

A PDE-based Adaptive Kernel Method for Solving Optimal Filtering Problems

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Abstract

In this paper, we introduce an adaptive kernel method for solving the optimal Itering problem. The computational framework that we adopt is the Bayesian Iter, in which we recursively generate an optimal estimate for the state of a target stochastic dynamical system based on partial noisy observational data. The mathematical model that we use to formulate the propagation of the state dynamics is the Fokker-Planck equation, and we introduce an operator decomposition method to efficiently solve the Fokker-Planck equation. An adaptive kernel method is introduced to adaptively construct Gaussian kernels to approximate the probability distribution of the target state. Bayesian inference is applied to incorporate the observational data into the state model simulation. Numerical experiments have been carried out to validate the performance of our kernel method.

Keywords: Optimal Itering problem, Bayesian inference, partial differential equation, kernel approximation

1 Introduction

Data assimilation is an important topic in data science. It aims to optimally combine a mathematical model with observational data. The key mission in data assimilation is the optimal Itering problem, in which we try to find the best estimate for the state of a stochastic dynamic model. Such a stochastic dynamic model is typically in the form of a system of stochastic differential equations (SDEs), and we call it the ‘state process’. In many practical situations, the true value of the state process is not available, and we can only use partial noisy observations to find the best estimate for the state. In the optimal Itering problem, the ‘best estimate’ that we want to find is dened as the conditional expectation of the state conditioning on the observations.

When both the state dynamics and the observations are linear, the optimal Itering problem is a linear Itering problem, which can be analytically solved by the classic Kalman Iter [20]. In the case of nonlinear Itering problem, one needs to derive an approximation for the conditional probability of the state { instead of calculating the conditional expectation directly, and we call this conditional probability the ‘Itering density’. There are two well-known nonlinear Itering methods, e.g., the Zakai’s approach and the Bayesian Iter. The Zakai’s approach formulates the Itering density as the solution of a parabolic type stochastic partial differential equation [32], e.g., the Zakai equation, then we solve the Zakai equation numerically to obtain an approximation for the Itering density [5, 6, 14, 34]. The Bayesian Iter solves the nonlinear Itering problem in a recursive

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two-step procedure: a prediction step and an update step. In the prediction step, we predict the Itering density of the state before reception of the observational data. Then, when the observational data is available in the update step, we let the predicted Itering density be the prior and apply Bayesian inference to incorporate the observational information into the prediction and obtain an updated Itering density as the posterior in the Bayesian inference. Besides the Zakai's approach and the Bayesian Iter, recently we developed a new approach to solve the optimal Itering problem, and we named this approach the backward SDE Iter [4, 9]. The backward SDE Iter is similar to Zakai's approach in the sense that it utilizes a system of differential equations (e.g., the backward SDEs) to analytically propagate the Itering density [3, 8]. At the same time, taking advantage of the SDE nature, the backward SDE Iter is highly scalable, which can be implemented efficiently on parallel computers.

Among the aforementioned approaches, the Bayesian Iter is widely used for solving the nonlinear Itering problem in practice. The state-of-the-art Bayesian Iter methods include the particle Iter [1, 16] and the ensemble Kalman Iter [12, 13]. Both the particle Iter and the ensemble Kalman Iter use samples (particles) to create an empirical distribution to describe the predicted Itering density (i.e. the prior) in the prediction step. In the update step, the particle Iter applies Bayesian inference to assign weights to particles and use weighted particles to represent the updated Itering density (i.e. the posterior). On the other hand, the ensemble Kalman Iter linearizes the observations and then adopts the Kalman update in the Kalman Iter method to derive an updated Itering density. Since the Kalman Iter is designed for linear problems, in the case that the optimal Itering problem is highly nonlinear, the ensemble Kalman Iter does not provide accurate estimates for the target state [29, 30]. The major drawback of the particle Iter is the degeneracy issue [21, 27]. When the observational data lies on the tail of the predicted Itering density, only very few particles will receive high likelihood weights in the Bayesian inference procedure, which significantly reduces the effective particle size in the particle Iter.

In addition to the methodology of using particles to propagate the state process, another approach that can transport the probability density forward in time is to solve the Fokker-Planck equation, which is a parabolic type particle differential equation (PDE). Although the PDE-based Fokker-Planck approach analytically formulates the propagation of the state model, solving a PDE in high dimensional state space is computationally expensive, which makes PDE-based optimal Itering solvers difficult to be practically applied.

In this work, we will develop a novel kernel method to efficiently solve the Fokker-Planck equation, and the kernel approximated solution for the Fokker-Planck equation will be used as our estimate for the predicted Itering density in the prediction step. Then, we will adopt Bayesian inference to incorporate the observational data into the kernel approximated Itering density.

Kernel method recently attracted extensive attentions in machine learning and function approximation [15, 18]. When solving the optimal Itering problem, the target function that we approximate with kernels is the Itering density, which is a probability density function (PDF). In many scenarios in the optimal Itering problem, the Itering density appears to be a bell-shaped function. This makes kernel method (especially with Gaussian type kernels) an effective way to construct approximations for the target Itering density [2]. Since optimal Itering is often used to solve practical application problems in real time, efficiency of an optimal Itering method is essential. In this paper, we will introduce an operator decomposition method to decompose PDF propagation in the Fokker-Planck equation into a linear component and a nonlinear component. The linear component of propagation can be analytically derived, and the nonlinear component needs to be carried out numerically. Numerical solver for the nonlinear component in the Fokker-Planck equation will be formulated as an optimization problem, which aims to determine kernel parameters that describe the nonlinear propagation of the Itering density. To implement the optimization procedure efficiently, we will introduce a boosting algorithm [23] to adaptively generate kernels to capture the

main features of the state distribution. This allows us to use minimum amount of active kernels to characterize the Itering density, which will be used to estimate the target state.

The rest of this paper is organized as follows. In Section 2, we introduce some preliminaries that we need to design the PDE-based adaptive kernel method for solving the optimal Itering problem. Then, we shall give a detailed description for our adaptive kernel method in Section 3. Numerical examples that validate the effectiveness of the kernel approach in solving the optimal Itering problem and comparison experiments will be presented in Section 4. Finally, summary and concluding remarks will be given in Section 5.

2 Preliminaries

In this section, we provide the preliminaries to formulate our adaptive kernel method for solving the optimal Itering problem. We shall first briefly introduce the optimal Itering problem. Then, we will discuss one of the most important optimal Itering approaches, i.e., the Bayesian Iter, and we will describe the mathematical framework of the adaptive kernel method as a Bayesian Iter type approach.

2.1 The optimal Itering problem

In the optimal Itering problem, we consider the following stochastic dynamical system in the form of a stochastic differential equation (SDE) in the probability space $(\Omega; \mathcal{F}; \mathcal{P})$

$$dX_t = b(t; X_t)dt + \sigma_t dW_t; \quad (1)$$

where $b : \mathbb{R}^+ \times \mathbb{R}^d \rightarrow \mathbb{R}^d$ is the drift coefficient, $\sigma : \mathbb{R}^+ \times \mathbb{R}^d \rightarrow \mathbb{R}^{d \times d}$ is the diffusion coefficient of the SDE, W is a standard d -dimensional Brownian motion under \mathcal{P} , and the $\sigma_t dW_t$ term is a standard Itô type stochastic integral, which brings additive noises to the dynamical model. The d -dimensional stochastic process $X := (X_t)_{t \geq 0}$ is called the 'state process', which represents the state of the dynamical model. In order to estimate the state of X_t when the true value of X_t is not available, we collect partial noisy observational data for X_t , denoted by Y_t , which is denoted by

$$Y_t = h(X_t)dt + dB_t; \quad (2)$$

where $h : \mathbb{R}^d \rightarrow \mathbb{R}^l$ is an observation function that measures the state of X_t and B is another Brownian motion independent of W with covariance R at any given time t . The stochastic process Y is often called the 'observation process'.

The goal of the optimal Itering problem is to find the best estimate for \hat{X}_t given the observational information Y_t , where $\mathcal{Y}_t := (Y_s; 0 \leq s \leq t)$ is the σ -algebra generated by the observation process Y , and \hat{X}_t is a given test function. In mathematics, the best estimate for \hat{X}_t is denoted by the 'optimal Iter', denoted by \hat{X}_t , which is the conditional expectation of X_t , i.e.

$$\hat{X}_t := E[\hat{X}_t | \mathcal{Y}_t]; \quad (3)$$

In this paper, we focus on the case that f (in the state process) and/or h (in the observation process) are nonlinear functions. The linear Itering problem is well-solved by the Kalman Iter (except for the extremely high dimensional cases). To solve the nonlinear optimal Itering problem, the standard approach aims to estimate the conditional probability of the state, i.e. $P(X_t | Y_t)$, which is also called the 'Itering density'. Then, we can calculate the conditional expectation in Eq. (3) through the integration formula

$$E[\hat{X}_t | \mathcal{Y}_t] = \int_Z \hat{X}_t(x) P(x | Y_t) dx;$$

In what follows, we will introduce the Bayesian Iter, which provides a two-step procedure to estimate the Itering density $P(X_t | Y_t)$ recursively.

2.2 The recursive Bayesian Iter

The Bayesian Iter recursively estimates the target state X_t on a sequence of discrete time instants $0 = t_1 < t_2 < \dots < t_n < \dots$, and the Bayesian Iter framework is composed of two steps: the prediction step and the update step.

Prediction step.

Assume that the Itering density $p(X_t | Y_{t_n})$ is given at time t_n . In the prediction step, we propagate the Itering density from time t_n to time t_{n+1} without usage of the new observational data $Y_{t_{n+1}}$, and we want to get the predicted Itering density, i.e. $p(X_{t_{n+1}} | Y_{t_n})$.

There are three major methods to achieve this goal:

The first method is designed to find the predicted Itering density through the following Chapman-Kolmogorov formula

$$p(X_{t_{n+1}} | Y_{t_n}) = \int p(X_{t_{n+1}} | X_{t_n}) p(X_{t_n} | Y_{t_n}) dX_{t_n};$$

where $p(X_{t_{n+1}} | X_{t_n})$ is the transition probability of the state equation (1) that transports the previous Itering density $p(X_t | Y_{t_n})$ from t_n to t_{n+1} . The above Chapman-Kolmogorov formula is often carried out by independent sample simulations, and it's the primary prediction technique in particle-based optimal Itering methods, such like the particle Iter and the ensemble Kalman Iter. As a result of the particle propagation of the Itering density, one may obtain an empirical representation for the predicted Itering density.

The second method utilizes the following (time-inverse) backward stochastic differential equation (BSDE) to generate the predicted Itering density:

$$P_{t_{n+1}} = P_{t_n} \int_{t_n}^{t_{n+1}} \sum_{i=1}^d \frac{\partial b_i}{\partial x_i}(X_t) P_t dt - \int_{t_n}^{t_{n+1}} Q_t dW_t; \quad P_{t_n} = p(X_{t_n} | Y_{t_n});$$

where X_t is the state process, and the $\int_{t_n}^{t_{n+1}} dW_t$ is a backward Itô integral, which is an Itô type stochastic integral integrated backwards [7, 24]. The solutions of the above BSDE is a pair (P, Q) , where Q is the martingale representation of P with respect to W [11]. We refer to [4, 8, 9] for more details of the BSDE method.

The third method, which is also the method that we are going to discuss in this paper, describes the propagation of the Itering density through the following Fokker-Planck equation over the time interval $[t_n; t_{n+1}]$

$$\frac{\partial p(x; t)}{\partial t} = \sum_{i=1}^d \frac{\partial}{\partial x_i} b_i(x; t) p(x; t) + \sum_{i,j=1}^d \frac{\partial^2}{\partial x_i \partial x_j} D_{i,j} p(x; t) \quad (4)$$

with initial condition $p(x; t_n) = p(X_{t_n} = x | Y_{t_n})$, where b_i is the i -th component of the drift function b , and the matrix D is dened by $D = \frac{\partial^2}{\partial x_i \partial x_j}$. As a result, solution $p(x; t_{n+1})$ of the Fokker-Planck equation (4) gives us the desired predicted Itering density $p(X_{t_{n+1}} = x | Y_{t_n})$.

Update step.

With an approximation for the predicted Itering density (obtained through either one of the aforementioned method), the Bayesian Iter updates the predicted Itering density to the (posterior) Itering density via the following Bayesian inference formula

$$p(X_{t_{n+1}} | Y_{t_{n+1}}) = \frac{p(X_{t_{n+1}} | Y_{t_n}) p(Y_{t_{n+1}} | X_{t_{n+1}})}{p(Y_{t_{n+1}} | Y_{t_n})}; \quad (5)$$

where

$$p(Y_{t_{n+1}} | X_{t_{n+1}}) = \exp \frac{Y_{t_{n+1}} - h(X_{t_{n+1}})^2}{R} \quad (6)$$

is the likelihood function, and $p(Y_{t_{n+1}} | Y_{t_n})$ in the denominator normalizes the Itering density at the time instant t_{n+1} .

Then, we carry out the above prediction-update procedure recursively to propagate the Itering density $p(X_t | Y_t)$ over time.

3 Adaptive Kernel Approximation Approach

In this paper, we solve the Fokker-Planck equation (4) numerically to generate an approximation for the predicted Itering density $p(X_{t_{n+1}} | Y_{t_n})$, and we apply the Bayesian inference (5) to calculate the estimated (posterior) Itering density $p(X_{t_{n+1}} | Y_{t_{n+1}})$. In what follows, we shall give detailed discussions on the computational framework that we construct to apply the adaptive kernel approximation method to solve the optimal Itering problem.

3.1 Prediction through Fokker-Planck equation

For convenience of presentation, we denote

$$L_b; p_t := \sum_{i=1}^{X^d} \frac{\partial b_i(x; t) p(x; t)}{\partial x_i} + \sum_{i,j=1}^{X^d} \frac{\partial^2 D_{i,j}}{\partial x_i \partial x_j} p(x; t);$$

and we call L_b the the Fokker-Planck operator in this paper. The Prediction step in our adaptive kernel approximation approach will focus on deriving a numerical solver for the Fokker-Planck equation

$$\frac{\partial p(x; t)}{\partial t} = L_b; p; \quad (7)$$

and the numerical solution to Eq. (7) will be our approximation to the predicted Itering density, which will be combined with the likelihood function to generate an estimated posterior Itering density.

Numerical methods for solving parabolic type PDEs, such like the Fokker-Planck equation, have been extensively studied [10, 17, 22, 31]. However, when the dimension of the problem is high, solving Eq. (7) becomes an extremely expensive computational task [33]. The primary challenge in obtaining numerical solutions to the Fokker-Planck equation is how to eiently and eectively implement spatial dimensional approximation. Traditional mesh-based numerical methods, such like nite dierence methods and nite element methods typically utilize polynomial approximations to describe solutions of the equation. However, due to the so-called \curse of dimensionality", the computational cost of solving the Fokker-Planck equation increases exponentially as the dimension of the problem increases.

In this work, we adopt the following kernel approximation scheme to approximate the solution of the Fokker-Planck equation

$$p(x; t_n) = \sum_{k=1}^K \phi_k(x); \quad (8)$$

where K is the total number of kernels, and

$$\phi_n(x) := \exp \frac{1}{2} (x - \mu_n)^T \Sigma_n^{-1} (x - \mu_n) \quad (9)$$

is a Gaussian type kernel function, which is parameterized by weight h^k , mean μ^k and covariance matrix Σ^k . Numerical analysis results have been derived to verify that the kernel approximation scheme (8) is capable of generating accurate approximations to wide range of function when the number of kernels K is sufficiently large [19, 26, 28]. The reason that we pick Gaussian type kernels to approximate the target function p is that p is the Itering density, which describes a conditional probability distribution. In many situations in the optimal Itering problem, the Itering density is a bell-shaped function, which can be effectively approximated by Gaussian type functions.

Then, assuming that we have a kernel approximation p_n for the Itering density $p(X_t | Y_t)$, we introduce the following temporal discretization scheme to solve the Fokker-Planck equation

$$p_{n+1} = p_n + L_b p_n t_n; \quad (10)$$

where $t_n := t_{n+1} - t_n$ is the time step-size, and p_{n+1} is a kernel approximation for the predicted Itering density $p(X_{t_{n+1}} | Y_{t_n})$. Given kernels $f^k g_{n+1}^k$ for the approximated Itering density p_n and the approximation scheme

$$p_n := \sum_{k=1}^K f^k g_n^k(x); \quad (11)$$

we can rewrite Eq. (10) as

$$p_{n+1} = \sum_{k=1}^K f^k g_{n+1}^k(x) + t_n L_b; \quad \sum_{k=1}^K f^k g_n^k(x); \quad (12)$$

and we let

$$p_{n+1} := \sum_{k=1}^K \tilde{g}_{n+1}^k;$$

where $f^k g_{n+1}^k$ is a set of kernels that approximates p_{n+1} . We can see from the temporal discretization scheme (12) that obtaining an approximation p_{n+1} for the predicted Itering density $p(X_{t_{n+1}} | Y_{t_n})$ is equivalent to finding parameters for kernels $f^k \sim \tilde{g}_{n+1}^k$. Note that the kernels $f^k g_{n+1}^k$ on the right hand side of Eq. (12) are Gaussian (as introduced in Eq. (9)). Hence the Fokker-Planck operator part, i.e. $L_b = \sum_{k=1}^K \tilde{g}_{n+1}^k(x)$ can be derived analytically. In this way, we transfer the computational cost of solving the Fokker-Planck equation from high dimensional spatial approximation to solving an optimization problem for kernel parameters.

Since the target function for kernel approximation is a PDF, a relatively small number of Gaussian kernels may be sufficient to provide a reasonable description for the Itering density. On the other hand, solving the Fokker-Planck equation through Eq. (12) suffers from the stability issue. When values of the drift function b in the state equation Eq. (1) are large (or the time step-size t_n is large), the drift term will generate a strong force that pushes the Itering density far from its current location. However, due to exponential decay of Gaussian tails, which would typically cause local behaviors of Gaussian kernels, the Itering density approximated by the kernel approximation scheme (11) can only be transported to a limited distance. This can make our method difficult to track targets driven by state equations with large drift terms.

In the following subsection, we shall introduce an operator decomposition method to alleviate the above stability issue.

3.2 Operator decomposition

The central idea of our operator decomposition method is to divide the Fokker-Planck operator into a drift operator and a diffusion operator. Then, we further decompose the drift operator into a

linear component and a nonlinear component, and we provide analytical and numerical methods to characterize the linear component and the nonlinear component separately.

Before we introduce our decomposition strategy, we would like to point out the following facts of the Fokker-Planck operator:

Fact 1. Given a PDF p , in the case that the diusion coecient does not contain state X , we have

$$L_b; p = L_{b,0}p + L_0;p:$$

Fact 2. The Fokker-Planck operator $L_b;$ is linear, i.e., for two constants a, b and two PDFs p, q , we have

$$L_b;[ap + bq] = aL_b;p + bL_b;q:$$

Therefore, the kernel approximated Itering density under the Fokker-Planck operator can be written as

$$L_b;p_n = \sum_{k=1}^{X^K} L_{b,n}(x)^k$$

and the right hand side of Eq. (12) becomes

$$\sum_{k=1}^{X^L} L_{b,n}^k(x) + t_n \sum_{k=1}^{X^K} L_{b,n}^k(x) = \sum_{k=1}^{X^K} L_{b,n}(x) + t_n L_{b,n}(x) : n \quad (13)$$

The linearity of the Fokker-Planck operator allows us to discuss the propagation of each Gaussian kernel separately.

In light of Fact 1, we can handle the drift term rst and then incorporate diusion into the state propagation. Fact 2 allows us to discuss state propagation kernel-by-kernel when necessary.

In this work, instead of deriving the operator decomposition method directly under the numerical PDE framework, we rst switch back to the state equation, and we consider the following Euler-Maruyama scheme that propagates each kernel n through the state equation

$$X_{n+1}^k = X_n^k + b(t_n; X_n^k)t_n + \epsilon_{t_n} W_{t_n}; \quad k = 1; 2; \dots; K; \quad (14)$$

where the initial state X_n^k , i.e. X^k follows the distribution of the k -th Gaussian kernel, and $W_t := W_t - W_{t_n} \sim N(0; t_n I_d)$. In this way, by combining distributions for X_{n+1}^k obtained through the discretized SDE scheme (14), we get a description for the predicted Itering density, which can also be considered as an approximation for the right hand side of Eq. (13).

To address the stability issue through operator decomposition and to transport Gaussian kernels eectively to the next time step, we introduce a linear approximation to the (nonlinear) drift function, and we denote it by $b^L(t_n; X_n^k) := A X_n^k + \epsilon$, where $A \in \mathbb{R}^{dd}$ and $\epsilon \in \mathbb{R}^d$. The linear operator b^L will be determined as the best linear approximation to b in the sense of least square. In other words, we aim to nd A and ϵ that will minimize the mean square error between the original drift function b and the linear approximation b^L , i.e.

$$\min_{A, \epsilon} E \left[b(t_n; X_n^k) - (A X_n^k + \epsilon) \right]^2 : \quad (15)$$

To maintain the nonlinearity of the state dynamics, we introduce a residual function $b^N(t_n; X_n^k) := b(t_n; X_n^k) - b^L(t_n; X_n^k)$ that models the nonlinear component of b . Hence, the drift function is decomposed into a linear component b^L and a nonlinear component b^N , i.e., $b(t_n; X_n^k) = b^L(t_n; X_n^k) + b^N(t_n; X_n^k)$.

$b^N(t_n; X_n^k)$, and the Euler-Maruyama scheme for the state equation can be interpreted as

$$X_{n+1} = X_n + b^L(t_n; X_n) + b^N(t_n; X_n)t_n + W_{t_n};$$

In what follows, we will introduce a three-step operator decomposition procedure to compute the predicted Itering density p_{n+1} .

In the first step, we only transport the Itering density via the linear component b^L . Specifically, we implement the following scheme

$$\begin{aligned} X_{n+1}^{k;L} &:= X_n^k + b^L(t_n; X_n) t_n \\ &= (A t_n + I) X_n + t_n \end{aligned} \quad (16)$$

to propagate the Itering density at the time step t_n , and we let

$$T(X_n^k) := (A t_n + I) X_n + t_n$$

be the operator that formulates the linear component of the drift function, i.e. $X_{n+1}^{k;L} = T(X_n^k)$. Note that a linear function will map a Gaussian distribution to a Gaussian distribution. Since X_n^k follows a Gaussian distribution, $X_{n+1}^{k;L}$ will also follow a Gaussian distribution, which can be determined by the linear operator $T()$, and we denote the distribution for $X_{n+1}^{k;L}$ by $p_{n+1}^{k;L}$.

In the second step, we incorporate the nonlinear component b^N of the drift function to the Itering density so that both the linear and the nonlinear components are considered in the Itering density propagation. Since b^N does not linearly propagate $X_{n+1}^{k;L}$, we can not derive a Gaussian kernel directly from $p_{n+1}^{k;L}$ to obtain a kernel that describes the nonlinear component of the drift. In order to derive a kernel approximation for the predicted Itering density, which have considered the nonlinear component of the drift, we define an operator

$$b^{N;T}(t_n; X_{n+1}^{k;L}) := b^N(t_n; T^{-1}(X_{n+1}^{k;L})) = b^N(t_n; X_n^k);$$

Then, with Gaussian distributions $f p_{n+1}^{k;L} g_{k=1}^K$ that describe random variables $f X_{n+1}^{k;L} g_{k=1}^K$ (introduced in Eq. (16)), we introduce the following PDE type solver to calculate a distribution \hat{p}_{n+1} dened by

$$\hat{p}_{n+1} = \sum_{k=1}^K p_{k+1}^{k;L} + L_{b^{N;T};0} p_{k+1}^{k;L} t_n; \quad (17)$$

where $L_{b^{N;T};0}$ is a Fokker-Planck operator with drift $b^{N;T}$, and the diusion is chosen as 0. The PDF \hat{p}_{n+1} on the left hand side of Eq. (17) is an approximation for the predicted Itering density before incorporation of the diusion term, and we use kernel approximation scheme to represent \hat{p}_{n+1} , i.e.

$$\hat{p}_{n+1} = \sum_{k=1}^K \hat{f}_{n+1}^{k;L}(x); \quad (18)$$

where $\hat{f}_{n+1}^{k;L} g_{k=1}^K$ is a set of Gaussian kernels, and we will introduce the procedure to determine parameters for $\hat{f}_{n+1}^{k;L} g_{k=1}^K$ in the next subsection.

Finally, in the third step we add diusion back to the predicted Itering density. Since we assume that the state dynamics are perturbed by additive noises in this work, for each Gaussian kernel $\hat{f}_{n+1}^{k;L}$ that approximates \hat{p}_{n+1} in Eq. (18), we can simply introduce the extra diusion information by adding t_n to the covariance of $\hat{f}_{n+1}^{k;L}$ and get a kernel $\hat{f}_{n+1}^{k;L}$ to approximate the predicted

Itering density at time stage t_{n+1} . As a result, we obtain the kernel approximation for the predicted Itering density as follows

$$p_{n+1} = \sum_{k=1}^K \tilde{p}_{n+1}^k : \quad (19)$$

In the above three-step procedure, we can see that the first step and the third step can be implemented analytically, and the second step incorporates the nonlinear behavior of the dynamical model, which needs an optimization procedure to determine kernel parameters. In what follows, we will introduce an adaptive boosting algorithm to achieve this goal.

3.3 Adaptive boosting algorithm for kernel training

Recall that each kernel in Eq. (18) is Gaussian and has the expression

$$\tilde{p}_{n+1}^k(x) = \frac{1}{2} \exp \left(-\frac{1}{2} (x - \tilde{\mu}_{n+1}^k)^2 \right) \left(\frac{1}{2} \right)^{k-1} (x - \tilde{\mu}_{n+1}^k)^k$$

Our optimization procedure aims to find kernel parameters $f(\tilde{\mu}_{n+1}^k; \tilde{\sigma}_{n+1}^k, \tilde{\sigma}_{n+1}^k g_{k=1}^K)$ so that the left hand side of Eq. (17), which is determined by $f(\tilde{\mu}_{n+1}^k; \tilde{\sigma}_{n+1}^k g_{k=1}^K)$, will be equal to the right hand side, which is dened by the linear transformed Gaussian distributions $f(p_{n+1}^k; L_{b^{n+1}; 0} p_{n+1}^k t_n)$. We denote

$$g_{n+1} := \sum_{k=1}^K p_{n+1}^k L_{b^{n+1}; 0} p_{n+1}^k t_n \quad (20)$$

for convenience of presentation. Since $f(p_{n+1}^k; L_{b^{n+1}; 0} p_{n+1}^k t_n)$ are Gaussian functions, g_{n+1} dened in Eq. (20) can be derived analytically.

In this work, instead of finding all the kernel parameters at the same time by solving a large scale optimization problem, we adopt the so-called 'boosting algorithm', which sequentially minimizes the approximation error. Specifically, we introduce the Boosting Algorithm in Table 1 to determine the parameter set $f(\tilde{\mu}_{n+1}^k; \tilde{\sigma}_{n+1}^k, \tilde{\sigma}_{n+1}^k g_{k=1}^K)$.

The boosting algorithm introduced in Table 1 will adaptively generate kernels, and this adaptive kernel approximation procedure allows us to capture more important features (modes) in the Itering density. Also, the Gaussian tails of the kernels can provide reasonable description for low density regions in the Itering density, which will make our method stable.

3.4 Bayesian update for Itering density

To incorporate the observational information to the predicted Itering density, we apply Bayesian inference (5). Since the predicted Itering density is described by multiple kernels, we apply Bayesian inference to each Gaussian kernel and obtain a kernel for the posterior Itering density. Specifically, for each state point x , let

$$p_{n+1}^{k; \text{post}}(x) = \tilde{p}_{n+1}^k(x) p(Y_{t_{n+1}} | x);$$

where $p(Y_{t_{n+1}} | x)$ is the likelihood function introduced in Eq. (6) with a given state position $X_{t_{n+1}} = x$ and \tilde{p}_{n+1}^k is a Gaussian kernel in Eq. (19) that approximates the predicted Itering density p_{n+1} . In this way, the entire posterior Itering density is approximated by

$$p_{n+1}^{\text{post}} = \sum_{k=1}^K p_{n+1}^{k; \text{post}} : \quad (21)$$

Table 1: Boosting Algorithm

Algorithm 1: Boosting algorithm to adaptively generate kernels.

Initialize the kernel approximation as $\phi_{n+1}(x) = 0$; define target function g_{n+1} through Eq. (20); set global approximation tolerance tol.

while $k = 1; 2; ; K$, do

- Generate M global state samples, denoted by $f_{n+1}^{(m)} g_{m=1}^M$, from the kernel approximated distribution based on $f_{n+1}^{k;L} g_{k=1}^K$.
- Evaluate the approximation error on each state sample and calculate $e_m := g(\hat{x}_m) - \phi_{n+1}(\hat{x}_m)$ for $m = 1; 2; ; M$.
- Compute global error $E_g = \frac{1}{M} \sum_{m=1}^M (e_m)^2$. If $E_g < \text{tol}$, break and set weights for other kernels 0, i.e. $w_j = 0$, $k < j \leq K$. Otherwise, continue.
- Locate the state sample with the largest approximation error, i.e. $\text{nd } m \text{ s.t. } e_m = \max_m e_m$.
- Generate a Gaussian kernel \hat{g}_{n+1}^k centered at the state sample that suffers from the largest error, i.e. choose the initial guess for the mean as $\hat{x}_{n+1}^k = \hat{x}_m$.
- Solve a local optimization problem to determine the weight and covariance for the kernel \hat{g}_{n+1}^k by comparing values of \hat{g}_{n+1}^k (treated as the left hand side of Eq. (17)) with g_{n+1} on locally generated state samples near the kernel center \hat{x}_{n+1}^k .
- Add the locally trained kernel \hat{g}_{n+1}^k to kernel approximation ϕ_{n+1} , i.e. let $\phi_{n+1} = \phi_{n+1} + \hat{g}_{n+1}^k$.

end while

Note that each kernel \hat{g}_{n+1}^k that we use to approximate the overall posterior Itering density p_{n+1}^{post} may not be Gaussian due to the nonlinear observation. To derive an approximation by Gaussian kernels, we train a new set of Gaussian kernels to describe the posterior Itering density. Specifically, we introduce a kernel approximation

$$p_{n+1} := \sum_{k=1}^K \hat{g}_{n+1}^k;$$

and we let p_{n+1} be an approximation to the approximated posterior Itering density p_{n+1}^{post} , i.e. p_{n+1} is the normalized version of \hat{g}_{n+1}^k . To this end, we adopt the same Boosting Algorithm framework introduced in Table 1 again to adaptively generate Gaussian kernels $f_{n+1}^k g_{k=1}^K$, and a normalization procedure will be implemented to $f_{n+1}^k g_{k=1}^K$ to make p_{n+1} a PDF.

3.5 Summary of the algorithm

In this subsection, we summarize our algorithm in Table 2.

Table 2: Summary of the algorithm

Algorithm 2: Algorithm of the adaptive kernel method.

Initialize the Itering density p_0 with kernels $f^k g_{k=1}^K$.

For $n = 0; 1; 2; 3;$

Prediction Step:

- Generate $f^{k,L} g_{k=1}^K$ through Eq. (16) to incorporate the linear component (determined through Eq. (15)) of the drift function.
- Use the Boosting Algorithm described in Table 1 to incorporate the nonlinear component of the drift function and generate Gaussian kernels $f^{k,A} g_{k=1}^K$ from g_{n+1} (dened in Eq. (20)) to approximate p_{n+1} .
- Add $t_{n+1} > t_{n+1}$ the covariance of each Gaussian kernel g_{n+1} to incorporate state diusion and get the kernel \tilde{g}_{n+1}^k to approximate the predicted Itering density p_{n+1} via Eq. (19).

Update Step

- Carry out Bayesian inference to generate a posterior Itering density p_{n+1}^{post} defined in Eq. (21).
- Carry out Boosting Algorithm in Table 1 again to obtain a Gaussian kernel approximation $p_{n+1} = f_{n+1}^k g_{k=1}^K$ to approximate p_{n+1}^{post} .
- Normalize $f_{n+1}^k g_{k=1}^K$ to make p_{n+1} a PDF, and p_{n+1} is the estimated Itering density at time stage $n + 1$.

end

4 Numerical Experiments

In this section, we present three numerical examples to demonstrate the performance of our adaptive kernel method for solving the optimal Itering problem. We rst present a demonstration example to show how our adaptive kernel approximation method will adaptively capture the main features of the Itering density in state propagation. In the second example, we solve a benchmark optimal Itering problem, i.e. the bearing-only tracking problem, and we compare our method with the particle Iter method [25] and the ensemble Kalman Iter method [13] to show accuracy and eciency of the adaptive kernel method. Then, in Example 3 we solve a high dimensional Lorenz-96 tracking problem, which is a well-known challenging optimal Itering problem due to the chaotic behavior of the state model.

4.1 Example 1: Demonstration for adaptive kernel approximation.

We use the rst numerical example to demonstrate the performance of our adaptive kernel approximation method in propagating state dynamics. Instead of solving an entire optimal Itering problem, we only present the eectiveness of our method in transporting a probability distribution through the Fokker-Planck equation, and the primary computational eort of our approach lies on using kernels

to approximate the Fokker-Planck operator. Since the Itering density is approximated by Gaussian kernels, Gaussian type diusions can be directly added to the target distribution. Therefore, in this example we shall focus on the drift part of the Fokker-Planck operator, i.e. $L_{b;0}$, and the drift term is dened by the following 2D function:

$$b(x_1; x_2) = x_1^2 + \frac{3}{4} x_1 x_2 + \frac{1}{32} :$$

For convenience of presentation, we consider state propagation in time with step-size be 1. Then, we choose the initial distribution as a standard Gaussian distribution, denoted by ρ_0 , and we apply the drift operator $L_{b;0}$ to ρ_0 . In this way, the target function that we try to use our kernel method to approximate is $F := \rho_0 + L_{b;0}\rho_0$. In Figure 1, we present the original target function F driven by the operator $L_{b;0}$ on left, and the linear approximation for function F obtained by the linear transportation Eq. (16) is presented on the right. From this gure, we can see that the linear component can roughly capture the main feature of the target function.

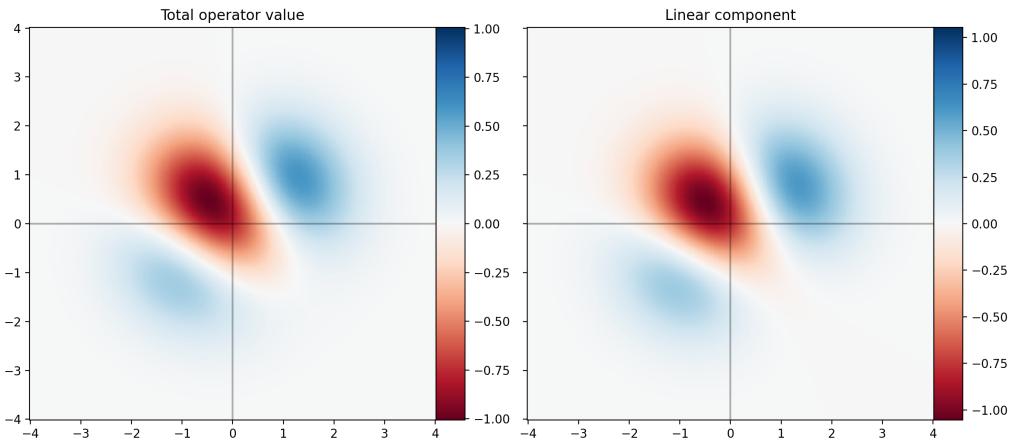


Figure 1: Example 1. Linear component in describing the Fokker-Planck operator

To demonstrate the performance of kernel method in approximating the nonlinear component (described in Eq. (17)) of the operator and the eectiveness of the adaptive boosting algorithm, we compare the analytically derived true nonlinear component of the function with the approximated nonlinear component in Figure 2. The subplot on the left shows the true function that we aim to approximate, and the subplot on the right is our approximated function by using the boosting algorithm introduced in Table 1. We use blue-to-red colors to represent function values, and we can see from this gure that the boosting algorithm can accurately capture the true function, which describes the nonlinear component of the Fokker-Planck operator.

To show more details of the performance of the adaptive kernel construction in the boosting algorithm, we present the approximation errors after tting up to 6 kernels in Figure 3. From this gure, we can see that by using only one kernel to describe the nonlinear component of the Fokker-Planck operator, the main part of the function in the region $[-1; 0] \cup [1; 1]$ (presented in the left subplot in Figure 2) is well tted, and two remaining features that represent two tails in the function (plotted in Figure 2) need to be tted. Then, by adding the second and the third kernels, we can successfully approximate those two tails and get low overall tting errors. As more and more kernels are added, we get rid of higher error regions one-by-one. As a result, we obtain more and more accurate approximations to the nonlinear component of the drift operator.

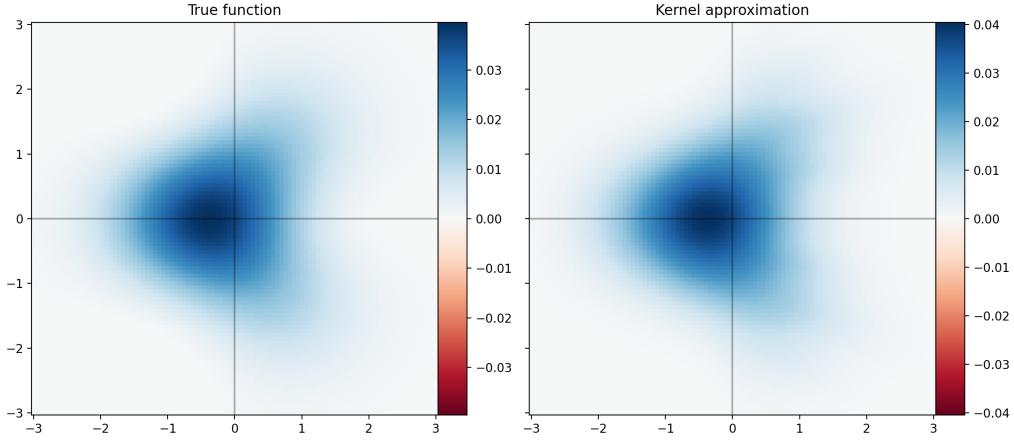


Figure 2: Example 1. Accuracy of approximation obtained by the boosting algorithm.

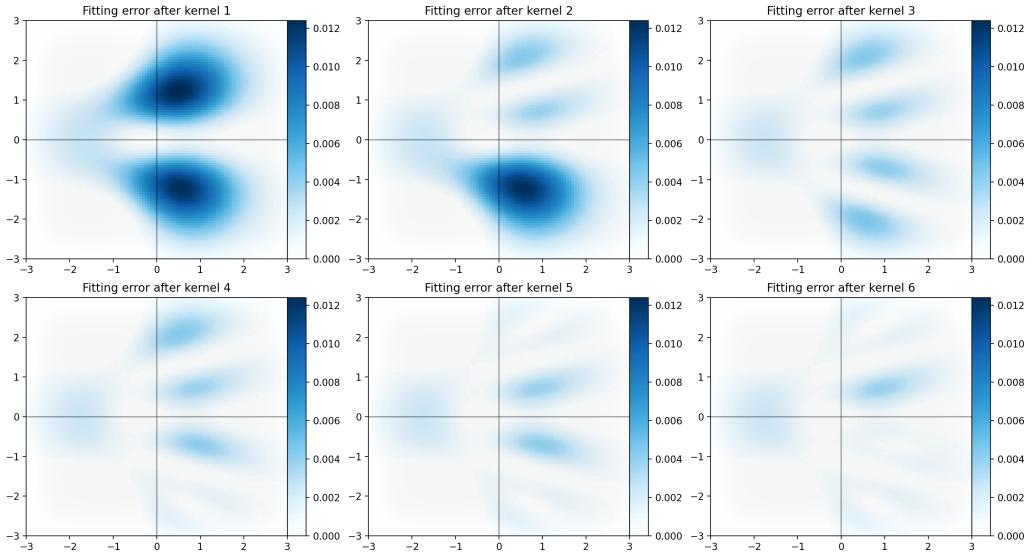


Figure 3: Example 1. Performance of the adaptive boosting algorithm in reducing approximation errors in fitting the nonlinear component of the operator.

4.2 Example 2: Bearing-only tracking

In this example, we solve the bearing-only tracking problem, which is a benchmark optimal filtering problem in practice. Specifically, we aim to track a moving target driven by the following state dynamics

$$dX_t = \begin{pmatrix} 2 & 3 & 2 & 0 & 0 & 0 & 3 & 2 \\ 6 & v_t^1 & 6 & 0 & 2 & 0 & 0 & dW_t^1 \\ 4 & v_t^2 & 4 & 0 & 0 & 3 & 0 & dW_t^2 \\ 0 & 5 & dt + & 0 & 0 & 0 & 0 & dW_t^3 \\ 0 & 0 & & 0 & 0 & 0 & 0 & dW_t^4 \end{pmatrix}; \quad (22)$$

where $X_t = [x_t^1; x_t^2; v_t^1; v_t^2]^>$, $[x_t^1; x_t^2]^>$ describes the 2D location of the target, and v_t^1, v_t^2 are the velocities in x_1 and x_2 directions, respectively. $W_t = [W_t^1; W_t^2; W_t^3; W_t^4]$ is a 4D Brownian motion that brings uncertainty to the state model, which is driven by the diusion coecient

$$:= \begin{bmatrix} 1 & 0 & 0 & 0 \\ 6 & 0 & 2 & 0 \\ 4 & 0 & 0 & 3 \\ 0 & 0 & 0 & 4 \end{bmatrix}.$$

In order to estimate the location of the target, we place two detectors on dierent observation platforms to collect bearing angles as observational data. Specically, the observational data is given by the following observational function

$$Y_t^i = \arctan \frac{x_t^2 - x_{i\text{-platform}}^2}{x_t^1 - x_{i\text{-platform}}^1} + \iota_i, \quad i = 1, 2; \quad (23)$$

where $(x_{i\text{-platform}}^1; x_{i\text{-platform}}^2)^>$ gives the location of the i -th platform, and ι_i is the observation noise of the i -th detector.

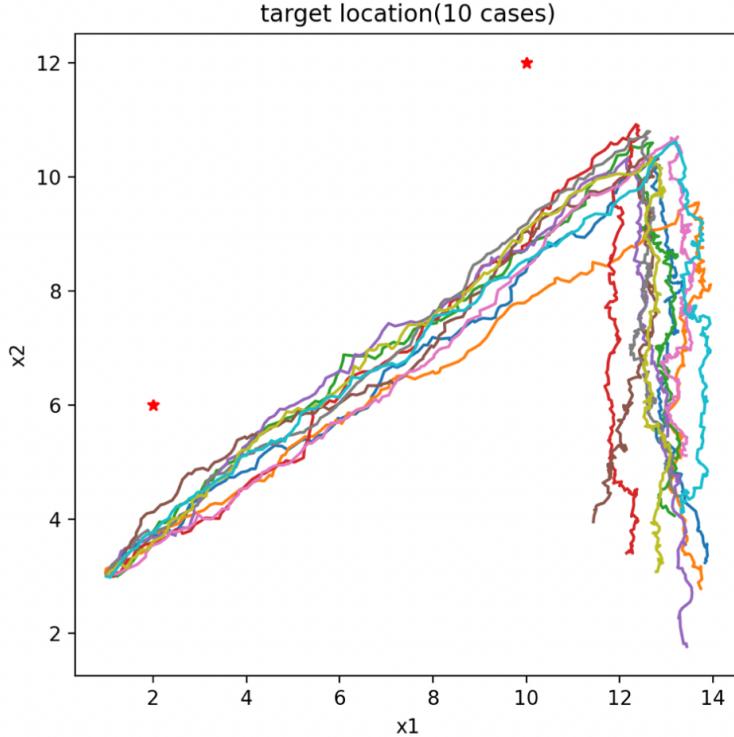


Figure 4: Example 2. Demonstration of 10 sample trajectories of the target.

In this example, we track the target over the time period $t \in [0; 3]$ with initial state $X_0 = [1; 3; 10; 6]^>$, and we let $t = 0:01$, i.e. we track 300 time steps. The diusion coecient is chosen as $1 = 2 = 0:5$, $3 = 4 = 0:3$, and we locate two platforms at $(2; 6)^>$ and $(10; 12)^>$, respectively. To demonstrate the stability of our method compared with other state-of-the-art methods, we assume that there's an unexpected turn in the target moving direction at the time instant $t = 1:2$, which would challenge the robustness of optimal Itering methods. In Figure 4, we plot 10 sample target

trajectories (by using different colors), and we mark the observation platforms with red stars. From this figure, we can see that the target is designed to move in front of the observation platforms and then it makes a sharp turn downward.

In Figure 5, we present a comparison experiment, in which we compare the tracking accuracy between our adaptive kernel method with two state-of-the-art optimal Itering methods, i.e. the ensemble Kalman Iter and the particle Iter. To implement our adaptive kernel method, we use up

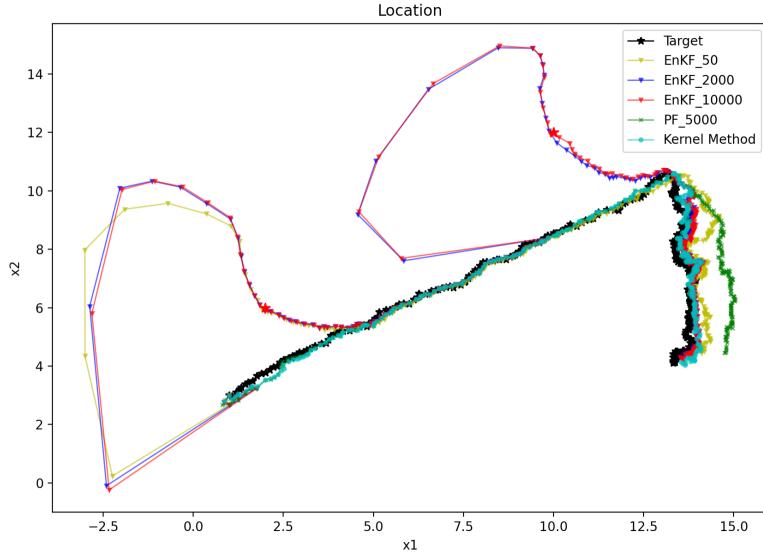


Figure 5: Example 2. Comparison of tracking performance in solving the bearing-only tracking problem.

to 20 kernels to approximate the Itering density, and active kernels are adaptively selected by the boosting algorithm (described in Table 1). For the ensemble Kalman Iter, we choose 50, 2;000 and 10;000 realizations of Kalman Iter samples to implement this tracking task. In the particle Iter, we use 5000 particles to generate empirical distributions for the Itering density. In the figure, we use the black curve (marked by stars) to represent a sample of real target trajectory and use other colored curves to represent the estimates obtained by various optimal Itering methods. The yellow, blue, and red curves (marked by triangles) are estimates for the target location obtained by using the ensemble Kalman Iter (EnKF) with 50, 2;000, and 10;000 realizations of Kalman Iter samples, respectively. The green curve (marked by crosses) gives the particle Iter (PF) estimates (obtained by using 5;000 particles). The cyan curve (marked by dots) describes the estimates obtained by our adaptive kernel method.

From this figure, we can see that the EnKF doesn't provide accurate estimates for the target location when the target is right below a detector { no matter how many realizations of samples we use in the EnKF. The poor performance of the EnKF is caused by the high nonlinearity of observational data (bearing angles introduced in Eq. (23)) when the target moves in front of detectors. For the PF, we can see that it provides accurate estimates until the sharp turn at the time instant $t = 1:2$. Then, the PF loses track of the target due to the degeneracy of particles when trying to adjust the change of the target location. On the other hand, the kernel method always keeps on track, and it gives accurate estimates all the time during the tracking period.

To further examine the performance of different optimal Itering methods in solving the bearing-only tracking problem (22)-(23), we repeat the above experiment 100 times and calculate the root mean square errors (RMSEs) of target tracking performance. The log scaled RMSEs of each method with respect to time are presented in Figure 6. From this figure, we can see that the adaptive kernel method (cyan curve marked by dots) has the lowest RMSEs, and it can provide good accuracy even after the sharp turn of the target. The PF (green curve marked by crosses) has low RMSEs at first. However, the errors increase dramatically at the turning point of the target trajectories. On the other hand, the EnKF estimates (yellow, blue and red curves marked by triangles) always suffer from low accuracy when the target passes the detectors. But the EnKF can recover quickly from inaccurate estimates, which indicates that the EnKF is a more stable method compared with the PF.

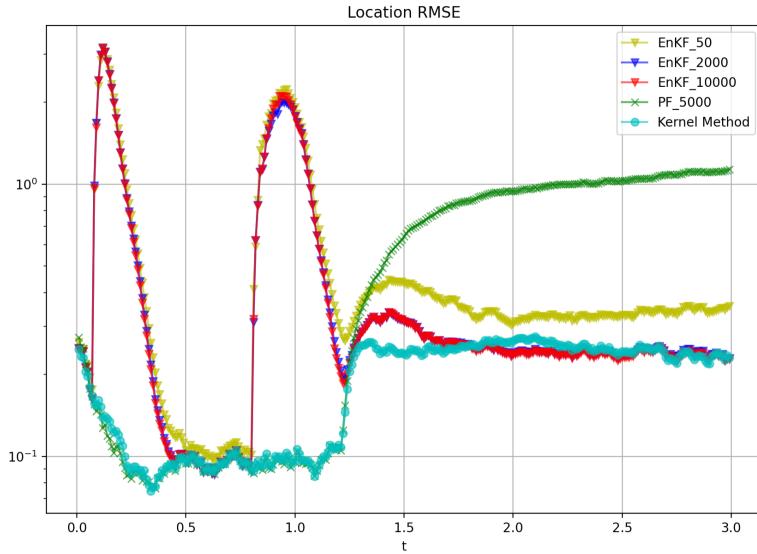


Figure 6: Example 2. Comparison of root mean square errors (RMSEs) with respect to time.

To summarize the general performance of each method, we present the accumulated RMSEs (the combined RMSEs over the tracking period) together with the CPU time of each method (average over the above 100 repeated tests) in Table 3. The CPU that we use is a AMD Ryzen 5 5600X

Table 3: Performance comparison

	EnKF 50	EnKF 2,000	EnKF 10,000	PF 5000	Kernel Method
Accumulated RMSEs	158:99	134:75	134:87	169:58	56:75
CPU time (seconds)	0:32	11	56	70	50

with 6 core 12 processing threads. We can see from this table that the PF has the lowest accuracy with the highest computational cost, which is mainly caused by the degeneracy of particles. The EnKF can solve the problem with very low computational cost. However, the accuracy of the EnKF does not improve much even we use a lot more realizations of Kalman Iter samples. The kernel

learning method, on the other hand, has much lower RMSEs compared with the EnKF and the PF with moderate cost.

4.3 Example 3: Lorenz-96 model

To examine the performance of the adaptive kernel method in solving high dimensional problems, in this example we solve the Lorenz-96 tracking problem, which is a benchmark high dimensional optimal Itering problem. The state model is given by the following stochastic dynamical system

$$\mathbf{x}_t^i = ((\mathbf{x}_t^{i+1} - \mathbf{x}_t^{i-2})\mathbf{x}_t^{i-1} - \mathbf{x}_t^i + \mathbf{F})dt + \mathbf{d}W_t^i; \quad i = 1, 2, \dots, d \quad (24)$$

where $\mathbf{X}_t = [\mathbf{x}_t^1; \mathbf{x}_t^2; \dots; \mathbf{x}_t^d]^T$ is the target state. In the Lorenz-96 model (24), we let $\mathbf{x}_t^1 = \mathbf{x}_t^d$, $\mathbf{x}_t^0 = \mathbf{x}_t^d$, $\mathbf{x}_t^1 = \mathbf{x}_t^{d+1}$, $\mathbf{W}_t = \mathbf{f}W_t^1; W_t^2; \dots; W_t^d$ is a d -dimensional Brownian motion, and $\mathbf{F} = [1; 2; \dots; d]^T$ is the diusion coecient. It is well-known that when $\mathbf{F} = 8$, the Lorenz-96 model has chaotic behavior, which makes the corresponding optimal Itering problem very challenging. In this example, we track the state \mathbf{X} of the Lorenz-96 model over the time period $t \in [0; 3]$, and we let $d = 10$. As a commonly used scenario when tracking the Lorenz-96 model, we simulate the Lorenz-96 model with time step-size $t = 0:001$, and we assume that we receive data of the state with time step-size $t = 0:1$. Therefore, the Bayesian inference procedure is implemented after every 100 simulation steps. In other words, we carry out one update step in every 100 predication steps.

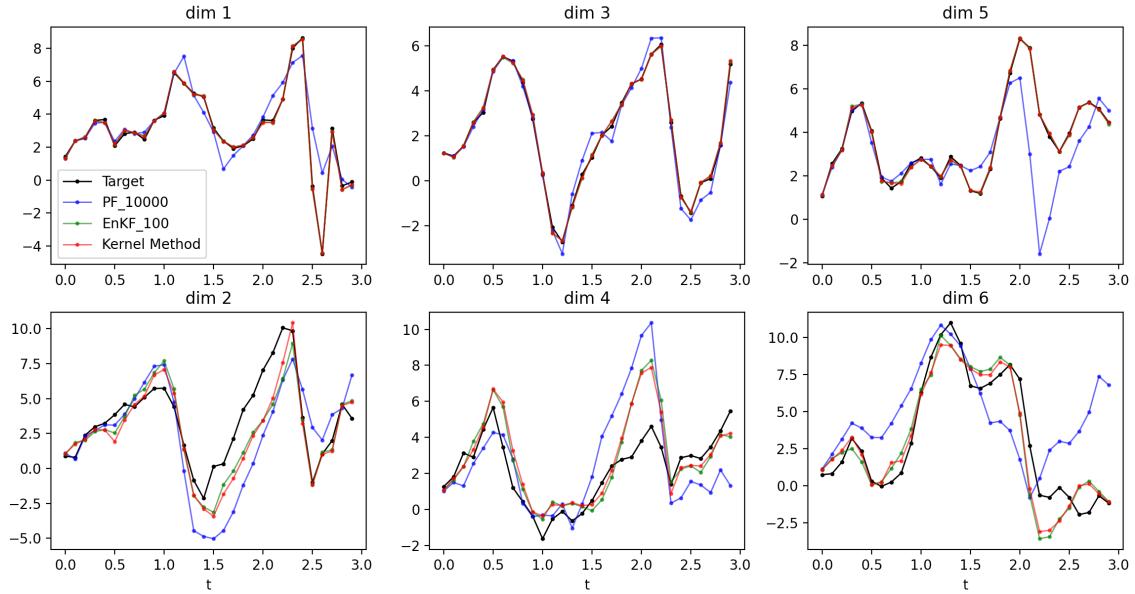


Figure 7: Example 3. Comparison of tracking performance in dimensions 1 to 6.

In this example, the observational data that we receive to estimate the state of the Lorenz-96 model are noise perturbed direct state observations in odd dimensions, i.e.

$$\mathbf{Y}_t = [\mathbf{x}_t^1; \mathbf{x}_t^3; \mathbf{x}_t^5; \mathbf{x}_t^7; \mathbf{x}_t^9]^T + \mathbf{v}_t;$$

where $\zeta \sim N(0; 1)$ is a standard Gaussian noise.

In Figure 7, we compare our kernel method with the PF and the EnKF, and we present the state estimation performance of each method in the first six dimensions. In each subplot, the black curve shows a sample of real target trajectory of the Lorenz-96 model state. The blue curve is the PF estimates obtained by using 10,000 particles to represent the empirical distribution of the state. The green curve is the EnKF estimates obtained by using 100 realizations of Kalman filter samples. The red curve gives the estimates obtained by our kernel method, and we use at most 20 kernels to approximate the filtering density in the adaptive boosting algorithm when fitting the nonlinear component of the state drift. From this figure, we can see that the EnKF has comparable estimation performance to the kernel method due to the linear observations, and the usage of "ensemble estimation" in the EnKF can handle the nonlinearity of the state dynamics. On the other hand, the PF provides low tracking accuracy. Especially, the long simulation period (without an update) in this example would cause more severe degeneracy issue since no data can be used to resample the particles.

To confirm the comparison result presented in Figure 7, we repeat the above experiment 100 times and present the log scaled RMSEs of each method with respect to time in Figure 8. We can see from this figure that the PF has much higher errors compared with the EnKF and the kernel method while both the EnKF and the kernel method have similar RMSEs in this Lorenz-96 tracking problem.

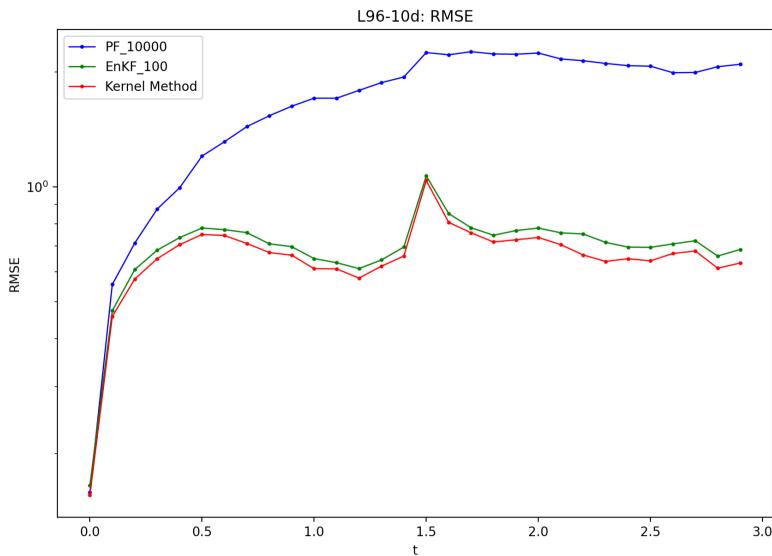


Figure 8: Example 3. Comparison of RMSEs with respect to time.

5 Summary and conclusions

In this paper, we developed an adaptive kernel method to solve the optimal filtering problem. The main idea of our method is to use a set of Gaussian kernels to approximate the filtering density of a target dynamical state model. Due to the fact that the filtering density describes a probabilistic

distribution, Gaussian kernels can effectively characterize the distribution, which is often a bell-shaped function. Then, an operator decomposition method is introduced to efficiently propagate the state of the model, and adaptive boosting algorithm is applied to adaptively capture important features of the Itering density.

Three numerical experiments are presented to examine the performance of our kernel method. In the first example, we presented the effectiveness of the adaptive kernel method in characterizing propagation of the Itering density. In the second example and the third example, we compared the performance of the kernel method with two state-of-the-art methods, i.e. the particle Iter and the ensemble Kalman Iter, in solving benchmark optimal Itering problems. Results in our numerical experiments indicate that our method has high accuracy and high stability advantage compared with the particle Iter, and it outperforms the ensemble Kalman Iter when data provide highly nonlinear state observations.

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