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Abstract. The solution of an inverse problem involves the estimation of variables and parameters values given by the state-space system. While a general (infinite-dimensional) optimal filter theory [1, 2] exists for nonlinear systems with Gaussian or non-Gaussian noise, applications rely on (finite-dimensional) suboptimal approximations to the optimal filter for practical implementations. The most widely-studied filters of this kind include the Regularized Particle Filter (RPF) [3, 4] and the Ensemble Square Root Filter (EnSRF) [5]. The latter is an ad-hoc approximation to the Bayes Filter, while the former is rigorously formulated, based upon the Glivenko-Cantelli theorem. By introducing a new global resampling step to the RPF, the EnSRF is proved to approximate the RPF in a special case.

Keywords: Ensemble Square Root Filter, Regularized Particle Filter with Langevin Resampling

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INTRODUCTION

For linear systems with Gaussian noise, the problem is completely solved by the Kalman filter (KF). The Ensemble Square Root Filter (EnSRF) originated as a version of the KF for large nonlinear problems and it is now an important data assimilation component of ensemble forecasting. The EnSRF is only strictly valid when all probability distributions are Gaussians, and the forward model is linear. It captures unbiasedness of the mean and the variance of the approximate posterior distribution. Rigorous methods such as the Regularized Particle Filter (RPF) [6, 7] approximate the posterior distribution more accurately without bias in higher moments.

Due to the nonlinearity of the system and the measurement error, sample impoverishment is the most common, key implementation issue of the RPF. The resampling step, which involves drawing samples from the posterior distribution, is designed to solve this problem. The traditional resampling methods, such as Residual, Stratified and Systematic Resampling [8, 9], only sample the local function space. If all the particles are located in the tails of the posterior distribution, such resampling schemes will not solve the problem.

The Langevin Algorithm is one of the most famous methods for drawing samples from a target distribution. It has a random forcing term at each pseudo time step and is more likely to break away from a local region of the sampling function space, and is more efficient at sampling the global sampling function space. We begin with the derivation of the Langevin resampling step. Then we state the algorithm of the RPF with Langevin step (RPFLR). Finally the EnSRF is proved to be a special case of our RPFLR for a Gaussian Kernel, with some assumptions.

DERIVATION OF LANGEVIN RESAMPLING

We consider the state-space system, characterized with additive observation noise as follows:

$$\text{the state equation: } x_k = f_{k-1}(x_{k-1}); \quad (1a)$$

$$\text{the measurement equation: } s_k = H_k x_k + v_k. \quad (1b)$$

Here, the subscript k denotes the time index, x_k is the state, $f_k(\cdot)$ is the nonlinear system, s_k is the measurement, H_k is the measurement matrix and v_k is the measurement noise. Both x_k and f_k are n_x -dimensional, s_k and v_k are each n_s -dimensional, while H_k has dimension $n_s \times n_x$. We denote the array of observations $\{s_1, s_2, \dots, s_{m-1}, s_m\}$ by S_M .

Assuming a prior probability density function (pdf), $\pi_0(x_0)$, for x_0 has been provided, we will focus on the filtering problem of determining the posterior pdf $\pi(x_k|S_k)$ when measurement s_k is assimilated at time step k . The RPF approximates the posterior pdf $\pi(x_k|S_k)$ using a continuous kernel density function, by assigning a kernel density function and a weight $w_{k,i}$ to each particle $x_{k,i}$ as shown in eq. (9). Here, we use the Langevin equation to construct a

random walk for each of our particles $x_{k,i}$, such that the invariant measure of the particles is $\pi(x_k|S_k)$:

$$d\mathbf{X}_\tau^i = \mathcal{A}D(x, \tau)d\tau + \sqrt{2\mathcal{A}}d\sigma_\tau. \quad (2)$$

Here, the superscript i is the particle index, τ is the pseudo-time, $\mathbf{X}_\tau \in \mathbb{R}^{n_x}$ are the particle states, \mathcal{A} is any positive-definite self-adjoint matrix, $D(x, \tau)$ is the drift vector and $\sigma_\tau \in \mathbb{R}^{n_x} \sim \mathcal{N}(0, I^{n_x})$ is a standard Brownian motion. Initially, $\mathbf{X}_0^i = x_{0,i}$ for all $i = 1, \dots, N$. It is well known that the corresponding evolution for the measurement is the Fokker-Planck equation:

$$\frac{\partial \pi(x, \tau)}{\partial \tau} = \nabla \cdot [-\mathcal{A}D(x, \tau)\pi(x, \tau) + \mathcal{A}\nabla\pi(x, \tau)]. \quad (3)$$

Introducing the potential v such that: $D(x, \tau) = -\mathcal{A}\nabla v(x, \tau)$, equations (2) and (3) become

$$d\mathbf{X}_\tau^i = -\nabla v(x, \tau)d\tau + \sqrt{2\mathcal{A}}d\sigma_\tau, \quad (4a)$$

$$\frac{\partial \pi(x, \tau)}{\partial \tau} = \nabla \cdot [\pi(x, \tau)\nabla v(x, \tau) + \mathcal{A}\nabla\pi(x, \tau)]. \quad (4b)$$

Using the fact that $\pi(x, \tau) \rightarrow \pi(x_k|S_k)$ when $\tau \rightarrow \infty$ and combining (4a,b), gives:

$$d\mathbf{X}_\tau^i = \mathcal{A}\nabla\{\ln[\pi(x_k|S_k)]\}d\tau + \sqrt{2\mathcal{A}}d\sigma_\tau. \quad (5)$$

REGULARIZED PARTICLE FILTER WITH A LANGEVIN RESAMPLING STEP (RPFLR)

The RPFLR for (1a, b) involves the following steps

1. Randomly generate N initial particles $x_{0,i}^a$ from a given initial pdf $\pi(x_0)$.
2. For $k = 1, 2, \dots$, generate the forecast particles $x_{k,i}^f$ using

$$x_{k,i}^f = f_k(x_{k-1,i}^a) \quad i = 1, \dots, N. \quad (6)$$

3. Calculate the mean and variance of the particles using

$$\hat{x}_k^f = \frac{1}{N} \sum_{i=1}^N x_{k,i}^f, \quad P_k^f = \frac{1}{N-1} \sum_{i=1}^N (x_{k,i}^f - \hat{x}_k^f)(x_{k,i}^f - \hat{x}_k^f)^T = \frac{1}{N-1} A_k A_k^T. \quad (7)$$

4. Update the weight $w_{k,i}$ of each particle using

$$w_{k,i} = \frac{w_{k,i}^*}{\sum_{i=1}^N w_{k,i}^*}, \quad w_{k,i}^* = \frac{w_{k-1,i}}{(2\pi)^{n_x/2} |R|^{1/2}} \exp\left(\frac{-(\tilde{s} - H_k x_{k,i}^f)^T R^{-1} (\tilde{s} - H_k x_{k,i}^f)}{2}\right). \quad (8)$$

5. Approximate the posterior $\pi(x_k|S_k)$ by

$$\pi(x_k|S_k) = \sum_{i=1}^N w_{k,i} K_h(x_k - x_{k,i}^f), \quad K_h(x) = \frac{\exp[-1/2 (A^{-1}x/h_{\text{opt}})^T (A^{-1}x/h_{\text{opt}})]}{(2\pi)^{n_x/2} h_{\text{opt}}^{n_x} (\det A)}, \quad (9)$$

Where, h_{opt} is a scalar, called the bandwidth of the regularized particle filter¹ [6, 7].

The Langevin Resampling step involves:

6. At pseudo time $\tau = 0$,

$$\forall i = 1, \dots, N: \quad \mathbf{x}_0^i = x_{k,i}^f. \quad (10)$$

¹ which minimizes the mean integrated error or the mean integrated square error between the approximate and exact posterior distributions

7. For $i = 1, 2, \dots, N$, choose an appropriate (small) pseudo time step $\Delta\tau$ and a positive-definite self-adjoint matrix \mathcal{A} .
8. Then, for $j = 1, 2, \dots$, proceed as follows until the proposal particle is accepted:
 - (a) Using the Crank-Nicolson numerical scheme for eq. (5), generate a proposal particle \mathbf{X}_j^i using

$$\mathbf{X}_j^i = \mathbf{X}_{j-1}^i + \frac{1}{2}\Delta\tau\mathcal{A}(\nabla\{\ln[\pi(x_k = \mathbf{X}_{j-1}^i|S_k)]\} + \nabla\{\ln[\pi(x_k = \mathbf{X}_j^i|S_k)]\}) + \sqrt{2\mathcal{A}\Delta\tau}\boldsymbol{\sigma}_\tau, \quad (11)$$

where $\boldsymbol{\sigma}_\tau \sim \mathcal{N}(0, I^{n_x})$ is n_x -dimensional white noise.

- (b) The proposal particle is then accepted if $|\mathbf{X}_j^i - \mathbf{X}_{j-1}^i| \leq \sqrt{2\mathcal{A}\Delta\tau}$ otherwise it is rejected.
- (c) The accepted particle is taken as our analysed particle at time step k :

$$x_{k,i}^a = \mathbf{x}_j^i \quad (12)$$

SPECIAL CASE OF RPFLR STEP: ENSRF

Taking only one stepping the update using eq. (11) of our Langevin Resampling and accept all the proposal particles as the analysed particles, so that:

$$x_{k,i}^a = x_{k,i}^f + \frac{\Delta\tau}{2}\mathcal{A}\nabla(\{\ln[\pi(x_k = x_{k,i}^f|S_k)]\} + \{\ln[\pi(x_k = x_{k,i}^a|S_k)]\}) + \sqrt{2\mathcal{A}\Delta\tau}\boldsymbol{\sigma}_\tau, \quad (13)$$

where $\boldsymbol{\sigma}_\tau \sim \mathcal{N}(0, I^{n_x})$ is n_x -dimensional white noise.

Choosing the bandwidth $h_{\text{opt}} = 1$, the prior pdf $\pi(x_k|S_{k-1})$ given by the forecasting step is:

$$\pi(x_k|S_{k-1}) = \frac{1}{N} \sum_{i=1}^N \mathcal{N}(x_{k,i}^f, P_k^f). \quad (14)$$

This is written in the same spirit as eqns (9). Here, $x_{k,i}^f$ and P_k^f are given by eqns (6) and (7), respectively.

Assuming the prior particles $x_{k,i}^f$ are very close to one another in the sampling space, using the axioms of Gaussian pdf addition, the prior pdf $\pi(x_k|S_{k-1})$ in eqn (14) is approximated as:

$$\pi(x_k|S_{k-1}) \approx \mathcal{N}(\hat{x}_k^f, P_k^f), \quad (15)$$

where \hat{x}_k^f is calculated using eqn (7).

Substituting the approximate prior pdf (15) and the measurement function (1b) into eqn (7), the posterior pdf $\pi(x_k|S_k)$ satisfies:

$$\pi(x_k|S_k) = \frac{1}{C_1} \exp\left\{-\frac{1}{2}[(x_k - \hat{x}_k^f)^T P_k^{f-1} (x_k - \hat{x}_k^f) + (s_k - Hx_k^f)^T R^{-1} (s_k - Hx_k^f)]\right\} \quad (16)$$

Here,

$$C_1 = (2\pi)^{n_x+n_s} (\det P_k^f)^{1/2} (\det R)^{1/2} \pi(s_k|S_{k-1})$$

is a constant. Hence, the key to our Langevin Resampling update will be to evaluate the drift term $\nabla\{\ln[\pi(x_k|S_k)]\}$ in eqn (13). Using eqn (16), this drift term becomes:

$$\begin{aligned} \nabla\{\ln[\pi(x_k|S_k)]\} &= -P_k^{f-1}(x_k - \hat{x}_k^f) - H^T R^{-1}(s_k - Hx_k) \\ &= (P_k^{f-1} + H^T R^{-1} H)[(P_k^{f-1} + H^T R^{-1} H)^{-1}(H^T R^{-1} s_k + P_k^{f-1} \hat{x}_k^f) - x_k] \end{aligned} \quad (17)$$

Introducing the Kalman gain matrix:

$$K_k = P_k^f H^T (H P_k^f H^T + R)^{-1} \quad (18)$$

and applying the matrix inversion lemma² $(P_k^{f-1} + H^T R^{-1} H)^{-1}$, equation (17) can be transformed as follows:

$$\begin{aligned} \nabla\{\ln[\pi(x_k|S_k)]\} &= (P_k^{f-1} + H^T R^{-1} H)\{[P_k^f - P_k^f H^T (H P_k^f H^T + R)^{-1} H P_k^f](H^T R^{-1} s_k + P_k^{f-1} \hat{x}_k^f) - x_k\} \\ &= (P_k^{f-1} + H^T R^{-1} H)\{(\hat{x}_k^f - x_k) + K_k(s_k - H\hat{x}_k^f)\}. \end{aligned} \quad (19)$$

Substituting eqn (19) into eqn (13), the analysed particles given by our special case Langevin Resampling step satisfy:

$$x_{k,i}^a = x_{k,i}^f + \frac{\Delta\tau}{2} \mathcal{A} (P_k^{f-1} + H^T R^{-1} H) [2\hat{x}_k^f - x_{k,i}^f + x_{k,i}^a + 2K_k(s_k - H\hat{x}_k^f)] + \sqrt{2\mathcal{A}\Delta\tau} \sigma_\tau, \quad (20)$$

where $\sigma_\tau \sim \mathcal{N}(0, I^{n_x})$ is an n_x dimensional white noise. It is interesting to note that matrix A and pseudo time step $\Delta\tau$ are operating together as a pre-conditioner on the update step. The requirement is for matrix A to be symmetric and positive-definite. To simplify our Langevin Resampling algorithm (20), we choose

$$\Delta\tau A = 2(P_k^{f-1} + H^T R^{-1} H)^{-1}. \quad (21)$$

With this choice, (20) becomes:

$$x_{k,i}^a = \hat{x}_k^f + K_k(s_k - H\hat{x}_k^f) + \sqrt{(P_k^{f-1} + H^T R^{-1} H)^{-1}} \sigma_\tau. \quad (22)$$

This is the exact form of the EnSRF because the stochastic part of the equation make the analysed particles satisfy the exact Kalman Filter covariance².

CONCLUDING DISCUSSION

It have been demonstrated that the Regularized Particle Filter is a more rigorous and general filter , compared to Ensemble Square Root Filter. By varying the pre-conditioner \mathcal{A} , the performance of our Regularized Particle Filter with Langevin Resampling step can be adjusted. Compared to the Ensemble Filters, the RPFLR has the capability of sampling the global function space of posterior pdfs. Further work is need to compare to other particle and kernel methods and the RPFLR regarding the efficienc y of the sampling.

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² Using the matrix inversion lemma: $(P_k^{f-1} + H^T R^{-1} H)^{-1} = P_k^f - P_k^f H^T (H P_k^f H^T + R)^{-1} H P_k^f = (I - K_k H^T) P_k^f$

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