Fast and stable estimation of macroscopic parameters in particle systems by data assimilation

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Abstract

In this paper we show a data assimilation framework which gives good estimation of the macroscopic parameter in particle systems. To give the fast and stable estimation, we employed the bounded Gaussian uniform mixture (BGUM) type dynamics that is originally introduced in the econophysics field. The result of the numerical experiment implies that BGUM type dynamics enable us to obtain appropriate estimation of macroscopic parameters from macroscopic observations faster than random walk type dynamics that is usually employed. It is also implied that mixing rate between Gaussian and uniform distribution can control the trade-off between fast detection and stability of macroscopic parameters. Those results suggest that the utility of the introduced framework for macroscopic parameter estimation in particle systems.

1 Introduction

As the development of high-performance computation, application fields of particle systems are broadening such as molecular dynamics, traffic flow, galaxy formation and granular material flows. Particle simulation method of complex water flow such as tsunami inundation simulation can be also regarded as the particle system. The characteristics of the particle system is that interactions among particles. Those interactions are calculated by simulation models to mimic actual phenomena.

However, unobservability of interaction parameters among particles imposes a limitation to applying particle simulations for realistic problems, especially to giving quantitative evaluation. For example, particle method of water flow simulations has the macroscopic parameter on interaction range among particles, which can not be determined accurately because it does not exist in real. In general, macroscopic parameters play an important role in particle systems and it is often difficult to be determined.

Data assimilation (DA, [1]) is one of the solutions to this problem. DA is the concept and algorithm that combine simulation models with observation data. It has been used in the meteorology and oceanography to generate appropriate initial values for forecast, but recently the application area is wide-spreadening, such as biology and geotechnical engineering. DA gives not only estimation of time varying states and initial conditions, but also that of empirical parameters and boundary conditions of target systems.

DA can be regarded as the state and parameter estimation in non-linear non-Gaussian state space model(SSM) from the viewpoint of statistical time series analysis and control theory. Therefore, state estimation algorithm for SSM can be used for DA. In the researches of DA, the extended Kalman filter[2], the ensemble Kalman filter (EnKF)[3], the four dimensional variational method (4DVAR)[4] and the particle filter (PF) [5, 6] are used. The EnKF and the 4DVAR are widely used in the meteorology and oceanography because the non-linearity of the system and multi-modality of estimated states are not problematic in those fields. On the other hand, the PF is used in the geotechnical engineering and biology because the non-linearity causes large estimation error in those fields.

In this paper, we will give the formulation of DA for estimation of macroscopic parameters of the particle systems. The difficulty of estimation of macroscopic parameters is derived from the difference between the time scale of macroscopic parameters and that of time varying states. Because of that, introduction of simple pseudo dynamics into macroscopic parameters causes unstable and inefficient parameter estimation. To overcome this difficulty, we adopt bounded Gaussian and uniform mixture (BGUM) for pseudo dynamics of macroscopic parameters, which is originally introduced in the field of econophysics[7]. To check efficacy and validity of introduction of BGUM dynamics for particle systems, we employ optimal velocity (OV) model which is one of the particle systems and mathematical models for traffic flow[8, 9].

2 Data Assimilation

2.1 State Space Modeling in Data Assimilation

In the DA, simulation models that are composed from some governing equations or empirical formula are employed for simulating time evolutionary phenomena. This computation process is usually deterministic, so
it is formulated as follows:

$$\tilde{x}_t = \hat{f}(\tilde{x}_{t-1})$$  \hspace{1cm} (1)

where \(\tilde{x}_t\) represents the simulation variables at the time step \(t\). At that time, variable \(\tilde{x}_t\) evolves deterministically in time. However, there are a lot of uncertainties among the simulations and real phenomena, such as round-off errors, discretization errors and modeling errors. There are also errors in observation process.

To formulate systems and observations with these uncertainties, non-linear non-Gaussian state space model (SSM) is used:

$$x_t = f_t(x_{t-1}, v_t), \quad (t = 1, \ldots, T)$$  \hspace{1cm} (2)

$$y_t = h_t(x_t, w_t), \quad (t = 1, \ldots, T)$$  \hspace{1cm} (3)

$$x_0 \sim p(x_0), \quad v_t \sim p(v_t), \quad w_t \sim p(w_t)$$

where \(x_t\) is state vector which corresponds to the set of all physical variables in the system at time \(t\), \(y_t\) is observation vector which corresponds to the set of all observations, \(v_t\) and \(w_t\) denote system and observation noise. Simulation model \(\hat{f}(\cdot)\) and observation process are suitably changed and included into the equation (2) and (3). Once the SSM is constructed, we can give state estimation by filtering methods such as particle filtering.

2.2 Particle Filter

Filtering algorithm such as the Kalman filter calculates estimates or the conditional probability distribution function (PDF) of the state vector, \(p(x_t|y_1:t)\), where \(y_1:t\) is the set of observations from time step 1 to time step \(t\), that is \(\{y_1, \ldots, y_t\}\). In Monte Carlo based filtering algorithms such as the particle filter, the conditional PDF of the state is approximated by the set of all realizations:

$$p(x_t|y_{1:t}) \approx \delta(x_t - x^{(i)}_{t|t}), \quad (i = 1, 2, \ldots, N)$$  \hspace{1cm} (4)

$$p(x_t|y_{1:t-1}) \approx \delta(x_t - x^{(i)}_{t|t-1}), \quad (i = 1, 2, \ldots, N)$$  \hspace{1cm} (5)

where \(\delta(\cdot)\) is Dirac’s delta and \(\{x^{(i)}_{t|t})_{i=1}^{N}\) is the set of \(N\) realizations of \(p(x_k|y_{1:t})\).

There are a lot of variants of the PF, we used sequential importance resampling (SIR) filter. The SIR filter algorithm of the non-linear non-Gaussian SSM is as follows:

1. Generate \(\{x^{(i)}_{0|1}\}_{i=1}^{N}\) from pre-determined PDF \(p(x_0)\) and set \(t \leftarrow 1\).

2. (One step ahead prediction) For each \(i = 1, \ldots, N\),

   (a) Generate \(\{v^{(i)}_t\}_{i=1}^{N}\) from \(p(v_t)\).
   (b) Calculate \(x^{(i)}_{t|t-1} = f_t(x_{t-1}, v^{(i)}_t)\).

3. (Filtering) If \(t\) is filtering time, do the following steps. Otherwise, go to the step 4.

   (a) Calculate weight of each state realization \(l^{(i)}_t = w^{(i)}_{t-1}p(y_t|x^{(i)}_{t|t-1})\) for all \(i\) using observation model (3).
   (b) Calculate normalized weight by \(w^{(i)}_t = \frac{l^{(i)}_t}{\sum_j l^{(j)}_t}\).
   (c) Calculate effective sample size \(N_{eff} = 1/(\sum_j (w^{(j)}_t)^2)\).
   (d) If \(N_{eff} < N_{threshold}\) for pre-determined \(N_{threshold}\), go to next step. Otherwise, set \(x_{t|i} = x^{(i)}_{t|t-1}\) and go to step 4.
   (e) Sample with replacement \(N\) times from \(\{x^{(i)}_{t|t-1}\}_{i=1}^{N}\) by the probability of \(\{w^{(i)}_t\}_{i=1}^{N}\) and set them as \(\{x^{(i)}_{t|i}\}_{i=1}^{N}\). Set \(w^{(j)}_t = 1/N\) for all \(i\).

4. If \(t\) is the stopping time \(T\), stop the algorithm.

   Otherwise, set \(t \leftarrow t + 1\) and go to step 2.

This SIR filter gives true estimates in terms of expectation convergence as \(N\) goes to infinity[10].

2.3 Construction of System Model for Macroscopic Parameters

In the particle systems, there are macroscopic parameters such as intensity of interactions among particles. For example, particle simulation method has an interaction range parameter that is determined empirically. It is often difficult to determine these macroscopic parameters because of the difficulty of direct observation. Therefore, these parameters should be modeled as random variables.

Usually, uncertainties in the physical variables are modeled as the initial state variable \(x_0\) and the system noise \(v_t\), whereas the errors in the observation process are modeled as \(w_t\). Because macroscopic parameters are physical variables and affect state variables, they should be included in the state vector \(x_t\) to obtain their estimates in principle.

It is also required to introduce pseudo dynamics of parameters, which does not exist in real. The reason of the requirement is that if initial guess of parameters does not cover the true one, posterior probability density at the true one always comes to zero. It is also the reason that Monte Carlo based estimation algorithm such as the PF can not avoid the problem called degeneracy that deficient number of realizations for representing PDF occurs. Pseudo dynamics solve these problems and enable the estimates of parameters to approach to the true one.

The problem is how to introduce these pseudo dynamics for fast and stable estimation. To obtain parameter estimation fast, the probability distribution function (PDF) of parameter values should have wide support in
the admissible parameter area. It means that if we use Gaussian distribution for random walk, variance should be large. On the other hand, large variance causes instability of parameter estimation. It also causes the degeneracy problem because the support range is often wide relative to the number of realizations. To avoid the degeneracy, variance should be small.

Bounded Gaussian and normal mixture (BGUM) can cope with this paradoxical situation:

\[(1 - \varepsilon)\text{trunc}N(\mu, \sigma^2; l, u) + \varepsilon U(l, u)\]  

(7)

where \(l\) and \(u\) represent lower and upper bound of parameters, \(\text{trunc}N(\mu, \sigma^2; l, u)\) is PDF of truncated Gaussian in the range \([l, u]\), \(U(l, u)\) is an uniform distribution with range \([l, u]\) and \(\varepsilon\) is the mixture rate. Fig. 1 illustrates the PDF of BGUM.

In order to work this dynamics, mixture rate \(\varepsilon\) and variance \(\sigma^2\) should be small. If we set \(\varepsilon = 1\), estimates of macroscopic parameters in the filtering steps are almost independent from previously estimated macroscopic parameters. In other words, we can find changed macroscopic parameters fast without the effect of the previous estimates. On the other hand, if we set \(\varepsilon = 0\) and very small variance for Gaussian part, estimates of the parameters stick to the previous estimates because the proposals of the parameters are restricted around the previous ones.

It also makes sense that the one step ahead prediction PDF of the macroscopic parameters should be changed only at the time just after resampling which occurs at \(N_{eff} < N_{threshold}\). The reason is that we do not take care of the degeneracy problem until \(N_{eff}\) goes to small value and it is checked at the filtering step. In the following, we employ this rule.

3 Numerical experiment

In this section, we check the validity and efficacy of introduction of BGUM for particle systems by numerical experiment of the optimal velocity (OV) model.

3.1 Optimal Velocity Model

The OV model is one of the traffic flow model proposed by Bando et al. In the OV model, each car has a position and a velocity. Its dynamics are written by ordinary differential equations

\[\dot{x}_i = a(-\ddot{x}_i + V(x_{i+1} - x_i))\],  

(8)

\[V(\Delta x) = \tanh(2 - \Delta x) + \tanh(2)\]  

(9)

where \(i(= 1, \ldots, M)\) represents the car number, \(x_i\) is the position of the cars in one dimensional periodic coordinate, \(a\) is sensitivity parameter and \(V(\cdot)\) is an optimal velocity function. Fig. 2 illustrates the setting.

The key feature of the OV model is that each car has dynamical optimal velocity \(V(\cdot)\) which is determined from the distance between the car itself and the one in front, and common sensitivity \(a\) which models reaction to the change from optimal velocity. The sensitivity parameter is the macroscopic one in this model.

3.2 Data Assimilation Settings

The simulation model of the OV model is constructed by Euler’s forward discretization. For the number of cars \(M\), the simulator of the OV model has \(2M\) variables because each car has two variables, speed and position. Macroscopic parameter \(\alpha\) is an additional one for state vector, therefore, the dimension of the state vector should be \(2M + 1\).

The settings of the simulation model and the SIR filter is shown in the Table 1. Because the integration time of the OV model is 1.9 and the step size of Euler scheme is \(1.0 \times 10^{-3}\), the last time step \((T)\) of the SSM is 1900.
Fig. 2: Setting of the optimal velocity model. Each car has two variables, position($x_i$) and speed($\dot{x}_i$). The acceleration of $i$th car is determined from its speed and the distance between itself and the one in front.

Table 1: Parameters for OV model.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Integration time $T_{OV}$</td>
<td>1.9</td>
</tr>
<tr>
<td>Step size $\Delta t$</td>
<td>0.001</td>
</tr>
<tr>
<td>Number of cars $M$</td>
<td>30</td>
</tr>
<tr>
<td>Circumferential length $L$</td>
<td>100</td>
</tr>
<tr>
<td>Number of particles $N$</td>
<td>30000</td>
</tr>
<tr>
<td>SD of observation noise $\sigma_{obs}$</td>
<td>0.01</td>
</tr>
<tr>
<td>Threshold for resampling $N_{threshold}$</td>
<td>27000</td>
</tr>
</tbody>
</table>

The true reaction parameter $a$ in the OV model is set as follows:

$$a = \begin{cases} 
2.0 & (0 \leq t \leq 1000) \\
0.9 & (t > 1000) 
\end{cases}$$

Observations are obtained from average flow of true parameter simulation at every 10 steps of numerical integration. Fig. 3 shows the average flow used for data assimilation.

BGUM parameters are set to $l = 0.1$, $u = 2.5$ and $\sigma = 0.05$ that is determined from the prior knowledge for this model, for example, $a$ should be positive.

3.3 Results

Fig. 4 shows the estimation result of the macroscopic parameter $a$ of the OV model. Red line represents true macroscopic parameter, blue($\epsilon = 0.01$), green($\epsilon = 0.03$) and orange($\epsilon = 0.05$) lines represent estimation results of parameters by BGUM parameter dynamics, and black line is that by Gaussian with $\sigma = 0.05$. Estimates are made by mean of filter distribution of $a$. We can confirm that estimation result of BGUM with $\epsilon = 0.01$ gives fast and stable estimation compared with others.

Table 2 shows the results of the arrival time at true parameter $a = 2$ RMS errors after arrival. RMSE are calculated for the time interval of $a = 2$. It also shows that $\epsilon$ is the trade-off parameter between fast detection and stable estimation. It also implies that introduction of BGUM dynamics is better than that of random walk dynamics for estimation of macroscopic parameters.

4 Conclusion

We formulated data assimilation framework and introduced BGUM dynamics with the SIR filter to find appropriate estimation of the macroscopic parameter in particle simulation systems. The result of numerical experiment implies that BGUM type dynamics enables us to obtain appropriate estimation of macroscopic parameters from macroscopic observations faster than Gaussian noise distribution that is usually employed. In ad-
Table 2: Results of the arrival time at true parameter $a = 2$ and RMSE after arrival. RMSE are calculated for the time interval of $a = 2$.

<table>
<thead>
<tr>
<th>Arrival time RMSE</th>
<th>BGUM($\varepsilon = 0.01$)</th>
<th>BGUM($\varepsilon = 0.03$)</th>
<th>BGUM($\varepsilon = 0.05$)</th>
<th>Gaussian</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>132</td>
<td>121</td>
<td>119</td>
<td>264</td>
</tr>
<tr>
<td></td>
<td>0.050</td>
<td>0.081</td>
<td>0.123</td>
<td>0.071</td>
</tr>
</tbody>
</table>

dition, mixing rate between Gaussian and uniform distribution can control the trade-off between fast detection and stability of estimation results. At present we do not have theoretical support for this approach and further theoretical investigation is required. However, because we can control the mixing rate for different purposes, the introduced framework can correspond with various situations in parameter estimation. It suggests the utility of the introduced framework.

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References


