density by empirical measures. Here we follow recently developed SMC methods which rely on appropriately defined modified evolution equations for particles \( z^i_l \), \( l = 1, \ldots, L \), such that

\[
\pi_t(z) \approx \frac{1}{N} \sum_{i=1}^L \delta(z - z^i_l).
\]

(5)

The feedback particle filter (FPF) [20, 21] is one of these, so called, particle flow filters, which is characterized by the modified SDE

\[
dz_t^j = \begin{bmatrix} f(z^j_t)dt + Q^{1/2}dW_t^j \\ 0 \end{bmatrix} + K^j_t \circ dl_t^j, \quad K^j_t = K_j(z^j_t) \quad \text{and innovation}
\]

\[
dl_t^j = dy_t - \frac{h(z^j_t) + \bar{h}_t}{2}dt.
\]

(7)

Here the Stratonovitch interpretation of the SDE (6) should be used [14]. The gain function \( K_j \) is determined by the elliptic partial differential equation

\[
- \nabla_{z^j} \cdot (\hat{\pi}_j K_j) = \hat{\pi}_j R^{-1}(h - \bar{h}_t)^T.
\]

(8)

Note that \( \hat{\pi}_j \) is unknown and needs to be approximated by (5). In other words, \( K_i \) is typically found as a weak approximation to (8). Different numerical approaches for solving (8) can be found in [17]. We mention that the innovation (7) can be replaced by the alternative form

\[
dl_t^j = dy_t - h(z^j_t)dt + R^{1/2}dU_t^j, \quad \text{where} \quad U_t^j \text{ denote standard } N_j \text{-dimensional Brownian motion independent of } W_t \text{ and } V_t. \quad \text{The statistical equivalence can be shown following the arguments of Appendix A in [17].}
\]

While (6) is very appealing, its numerical implementation can be demanding for high-dimensional systems which require a large number, \( L \), of particles \( z^i_l \). In order to address this issue we propose to rewrite the joint distribution \( \hat{\pi}_t \) in its desintegrated form, i.e.

\[
\hat{\pi}_t(z) = \hat{\pi}_t(x|\lambda)\hat{\pi}_t(\lambda).
\]

(10)

A corresponding particle approximation can be defined as follows:

\[
\hat{\pi}_t(z) \approx \frac{1}{M} \sum_{i=1}^M \delta(z - \hat{x}^i_t),
\]

(11)

where \( \hat{x}^i_t \sim \hat{\pi}_t(\lambda) \), \( i=1, \ldots, L \), are constant parameter values drawn from the prior parameter distribution with time-dependent weights \( w^i_t \), \( i=1, \ldots, L \). There is also a set of \( M \) time-dependent states \( \{ \hat{x}^i_\lambda \}_{i=1}^M \) for each parameter vector \( \hat{x}^i_\lambda \), \( i \in \{1, \ldots, M\} \). The evolution equations for these states are given by the FPF with the parameters \( \hat{x}^i_\lambda \) held fixed, i.e.,

\[
d\hat{x}^i_\lambda = \hat{f}(\hat{x}^i_\lambda, \hat{x}^i_\lambda)dt + \hat{Q}^{1/2}dW^i_t + \hat{K}^{i \lambda} \circ dl^i_t,
\]

(12)

where \( \hat{K}^{i \lambda} = K_i(z^i_t, \hat{x}^i_\lambda) \) is determined by an appropriate numerical approximation to

\[
- \nabla_{\lambda} \cdot (\hat{\pi}_i K_i) = \hat{\pi}_i R^{-1}(h - \hat{h}_t)^T.
\]

(13)
and $dI_{t}^{i,j}$ denotes the innovation, i.e.,

$$dI_{t}^{i,j} = dy_i - \frac{h(x_t^{i,j}) + \bar{h}_t}{2} dt \quad (14)$$

or

$$dI_{t}^{i,j} = dy_i - h(x_t^{i,j})dt + R^{1/2}dU_{t}^{i,j}, \quad (15)$$

respectively. The time evolution of the normalized importance weights $w_t^i$ are calculated according to

$$dw_t^i = w_t^i(h(x_t^{i,j}) - \bar{h}_t)^T R^{-1}(dy_i - \bar{h}_t)dt \quad (16)$$

with $w_t^0 := 1/L$ initially and

$$\bar{h}_t = \frac{1}{M} \sum_{j=1}^{M} h(x_t^{i,j}), \quad \bar{h}_t = \frac{1}{L} \sum_{i=1}^{L} \bar{h}_t^i. \quad (17)$$

Note again that the parameter values are kept constant in (11), i.e., $\lambda_t^{i} = \lambda_t^{j}$.

A special case of the FPF scheme arises when the gain factor is assumed to be constant, which results in the popular EnKBF:

$$d\tilde{x}_t^{i,j} = f(\tilde{x}_t^{i,j}, \lambda_t^{i})dt + Q^{1/2}dW_t^{i,j} + C_t^{i} R^{-1}dI_{t}^{i,j}, \quad (18)$$

where the covariance matrix $C_t^{i}$ is determined empirically, i.e.,

$$C_t^{i} = \frac{1}{M-1} \sum_{j=1}^{M} (\tilde{x}_t^{i,j} - \bar{x}_t^{i})(h(\tilde{x}_t^{i,j}) - \bar{h}_t)^\top, \quad \bar{x}_t^{i} = \frac{1}{M} \sum_{j=1}^{M} \tilde{x}_t^{i,j},$$

and the innovation $dI_{t}^{i,j}$ is either given by (14) or (15), respectively. The EnKBF produces asymptotically correct results in a linear model setting when the posterior is a Gaussian distribution but is also successfully employed for state estimation in the context of strongly nonlinear model scenarios [2]. In this paper, we employ the EnKBF to forward state samples, $\tilde{x}_t^{i,j}$, in time. In other words, we interpret (11) as a weighted Gaussian mixture approximation to the conditional filtering distribution, $\mathcal{F}_t$.

The effective mixture size, defined by

$$L_t^{eff} = \frac{1}{\sum_{i=1}^{L} (w_t^i)^2}, \quad (19)$$

will deteriorate as time progresses, in general. A classic approach would be to resample the parameter values $\lambda_t^{i}$ jointly with their state samples $\{\tilde{x}_t^{i,j}\}_{j=1}^{M}, i \in \{1, \ldots, L\}$ at an appropriate instance $t = t^*$ of time according to their weights $w_t^i$,

in order to produce an equally weighted mixture (11). However, resampling with replacement would produce identical sets of parameters and associated state samples. Hence, we propose an extension of the ETPF [15,16] to (11). Contrary to the EnKBF, the ETPF produces a consistent approximation of the gain factor of the FPF on the basis of an optimal transport problem [17]. The ETPF has also been shown to work well under relatively small number of particles and high dimensional systems when combined with localization [3,8].

3 Ensemble transform particle filter

As mentioned above, the ETPF is an numerical approximation of the feedback control law of the FPF induced by a linear transport problem [17]. A different interpretation is that the ETPF replaces the resampling step of the classical particle filter with a linear transformation [15,16]. The key idea is to choose a linear transformation that connects the empirical measure of the weighted prior ensemble with an equally weighted posterior ensemble in the sense of optimal transportation. Intuitively, one would like to achieve a high correlation between the prior and posterior samples. More generally, the optimal transport problem between two weighted empirical measures $v_1$ and $v_2$, given by

$$v_1(y) = \sum_{i=1}^{L} w_t^i \delta(y - y_t^i), \quad v_2(y) = \sum_{i=1}^{L} w_2^i \delta(y - y_2^i),$$

can be formulated as follows [16]. Introduce the set

$$U(W_1, W_2) = \{ T \in \mathbb{R}^{L \times L} : t_{ij} \geq 0, \sum_{j=1}^{L} t_{ij} w_1^i, \sum_{i=1}^{L} t_{ij} = w_2^j \}$$

of admissible bi-stochastic matrices $T$ and the $L \times L$ matrix of mutually distances $M_{Y_1, Y_2}$ with entries

$$(M_{Y_1, Y_2})_{ij} = \|y_1^i - y_2^j\|^2.$$ 

Then the Wasserstein distance between $v_1$ and $v_2$ is defined by

$$W_2^2(v_1, v_2) = \min_{T \in U(W_1, W_2)} \text{tr} (T^T M_{Y_1, Y_2}). \quad (20)$$

The matrix $T^* \in U(W_1, W_2)$, which achieves the minimum in (20), is called the optimal coupling between $v_1$ and $v_2$.

The ETPF relies on the special situation that the vector $W_1 = (w_1^1, \ldots, w_1^L)^\top$ represents the importance weights of the prior samples $y_t^i, i \in \{1, \ldots, L\}$, and $W_2 = (1/L, \ldots, 1/L)^\top$. Furthermore, the ETPF also uses $Y_1 = Y_2 = Y := (y_1^1, \ldots, y_1^L)^\top$ and the desired equally weighted posterior samples are defined by

$$\bar{y} = M \sum_{i=1}^{L} y_t^i t_{ij}^*.$$
Solving an optimal transport problem is computationally demanding for large sample sizes $L$. This issue has been addressed in [6, 7] via a Sinkhorn approximation which reduces the complexity of the optimal transport problem from $O(L^3 \log(L))$ to $O(L^2)$. It is shown in [8] how this approximation can be employed successfully in the context of sequential filtering.

In case of the weighted mixture approximation (11), the ETPF is implemented at an appropriate instance $t = r^*$ of time as follow. First, we define the distance matrix $M_{Y_1, Y_2}$. There are two choices. Either one sets $Y_1 = Y_2 = (\tilde{\lambda}_{1i}^t, \ldots, \tilde{\lambda}_{Li}^t)^T$ or one uses the extended vectors $\tilde{\xi}_i^t = ((\tilde{\lambda}_{1i}^t)^T, (\tilde{\xi}_{1i}^t)^T)^T \in \mathbb{R}_N^2$ instead of $\tilde{\lambda}_{1i}^t$ in both $Y_1$ and $Y_2$. Second, the weight vector $W_t$ is defined by $W_t = (w_{1}^t, \ldots, w_{L}^t)^T$. Denoting the solution of the optimal transport problem again by $T^*$, equally weighted parameter values are finally provided by

$$\tilde{\lambda}_{ij}^t = L \sum_{l=1}^{L} \tilde{\lambda}_{ij}^t.$$  \hspace{1cm} (21)

We also need to transform the associated state samples $\tilde{x}_i^t$. The obvious choice is

$$\tilde{x}_i^t = M \sum_{l=1}^{L} \tilde{x}_i^t, \quad \forall j \in \{1, \ldots, M\}. \hspace{1cm} (22)$$

This requires, however, that the state samples $\tilde{x}_i^t$ are optimally correlated for each fixed index $i \in \{1, \ldots, L\}$. This can be achieved either through an appropriate initialization of the state samples or through finding an appropriate permutation matrix $P_i \in \mathbb{R}^{M \times M}$ for each set of state samples $\{\tilde{x}_i^t\}_{i=1}^{M}$ via an associated Wasserstein barycenter problem [7]. More specifically, introduce $L$ equally weighted empirical measures

$$v_i(x) = \frac{1}{M} \sum_{j=1}^{M} \delta(x - \tilde{x}_i^t)$$

and the empirical measure

$$v(x) = \frac{1}{M} \sum_{i=1}^{M} \delta(x - \tilde{x}_i^t)$$

with its locations $x^j, \ j = 1, \ldots, M$, determined as the minimizer of the functional

$$f(v) = \sum_{i=1}^{L} W_i^2(v, v_i). \hspace{1cm} (23)$$

The desired permutation matrices are now given by

$$P^i = MT^i, \quad i \in \{1, \ldots, L\},$$

where $T^i$ denotes the optimal coupling matrix associated to $W_i^2(v, v_i)$. Efficient numerical methods for solving Wasserstein barycenter problems for empirical measures have been discussed in [7]. These permutation matrices $P$ are now used to rearrange the state samples prior to the application of (22).

While the transformation steps (21)–(22) in the parameters and the state samples is relatively complex, we emphasize that it only needs to be conducted whenever the effective sample size (19) drops below a certain threshold such as $L^* = 3L/4$, for example.

## 4 Algorithmic summary

The details of the proposed hybrid mixture model are laid out in form of pseudocode in Algorithm (1). In particular, the states $\tilde{x}_i^t$ are evolved numerically via a forward Euler discretization of the EnKBF (18) with step-size $\Delta t$ and the weight update formula (16) is discretized as

$$w_{n+1}^i = w_n^i \exp \left(-\frac{1}{2} \sum_{k=0}^{n} (\tilde{\delta}_n^i)^{\top} R^{-1}(\tilde{\delta}_n^i - \delta_n^i)^{\top} R^{-1} \Delta n \right) \hspace{1cm} (24)$$

in order to prevent negative weights. Here subscript $n$ denotes approximations at time-level $t_n = n\Delta t$.

Whenever the effective sample size (19) drops below a threshold value $L^* < L$, the parameters and the state samples are updated via the extended ETPF as described in Section 3 and the weights are reset to $1/L$. This step requires to solve a linear transport problem, i.e.,

$$T^* = \arg \min_{T \in \mathbb{R}^{L \times L}} \sum_{l=1}^{L} t_{lk} \| \tilde{\lambda}_n^l - \tilde{\lambda}_n^k \|^2 \hspace{1cm} (25)$$

subject to the constraints

$$\sum_{l=1}^{L} t_{lk} = 1/L, \quad \sum_{k=1}^{L} t_{lk} = w_n^l \quad \text{and} \quad t_{lk} \geq 0 \hspace{1cm} (26)$$

and, if necessary, the Wasserstein barycenter problem (23).

## 5 Numerical example

The proposed mixture ansatz is now numerically investigated for the stochastic wave equation

$$\dot{u}_t = c \triangle u_t + \gamma \triangle v_t + \delta W_t(x), \hspace{1cm} (27)$$

$$u_0 = v, \hspace{1cm} (28)$$

with unknown wave velocity parameter $c = e^x$, $\delta = 0.02, \gamma = 0.001$ and space-time white noise $W_t(x)$. Note that a more general case than discussed earlier is considered here, i.e., $u_t(x)$ and $v_t(x)$ are functions with respect to the spatial domain $x \in [0, 2\pi]$ at any given time $t$. We assume periodic boundary conditions and generate initial fields from a
Algorithm 1 Two step EnK-FETPF update

Input: $x_0^i$, $\hat{\lambda}^i_0$, $w_0^i := 1/L$, $i \in \{1, \ldots, L\}$, $j \in \{1, \ldots, M\}$
Output: $\hat{\lambda}_{[0,j]}, \tilde{x}_{[0,j]}^i$, $i \in \{1, \ldots, L\}$

1: for $n = 1$ to $t$
2: for $j = 1$ to $M$
3: Calculate $\tilde{x}_{t,j}$ according to eq. (18)
4: end for
5: for $i = 1$ to $L$
6: Compute weights weights $w_n^i$ via (24)
7: if $L_n^{\text{eff}} \leq L^*$ then
8: Solve minimization linear transport problem (25) to find $T^*$
9: If required, solve the Wasserstein Barycenter problem (23) and rearrange states $\tilde{x}_{t,j}^i$
10: Update samples $\tilde{x}_{t,j}^i$ and $\hat{\lambda}_{[0,j]}$ via (22) and (21)
11: Set weights $w_n^i := \frac{1}{L}$
12: end if
13: end for
14: Determine $\bar{\lambda}_n = \frac{1}{L} \sum_{i=1}^L \hat{\lambda}^i_n \forall n$
15: Compute $\bar{x}_n = \frac{1}{M} \sum_{j=1}^M \tilde{x}_{t,j}^i \forall n \forall i$
16: end for

6 Conclusions

We have presented a sequential state-parameter estimation algorithm suitable for high-dimensional state space models which depend on a relatively small number of parameters. In comparison to a direct approach based on the FPF formulation (6) for an extended state space model, the proposed methodology can be implemented as a parallel update of $L$ standard state estimation problems for given parameters using either the FPF, the EnKBF or other ensemble transform particle filter. If necessary, techniques such localization and ensemble inflation [10, 16] can also be used. The parameters, on the other hand, are adjusted using an extended version of the ETPF once the effective sample size of the parameters drops below a certain threshold value. This part of the algorithm is computationally more demanding than a standard resampling approach. However, it allows again for an application of localization to the estimation of spatially dependent parameters. A practical exploration of such an extension of the presented algorithm will be explored for stochastic wave equation (27)–(28) and spatially dependent wave velocities $c(x)$ in future work. Furthermore, the computational complexity of the parameter update step can be reduced by using alternative implementations of the ETPF such as provided by the Sinkhorn algorithm for the underlying linear transport problem [8].
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