From the Ensemble Kalman Filter to the Particle Filter: a comparative study in rainfall-runoff models

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Abstract: Rainfall-runoff models are hydrologic models and they play a very important role in flood forecasting. Hydrologic systems are featured by a non-linear behaviour, non-Gaussian distributions and the presence of large uncertainties in the model itself and in the input data. Therefore, the use of non-linear/non-Gaussian state estimation or data assimilation techniques is important in order to improve the model predictions. The objective of this paper is to present a comparative study between the performances of two sequential data assimilation techniques, which are based on Monte Carlo (MC) methods. The advantages and drawbacks of the well known ensemble Kalman Filter (EnKF) and the standard particle filter will be discussed in this study. Results show that both filters perform similar with the surface soil moisture as the estimated variable and using synthetic generated data.

Keywords: Non-linear state estimation, data assimilation, ensemble Kalman filter, particle filter.

1. INTRODUCTION

Rainfall-runoff models represent the physical processes of the hydrologic cycle such as runoff, infiltration, evapotranspiration, soil-water content, discharge. These processes are interdependent, making the construction of hydrologic models complex.

State estimation is used in order to adapt the results of model simulations using external observations. The state estimation using land observations (e.g., volumetric surface soil moisture) is also known as Land Data Assimilation. Data assimilation (DA) is used in many different disciplines such as earth sciences, space sciences, computer graphics and industrial applications.

In 1994, Evensen presented the Ensemble Kalman Filter (EnKF) [Evensen (1994)] as a Monte Carlo approach to the non-linear filtering problem; since then the EnKF has been successfully applied to a variety of complex non-linear systems.

The particle filter, which is a Sequential Monte Carlo (SMC) method for state estimation, has been widely applied in mobile robot localization with promising results [Arulampalam et al. (2002)]. Recently, the particle filter has been proposed as an alternative to the EnKF and it has been evaluated over non-linear systems. [Moradkhani et al. (2005), Jardak and Navon (2007)].

The goal of this study is to evaluate and compare the performances of the EnKF and the particle filter. The conceptual rainfall-runoff model used in this study is described in Section 2. A review of the methods is presented in Section 3. Finally the implementation issues and results are commented in Section 4.

2. RAINFALL-RUNOFF MODEL

A detailed description of the model is presented in section 2.1. The model is applied to the setting of the Alzette watershed, which is located in Luxembourg. The dataset contains daily precipitation, evapotranspiration, and discharge observations; this dataset was obtained from the Gabriel Lippman Research Center (CRP-GL). The precipitation and evapotranspiration data are used as the model inputs and the discharge observations are used in the identification of the model parameters. Synthetic volumetric soil moisture observations were generated and used in the comparison of the filter performances.

2.1 Model description

A modified version of the Hydrologiska Byråns Vattenbalansavdelning (HBV) model, which is developed and explained in [Lindström et al. (1997)] is used in the following paper;[Matgen et al. (2006)]. In this study, the simplified version of the HBV model is adopted in order to be able to evaluate different DA techniques.

Fig. 1 shows a schematic of the hydrologic model where the real discharge area is divided into three reservoirs, a
soil reservoir, a fast reacting reservoir, and a slow reacting reservoir. The slow flow unit characterizes the water that flows through the ground and eventually ends up in the discharge point. The fast flow unit represents the water that flows directly into the discharge point. The equations governing the water mass balance in the reservoirs are presented as follows:

\[
\begin{align*}
\dot{S}_{\text{soil}}(t) & = R_{in}(t) - E_{tr}(t) - P_{er}(t) \\
\dot{S}_{\text{slow}}(t) & = R_{\text{slow}}(t) - Q_{\text{slow}}(t) + P_{er}(t) \\
\dot{S}_{\text{fast}}(t) & = R_{\text{fast}}(t) - Q_{\text{fast}}(t)
\end{align*}
\]

The inputs of the system are the precipitation \( R_{\text{tot}} \) and the potential evapotranspiration \( E_{tp} \).

The model is able to represent some flows such as the actual evapotranspiration \( E_{tr} \), the infiltration \( R_{in} \), the effective precipitation \( R_{eff} \), the percolation \( P_{er} \), the fast reacting reservoir input \( R_{fast} \), the output flow of the fast reacting reservoir \( Q_{fast} \), the slow reacting reservoir input \( R_{slow} \) and the output flow of the slow reacting reservoir \( Q_{slow} \).

The model flows are related to the states according to the following relationships:

\[
\begin{align*}
E_{tr}(t) & = \frac{S_{\text{soil}}(t)}{\lambda S_{\text{max}}} E_{tp}(t) \\
R_{in}(t) & = \left(1 - \frac{S_{\text{soil}}(t)}{S_{\text{max}}} \right)^{b} R_{\text{tot}}(t) \\
R_{eff}(t) & = R_{\text{tot}}(t) - R_{in}(t) \\
P_{er}(t) & = P \left(1 - e^{-\beta \frac{S_{\text{soil}}(t)}{S_{\text{max}}}}\right) \\
R_{fast}(t) & = \alpha \frac{S_{\text{soil}}(t)}{S_{\text{max}}} R_{eff}(t) \\
Q_{fast}(t) & = \kappa_{2} \left(\frac{S_{fast}(t)}{S_{2,\text{max}}}\right)^{\gamma} \\
R_{slow}(t) & = R_{eff}(t) - R_{fast}(t) \\
Q_{slow}(t) & = \kappa_{4} S_{slow}(t)
\end{align*}
\]

where \( \lambda, b, \alpha, \beta, \gamma \) are dimensionless model parameters, \( S_{\text{max}} \) is the storage capacity of the soil reservoir (m³), \( P \) is the maximum percolation (m³s⁻¹), \( S_{2,\text{max}} \) is the storage capacity of the fast reacting reservoir (m³), \( \kappa_{2} \) (m³s⁻¹) and \( \kappa_{4} \) (s⁻¹) are model parameters.

From the three state variables we will focus on the estimation of \( S_{\text{slow}} \) since there is a direct relationship between the amount of water in the slow reacting reservoir and the volumetric soil moisture variable \( \theta(t) \) (m³m⁻³).

\[
\theta(t) = \frac{S_{\text{slow}}(t)}{v_{r}}
\]

where \( v_{r} \) (m³) is the approximate volume of the discharge watershed.

### 2.2 Model parameters identification

The optimal values of the parameters described in section 2.1 were identified using discharge observations and using a conventional parameter identification method, which is mainly used in the hydrologic field. The method applied in the identification of the parameters is the Shuffled complex evolution approach [Duan et al. (1993)].

Although SMC methods have been widely applied in the identification of static model parameters as it is reported in Kantas et al. (2009), in this paper we focus the study on the application of SMC methods to the state estimation problem.

### 3. STATE ESTIMATION TECHNIQUES

The well known Kalman filter (KF) [Kalman (1960)] is the optimal estimator for linear systems with Gaussian distributions. Several extensions to the Kalman filter have been developed mainly to deal with nonlinearities in the system and non-Gaussian distributions.

The Extended Kalman filter (EKF) is probably the most frequently used non-linear version of the KF. The EKF linearizes the system around the mean and covariance using the Taylor series. The Unscented Kalman Filter (UKF) [Wan and Merwe (2000)] is based on the unscented transformation; the transformation consists in the parametrization of the means and covariances of the probability distributions using a set of appropriately chosen weighting points.

In the field of Geosciences, where the systems are high-dimensional featured by a non-linear behaviour and most of the times without continuous measurements and non-Gaussian distributions, the ensemble Kalman filter [Evensen (2003)] was proposed as a solution to the estimation problem. Recently, research has been conducted in the application of the particle filter in geosciences for parameter and state estimation [Moradkhani et al. (2005), Nakano et al. (2007), Weerts and El Serafy (2006), Jardak and Navon (2007)].

A short description of the EnKF and the particle filter will be provided in this section.

#### 3.1 Ensemble Kalman filter

The Kalman filter (KF) and the extended Kalman filter (EKF) explicitly propagate the state error covariance
matrix. In contrast, the EnKF uses an ensemble of model trajectories to determine the error covariances directly from the spread of the states in an ensemble at a certain point in time, instead of obtaining a value for the error covariance matrix, which is computed with a linearized equation.

Considering the following non-linear system:

\[ x_t = f_t(x_{t-1}, u_{t-1}, v_{t-1}) \]
\[ y_t = h_t(x_t, n_t) \]

where, \( x_t \) is the state vector, \( u_t \) represents the inputs, \( f_t \) and \( h_t \) are non-linear functions, \( y_t \) is the observation model, \( v_t \) and \( n_t \) are the process and observation noises and \( t \) is the discrete time index.

The main difference among the KF/EKF and the EnKF is related to the model error \( v_t \), in the EnKF the model error is assessed and explicitly added to the model equations. The a priori estimated ensemble member \( \tilde{x}_t^{-i} \) (with \( i = 1, \ldots, N \)) and \( N \) the number of members in the ensemble is given by:

\[ \tilde{x}_t^{-i} = f_t(\tilde{x}_{t-1}^{-i}, u_{t-1}, v_t^{i-1}) \]

with \( v_t^{i-1} \) a random white noise with a predefined standard deviation. In the EnKF, the measurements \( y_t \) are perturbed using additive white noise \( n_t \). Therefore, the measurement set \( y_t^{i} \) is given by:

\[ y_t^{i} = y_t + n_t^{i} \]

The optimal estimate \( \tilde{x}_t^{i} \) of an ensemble member is given by:

\[ \tilde{x}_t^{i} = \tilde{x}_t^{-i} + K_t[y_t^{i} - h_t(\tilde{x}_t^{-i})], \forall i = 1, \ldots, N \]

The Kalman gain \( K_t \) is identical for all members and computed as in the KF and EKF:

\[ K_t = P_t^{-1/2} H_t^T (H_t P_t^{-1/2} H_t^T + R_t)^{-1} \]

where \( P_t^{-1} \) is the state error covariance matrix, \( H_t \) is a Jacobian matrix and \( R_t \) is the measurement error covariance matrix. For the EnKF, the a priori covariance \( P_t^{-1} \) is defined as:

\[ P_t^{-1} = E[(\tilde{x}_t^{-i} - \tilde{x}_t^{-i}) (\tilde{x}_t^{-i} - \tilde{x}_t^{-i})^T] \]

The ensemble mean of the a priori estimates \( \tilde{x}_t^{-i} \) is given by:

\[ \tilde{x}_t = \frac{1}{N} \sum_{i=1}^{N} \tilde{x}_t^{-i} \]

In practice, equation (17) can be approximated as:

\[ P_t^{-1} = \frac{1}{N-1} [\tilde{x}_t^{-1} - \tilde{x}_t^{-1}] \times \ldots [\tilde{x}_t^{-N} - \tilde{x}_t^{-N}]^T \]

### 3.2 Particle Filter

Particle filters are SMC methods, special attention to the sequential importance sampling (SIS) and sequential importance resampling (SIR) methods is addressed in this study.

**Sequential Importance Sampling** In Monte Carlo methods, the importance sampling approach is used as a variance reduction technique. The key idea around this approach is to circumvent the sampling difficulty from the posterior density function \( p(x_{0:t}|y_{1:t}) \) by proposing an importance density function \( q(x_{0:t}|y_{1:t}) \), from which the sampling should be easier.

For any integrable function \( g_t(x_{0:t}) \):

\[ E_{P_t}[g_t(x_{0:t})] = \int g_t(x_{0:t}) p(x_{0:t}|y_{1:t}) \, dx \]

\[ \ldots \int g_t(x_{0:t}) \frac{p(x_{0:t}|y_{1:t})}{q(x_{0:t}|y_{1:t})} q(x_{0:t}|y_{1:t}) \, dx \]

\[ \ldots \int g_t(x_{0:t}) \tilde{w}_t(x_{0:t}) q(x_{0:t}|y_{1:t}) \, dx \]

The notation \( q(.) \) has been used in order to remark the fact that the expectation is taken over the proposal distribution rather than the posterior \( E_{P_t}[.] \). The term \( w_t \) in (20) is referred to the importance weights.

Under the assumptions of a perfect MC simulation, equation (20) can be approximated as follows:

\[ \hat{E}[g_t(x_{0:t})] = \sum_{i=1}^{N} g_t(x_{0:t}^i) \tilde{w}_t(x_{0:t}^i) \]

where \( i = 1, \ldots, N \), \( N \) is the number of particles and \( x_{0:t}^i \) is the \( i \)th particle drawn from the proposal distribution. \( \tilde{w}_t^i \) is the normalized importance weight given by:

\[ \tilde{w}_t^i = \frac{w_t^i}{\sum_{j=1}^{N} w_t^j} \]

Considering that the system states evolve according to a Markov process and applying recursion to the filtering problem, the recursive expression for the importance weights is given by:

\[ w_t^i = w_{t-1}^i \frac{p(y_t|x_{t-1}) p(x_t^i|x_{t-1}^i)}{q(x_{t}^i|x_{t-1}^i, y_t)} \]

A common choice of the proposal is the transition prior function [Kitagawa (1996), Gordon et al. (1993)]:

\[ q(x_{t+1}|x_t, y_{1:t}) = p(x_{t+1}|x_t) \]

When comparing the transition prior and the optimal proposal function \( p(x_{t+1}|x_t, y_{1:t}) \), the absence of the most recent observations is noticeable. Consequently, the variance of the importance weights increases over time as it is stated in Kong et al. (1994) and Doucet et al. (2001).

**Sequential Importance Resampling** Resampling is basically the selection and replication of those particles with high importance weights. This additional step to the SIS filter involves mapping the Dirac random measure \( \{x_{0:t}^i, \tilde{w}_t^i\} \) into an equally random measure \( \{x_{0:t}^i, N^{-1}\} \). Gordon et al. (1993) proposed a methodology which consists in drawing samples uniformly from the discrete set \( \{x_{0:t}^i, \tilde{w}_t^i\} \) and it is referenced as the sequential importance resampling method (SIR).

Residual resampling is an improved version of the SIR method and was proposed by [Higuchi (1997), Liu and Chen (1998)]. The main characteristics of residual resampling are: the variance is smaller than the variance from the SIR method and the algorithm is computationally efficient.

The replication of particles poses a problem when the set of resampled particles collapses to a single particle in the
worst case and once more the particle set will suffer from
degeneracy.
The use of Markov chain Monte Carlo (MCMC) steps is a
valid strategy to overcome the extreme replication problem
[Andrieu et al. (1999)]. The main idea around MCMC
steps involves the assumption that if the particles \( x_{0:t} \)
are distributed according to the posterior \( p(x_{0:t}|y_{1:t}) \), then
applying a Markov chain transition kernel \( K(x_{0:t}|x_{0:t}) \)
results in a set of particles distributed according to the
posterior of interest \( p(x_{0:t}|y_{1:t}) \). Moreover, the spread of
the new particle set might have been moved covering more
interesting areas of the state space.

The application of the MCMC move step consists of two
steps: first, the new particles are drawn from a proposal
density function and these particles should be selected
according to standard MCMC methods such us the Gibbs
sampler and Metropolis Hastings (MH) algorithms.

4. IMPLEMENTATION AND RESULTS

The performance of the different state estimation tech-
niques introduced in section 3 will be presented in this
section. First, all the considerations around the hydrologic
model and the application of the filters are presented.

4.1 Implementation considerations

Considering additive noise in (11) and (12), the state space
model of the hydrologic system is given by:

\[
x_t = f_t(x_{t-1}, u_{t-1}) + v_{t-1}
\]

where the state vector is \( x = [S_{\text{soil}} S_{\text{fast}} S_{\text{slow}}] \), and
\( f_t(.) \) is the discretized version of the system defined in
(1), \( v_{t-1} \) is white Gaussian noise with variance \( Q_{t-1} \). The
measurement equation is given by:

\[
y_t = h_t(x_t) + n_t
\]

where the output of the system is the volumetric soil
moisture variable \( y_t = \theta_t \) and the mapping state to
observation function \( h_t(.) \) is the discretized version of (10),
\( n_t \) is white Gaussian noise with variance \( R_t \).

The state variable to estimate is the water content in the
slow reacting reservoir. Synthetic true soil moisture values
are generated after the perturbation of the optimal pa-
parameter values described in section 2.1. Random samples
referenced to ensembles (EnKF) or particles should be
generated sequentially from the transition prior density
function \( p(x_t|x_{t-1}) \), which is considered to be Gaussian
with variance \( Q_t \), the number of samples is 64 in order
to assure a good MC approximation.

The likelihood density function \( p(y_t|x_t) \) is considered to
be Gaussian with mean equal to \( h_t \) and variance equal
to \( R_t \). Finally, the scope of this study is limited to
the application of the standard particle filter with the
importance density function \( q(x_t|x_{t-1}, y_t) \) equal to the
transition prior function. In some cases, this selection
results in a poor performance of the particle since the
information from the last observation is not taken into
account by the prior density function thus MCMC move
steps are applied to overcome this deficiency.

4.2 Results

Some graphics of the state evolution over time are pre-
sented in this section in order to show the performance
of the different filters. The simulation period corresponds
to the first 160 days (01/Jan - 05/Jun) from year 2007.
The Root Mean Squared Error (RMSE) is used in order
to quantify the performance and for posterior comparison.
Table 1 presents the RMSE averaged values, computation
time and the figures associated to each filter for 100 MC
runs.

**Table 1.** Table of the applied filters, corresponding
figures, RMSE index and computation time

<table>
<thead>
<tr>
<th>Filters</th>
<th>Fig</th>
<th>RMSE[%]</th>
<th>time demand[s]</th>
</tr>
</thead>
<tbody>
<tr>
<td>SIR+MCMC</td>
<td>6</td>
<td>0.83</td>
<td>0.75</td>
</tr>
<tr>
<td>SIR filter</td>
<td>5</td>
<td>1.38</td>
<td>1.09</td>
</tr>
<tr>
<td>EnKF</td>
<td>2</td>
<td>1.77</td>
<td>1.30</td>
</tr>
<tr>
<td>SIS filter</td>
<td>3, 4</td>
<td>4.01</td>
<td>3.64</td>
</tr>
</tbody>
</table>

**EnKF** The EnKF performance depends on the MC
approximation of the covariance and the Gaussian
approximation of the posterior distribution. The MC approxi-
mation is an alternative to the local linearization used in
the EKF in order to deal with the nonlinearities of the
systems. Some assumptions were made in the development
of the conceptual rainfall-runoff model in order to preserve
the model as simple as possible and the nonlinearities in
the system mainly depend on the relationship between the
state and the parameters (equations 2-9). The non-linear
problem is limited to the states equation since the mea-
surement equation is linear. A reasonable approximation
of the posterior by the EnKF can be expected based on the
simplicity of the model and the linearity of the function
\( h_t \).

Fig. 2 shows the evolution of the 64 ensemble members in
light gray color, the corresponding ensemble mean in black
line, the true observations (true state) in red dotted line
and the deterministic run (control run) in blue dotted line.
A good approximation of the posterior can be seen from
fig. 2. The mean of the filter is frequently close to the true
state except for the time period corresponding to the last
days of April and first of May. The RMSE indexes indicate
small errors in the estimation.

**SIS filter** The application of the standard particle filter
involves a Gaussian prior density function and a Gaussian
likelihood density function, the same assumptions hold for
the EnKF and both methods are MC based. Consequently,
the performance is expected for both filters unless
internal limitations in the algorithms could degrade the
performances.

The RMSE measure shows that the SIS filter is the least
accurate of the algorithms at approximating the posterior
density function. This result is somehow expected mainly
due to the degeneracy of the importance weights. The
degeneracy problem can be noticed by monitoring the
importance weights.

As can be seen from fig. 3, the weighted mean is rarely close
to the true state, the filter seems to perform acceptable
only during the first time steps of the simulation.
Volumetric Soil Moisture

Fig. 2. EnKF performance. The lines in grey color correspond to the ensemble mean, the blue dotted line corresponds to the deterministic run and the red dotted line corresponds to the synthetic observations.

Fig. 3. SIS performance. The lines in gray color correspond to the particles evolution, the black line corresponds to the mean of the particles, the blue dotted line corresponds to the deterministic run and the red dotted line corresponds to the synthetic observations.

Fig. 4 shows the location and weights of the particles at the time initialization and time steps 1 (01/Jan), 50 (20/Feb), 125 (06/May). The plots in the upper part of fig. 4 show the importance weight transition from a uniform distribution at $t = 0$ to a normal distribution according to the Gaussian likelihood function at $t = 1$. For both plots in the lower part of fig. 4 it is clearly noticeable that after a few model time steps, one of the normalized importance weights reaches the value of 1, while the remaining set of weights falls to negligible values. Consequently a large number of samples are removed from the sample space because their weights become numerically insignificant. The set of samples and weights results in a wrong approximation of the posterior.

**SIR filter** As shown by fig. 5, the addition of the resampling step to the SIS filter improves the performance of this filter. The mean of the filter is frequently close to the true state except for the time period corresponding to the presence of the highest observation peak. This behaviour is similar to the EnKF performance. Moreover, the RMSE indexes indicate that the EnKF and the SIR filter performances are close to each other.

**SIR filter with MCMC move steps** As can be seen from fig 6 and according to the RMSE value, the use of the MCMC move steps in the SIR filter improves the performance. The main drawback regarding the use of MCMC steps is the computation time. MCMC steps involves the generation of new proposed particles, in the case of the standard particle filters the proposal density is the prior density function. Consequently a new model run should be carried out at every data assimilation step in order to obtain the new set of samples making this approach computationally expensive.
The advantage of incorporating MCMC steps can be seen from fig. 6. Comparing the different strategies around the highest observation peak, the benefit of moving the particles to more interesting parts of the posterior is noticeable. Although the estimates do not reach the true state, the particles spread covers the measurements providing better estimates.

Fig. 6. Improved SIR performance. The lines in gray color correspond to the particles evolution, the black line corresponds to the mean of the particles, the blue dotted line corresponds to the deterministic run and the red dotted line corresponds to the synthetic observations.

5. CONCLUSIONS

The performances of the EnKF and the standard particle filter applied to a rainfall-runoff model have been presented in this paper. Although, the EnKF equations concerning the calculation of the Kalman gain are limited to the linear case, the filter presents a good performance when it is evaluated over a non-linear hydrologic model.

Results show that the SIR filter with MCMC steps performs better compared to the EnKF, however, the use of MCMC steps increase the computational time demand. When using particle filters and when the computational time demand is not a limitation it is strongly recommended to improve the filter either increasing the number of particles or adding resampling steps in combination with MCMC move steps.

For the case of complex models such as high dimensional models or spatially distributed models it is recommended to explore possible alternatives for improving particle filters. The approximation of the posterior by a set of particles and weights allows to adapt important density functions to the specific study case.

REFERENCES


