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State estimation comparison for a high-dimensional nonlinear system by particle-based filtering methods

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ABSTRACT

The sequential filtering scheme provides a suitable framework for estimating and tracking geophysical states of systems as new data become available online. Mathematical foundations of sequential Bayesian filtering are reviewed with emphasis on practical issues for both particle filters and Kalman-based filters. In this study, we further investigate the study of Kim (2005) such that the sequential Importance resampling method (SIR), Ensemble Kalman Filter (EnKF), and the Maximum Entropy Filter (MEF) are tested in a relatively high dimensional ocean model that conceptually represents the Atlantic thermohaline circulation. The model exhibits large-amplitude transitions between strong (thermo-dominated) and weak (salinity-dominated) circulations that represent climate states between ice-age and normal climate.

The performance of the particle-based schemes is compared with the convergent results from SIR based on measurement errors, observation locations, and particle sizes in various sets of twin experiments. The sensitivity analysis shows strength and weakness of each filtering method when applied to multimodal non-linear systems. As the number of particles is increased, SIR achieves the convergent results that are mathematically optimal solutions. EnKF shows suboptimal results regardless of sample sizes, and MEF achieves the optimal solution even with a small sample size. Both EnKF, and MEF produces robust results with a relatively small sample size or increased measurement locations. Small measurement errors or short intervals of observations (or, more frequent observations) significantly improve the performances of SIR and EnKF, and MEF still show robust results even with a relatively small sample size or sparse measurement locations when the system experiences the transition between one region to the other region.

1. Introduction

Filtering is the problem of estimating the state of a system by assimilating into the system a set of observation available online. Various filtering techniques have been developed in the past decade partially due to the advances in theoretical signal processing and also partially due to the rapid increase in computational power. These methods are largely classified into the numerical sequential Monte Carlo (SMC) methods such as sequential Importance resampling method (SIR, [1,2]), and the Kalman framework, such as Ensemble Kalman filter (EnKF, [3,4]) and Maximum Entropy filter (MEF, [5,6]). All variants of such sequential Bayesian filters have been developed to perform better than the other filters for particular sets of problems. And, they are based on point-mass representation (called samples or particles) of the state probability density function (pdf), and employ the discrete approximation of the nonlinear Bayesian filter. That is, in the filters, the particles are integrated forward with the numerical model to propagate the predictive state pdf in time, and their assigned weights or assumed pdfs are updated whenever new observations are available.

The particle-based filters such as EnKF, and MEF have been explicitly designed for high-dimensional problems in geophysics. They employ fewer assumptions and require less computational cost. The filters have been compared with nonlinear but mostly low dimensional systems [7]. The dimensionalities of the models are sometimes too small to reveal characteristics of their performance. Kim [8] evaluates the performance of those filters for an intermediate and conceptual ocean model that is a high dimensional model with highly nonlinear transitions of ocean states. The results are significant in that they show the advantages of the filters when applied to a real-world model, but their results are

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rather preliminary as measurements are taken at only one location, and measurement errors are fixed.

The preceding results of the performance for the particle-based filters need to be qualitatively and quantitatively verified with the different circumstances. The goal of this study is to evaluate the performance of the particle-based filters on various circumstances such as measurement frequency, measurement errors, and different measurement locations. We employ the conceptual ocean model called the Stochastic Cessi–Young (SCY) model [9]. The SCY model is a partial differential equation that represents an idealized ocean of thermohaline circulation. This model captures important features of climate changes, bimodality, and abrupt transitions between the two modes. These features of the SCY model can provide a good testbed for filtering methods in a high dimensional nonlinear model. The SCY model is fastidious in either analytical or statistical linearization, so the *optimal* solution to the filtering problem can be obtained by the sequential importance resample (SIR) method, which is well known to be mathematically a convergent filtering scheme [10].

The paper is organized as follows. Section 2 describes the foundations of sequential Bayesian filtering formulation and its optimal solution. In Section 3, the formulations for the state estimation for a convergent particle filter and the particle-based filters are presented. In Section 4, the basic physical characteristics of an ocean thermohaline circulation in the simulation are described followed by the discussion of the performance of the filtering schemes and various sensitivity analyses. The concluding remarks are given in Section 5.

2. Sequential Bayesian formulations

The state–space model is defined by the two equations as follows:

$$x_t = f_t\left(x_{t-1}\right) + v_t, \tag{1}$$

$$y_t = h_t\left(x_t\right) + w_t. \tag{2}$$

The signal process (1) is called the state equation that describes the state evolution of x_t via a known function f_t. The observation process (2) is called the measurement equation that represents the relationship between the observations y_t and the state vector x_t through a known (measurement) function h_t. The noise vectors v_t, w_t are incorporated in the state and observation equations, and assumed to be additive and mutually independent of known probability density functions $p\left(v_t\right)$ and $q\left(w_t\right)$, respectively. The dimensionalities of the state and observation vectors are respectively n_x and n_y, and the step $t = 1, \ldots, T$ can be numerical iteration or time.

With the initial pdf $p\left(x_0\right)$ available, the sequential Bayesian framework formulates the joint pdf $p\left(X_t|Y_t\right)$ at step *t*, where $X_t = [x_1, x_2, \ldots, x_t]$ and $Y_t = [y_1, y_2, \ldots, y_t]$ are respectively the unknown sequences of state vectors and the set of available observed data at step *t*. Due to the computational cost and the statistical quantities of interest such as mean and variance, the formulation can be simplified by recursively estimating the marginal pdf $p\left(x_t|Y_t\right)$ (i.e. the posterior pdf) from the prediction pdf $p\left(x_t|Y_{t-1}\right)$ (i.e. the prior pdf).

The prediction pdf can be obtained by the Chapman–Kolmogorov equation with the first-order Markov chain assumption of x_t:

$$p\left(x_t|Y_{t-1}\right) = \int p\left(x_t|x_{t-1}, Y_{t-1}\right) \cdot p\left(x_{t-1}|Y_{t-1}\right) dx_{t-1} \tag{3}$$

$$= \int p\left(x_t|x_{t-1}\right) \cdot p\left(x_{t-1}|Y_{t-1}\right) dx_{t-1}. \tag{4}$$

The transition pdf $p\left(x_t|x_{t-1}\right)$ can be calculated by the state equation in Eq. (1) and the noise pdf $p\left(v_t\right)$. When a new measurement y_t becomes available at step *t*, the new state x_t in the posterior pdf $p\left(x_t|Y_t\right)$ can be obtained by the likelihood of the state vector $p\left(y_t|x_t\right)$ and the prior pdf $p\left(x_t|Y_{t-1}\right)$ via the Bayes theorem such that

$$p\left(x_t|Y_t\right) = \frac{p\left(y_t|x_t\right) \cdot p\left(x_t|Y_{t-1}\right)}{p\left(y_t|Y_{t-1}\right)}. \tag{5}$$

Table 1
Sequential importance resampling PF [1].

Predict : Sample new N_p particles at time t : $\{x_t^i\}_{i=1}^{N_p} \sim p\left(x_t|x_{t-1}\right)$ given $\{x_{t-1}^i\}_{i=1}^{N_p}$ Using $x_t^i = f(x_t^{i-1}, v_t^i)$ for $i = 1, \ldots, N_p$ where v_t^i are samples from the state noise PDF.
Update : • Compute the likelihood $p\left(y_t|x_t^i\right)$ for each x_t^i • Normalize the weights $w_t^i = \frac{p(y_t|x_t^i)}{\sum_{i=1}^{N_p} p(y_t|x_t^i)}$ • The posterior PDF is approximated by $p\left(x_t|Y_t\right) \approx \sum_{i=1}^{N_p} w_t^i \cdot \delta\left(x_t - x_t^i\right)$ where $\delta(x)$ denotes the Dirac-delta mass located in x
Resample : Resample N_p particles x_t^j with equal weights : $\{x_t^i, w_t^i\}_{i=1}^{N_p} \mapsto \left\{x_t^i, \frac{1}{N_p}\right\}_{i=1}^{N_p}$ such that $p\left(x_t|Y_t\right) \approx \sum_{j=1}^{N_p} \frac{1}{N_p} \cdot \delta\left(x_t - x_t^j\right)$

The normalization factor in the denominator in Eq. (3) ensures the integration of the marginal pdf to be unity, which can be written as:

$$p\left(y_t|Y_{t-1}\right) = \int p\left(y_t|x_t\right) \cdot p\left(x_t|Y_{t-1}\right) dx_t. \tag{6}$$

The posterior density $p\left(x_t|Y_t\right)$ contains all statistical information and any necessary quantities can be calculated by the integration of the marginal pdf in Eq. (3) such as mean, variance and *i*th marginal moments. This is called the filtering problem of data assimilation which determines the best estimate $p\left(x_t|Y_t\right)$ of the solution history of the dynamical system in Eq. (1) given some partial and incomplete data in Eq. (2). It is worth noting that the first-order Markov chain is too simple in some fields in which the higher order Markov chain is need for a prediction pdf, and this assumption could easily be generalized to the higher order Markov chain. For the filtering problem in the field of geoscience, a general assumption of the prediction pdf is generally accepted to be the first-order Markov chain.

3. Sequential filtering methods

To obtain the mathematically optimal solution for the posterior pdfs in Eq. (5) at time *t*, one can numerically discretize the Fokker–Planck equation to evolve the system statistics [11]. However, the algorithm is only feasible for simple models due to the computational cost. One way to overcome this problem is to adopt a cloud of particles $\{x_t^i\}_{i=1}^{N_p}$ to represent the posterior pdf, where N_p is the number of particles. In the following, sequential filtering methods for this study are summarized.

3.1. Sequential importance resampling filter

The Sequential Importance Resample (SIR) filter has been used as the most popular particle filter implementation since it is mathematically proven to be convergent to any given pdf in the limit of N_p [1,12]. In SIR, the prediction pdf is represented by the cloud of equally weighted particles $\{x_{t-1}^i\}_{i=1}^{N_p}$ each of whose weights is $w_{t-1}^i = \frac{1}{N_p}$. When assimilating measured data y_t available at time *t*, each weight w_{t-1}^i of particles is recalculated by the following likelihood in Eq. (5):

$$w_t^i \propto w_{t-1}^i p\left(y_t|x_t^i\right). \tag{7}$$

The sum of all new weights should be normalized so that their sum becomes 1. Then, new particles $\{x_t^i\}_{i=1}^{N_p}$ are drawn from the previous particle $\{x_{t-1}^i\}_{i=1}^{N_p}$ based on their weights w_t^i in Eq. (7). During this resampling procedure, all particles have equal weights $w_t^i = \frac{1}{N_p}$. The sampling stage proposed by Gordon et al., [1] creates more high-weight particles from the previous set of particles $\{x_{t-1}^i\}_{i=1}^{N_p}$. The process at step *t* is summarized in Table 1.

It is important to note that since the performance of the SIR method depends on the sample size of N_p, the method sometimes experiences