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ARTICLE

Convergence Monitoring of Markov Chains Generated for Inverse Tracking of Unknown Model Parameters in Atmospheric Dispersion

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The dependency within the sequential realizations in the generated Markov chains and their reliabilities are monitored by introducing the autocorrelation and the potential scale reduction factor (PSRF) by model parameters in the atmospheric dispersion. These two diagnostics have been applied for the posterior quantities of the release point and the release rate inferred through the inverse tracking of unknown model parameters for the Yonggwang atmospheric tracer experiment in Korea. The autocorrelations of model parameters are decreasing to low values approaching to zero with increase of lag, resulted in decrease of the dependencies within the two sequential realizations. Their PSRFs are reduced to within 1.2 and the adequate simulation number recognized from these results. From these two convergence diagnostics, the validation of Markov chains generated have been ensured and PSRF then is especially suggested as the efficient tool for convergence monitoring for the source reconstruction in atmospheric dispersion.

KEYWORDS: atmospheric dispersion, source reconstruction, Markov chain, convergence monitoring, autocorrelation, potential scale reduction factor

I. Introduction

A value from an interesting distribution π is only obtained when the iteration number of the Markov chain approaches infinity. In practice, this is not attainable and a value obtained at a sufficiently large iteration is taken instead of being drawn from π.[1,2)] There is a question that the simulation actually leads to draws from its target distribution and the most basic one is whether such Markov chain can always be constructed and all values sampled from the chain. The problem to be solved is, therefore, the determination of how large this iteration should be to achieve the target distribution. This problem can be answered as convergence monitoring. [3)]

There are two main ways for monitoring convergence. The first one is more theoretical and tries to measure distances and establish bounds on distribution functions generated from a Markov chain. The second one can be approached from a statistical perspective that analyzes the properties of the chain values generated. This is an empirical as opposed to a theoretical treatment and is obviously more practical. However, the difficulty with this approach is that it can never guarantee convergence because it is only based on observations from the chain.

Although two approaches for monitoring convergence are valid and complement each other, theoretical results have been proved to be more difficult to obtain and apply to practical problems. In this study, the convergence monitoring will be only provided for a detailed description based on the statistical properties of the chain generated. The autocorrelation and the potential scale reduction factor (PSRF) will be introduced for the convergence monitoring.[3)] Posterior distributions of interesting model parameters, which are the release point (x, y) and the release rate (Q), have been already obtained through another literature.[4)] The two convergence diagnostics will be tried out for the three posterior distributions.

Since the convergence monitoring for the Bayesian inference has not been defined well, the methods tried out in this study can be applied as useful tools for answering how the reliability of posterior distributions can be ensured and how large the simulation should be considered for achieving the target distributions for all model parameters in this source reconstruction.

II. Materials and Method

1. Autocorrelation

The first form is to consider a single chain and then explore autocorrelations within two sequential results. After convergence, all chain values are given as the target distribution π. The autocorrelation is to examine the dependency within the two sequential sample values at every kth lag after burn-in process. As the lag between iterations increases, the two sequential values become less and less correlated and are virtually independent for a large value of the lag k.

Consider a sequence $\left\{\varphi^{(1)}, \varphi^{(2)}, \cdots, \varphi^{(n)}\right\}$ of length n. Correlations can occur between adjacent members $\left\{\rho(\varphi^{(i)}, \varphi^{(i+1)}\right\}$, and between more distant members $\left\{\rho(\varphi^{(i)}, \varphi^{(i+k)} \approx 0)\right\}$. The kth lag autocorrelation $\hat{\rho}_k$ can be estimated by

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$$\hat{\rho}_k = \frac{Cov\left(\varphi^{(i)}, \varphi^{(i+k)}\right)}{Var\left(\varphi^{(i)}\right)} = \frac{\sum_{i=1}^{n-k}\left(\varphi^{(i)} - \bar{\varphi}\right)\left(\varphi^{(i+k)} - \bar{\varphi}\right)}{\sum_{i=1}^{n-k}\left(\varphi^{(i)} - \bar{\varphi}\right)^2} \quad . \qquad (1)$$

$$with \ \bar{\varphi} = \frac{1}{n}\sum_{i=1}^{n}\varphi^{(i)}$$

BOA (Bayesian Output Analysis) program[5] is especially used for calculating the autocorrelations of the posterior quantities for x, y and Q.

2. Potential scale reduction factor

The second form to monitor convergence is to process m chains in parallel until convergence, say after n iterations, and take as sample elements the nth chain value from each of the m chains. The generation procedure will then require mn generations from the chains. If chains are initialized independently, the sample consists of independent values from π. This diagnostic is named as potential scale reduction factor.[3]

This technique is begun by independently simulating $m \geq 2$ sequences of length $2n$ beginning at starting points over-dispersed with respect to the stationary distribution, and the first n iterations discarded, retaining only the last n ones. Considering m parallel chains and a real function $\varphi = t(\theta)$, there are m trajectories $\left\{\varphi_i^{(1)}, \varphi_i^{(2)}, \cdots, \varphi_i^{(n)}\right\}$, $i = 1, 2, \cdots, m$, for φ. The variances between chains B and within chains W are given by

$$B = \frac{n}{m-1}\sum_{i=1}^{m}\left(\bar{\varphi}_i - \bar{\varphi}\right)^2$$
$$W = \frac{1}{m(n-1)}\sum_{i=1}^{m}\sum_{j=1}^{n}\left(\varphi_i^{(j)} - \bar{\varphi}_2\right)^2, \qquad (2)$$

where $\bar{\varphi}_i$ is the average of observations of chain i, $i = 1, 2, \cdots, m$, and $\bar{\varphi}$ is the average of these averages. Under convergence, all these mn values are drawn from the posterior distributions and $\hat{\sigma}_\varphi^2$, the variance of φ, can be consistently estimated by W, B and the weighted average $\hat{\sigma}_\varphi^2 = \frac{n-1}{n}W + \frac{B}{n}$.

If the chains have not yet converged, then initial values will still be influencing their trajectories. Due to their over-dispersion, they will force $\hat{\sigma}_\varphi^2$ to overestimate σ_φ^2 until the stationary condition is reached. Following this reasoning, an indicator of convergence can be formed by PSRF given as $\hat{R} = \sqrt{\hat{\sigma}_\varphi^2 / W}$, that is always larger than 1. As n approaches to infinity, convergence can be evaluated by the proximity of $\hat{R}$ to 1.

Strictly speaking, if the PSRF approaches to 1.2 with the process of simulation, the convergence of Markov chain is ensured and the optimal iteration number for achieving its target distribution is one corresponding to 1.2.[3] One consideration is that 1.2 is 97.5%ile PSRF. That is, though a conservative estimation is applied for monitoring the PSRF, the converging condition of Markov chain should be satisfied within PSRF of 1.2.

There is no general agreement on the subject of the convergence. Although it is generally agreed that running n parallel chains in practice is computationally inefficient and unnecessary, running multiple parallel chains is generally applied for the convergence monitoring due to easy implementation. The main debate for PSRF is the number of parallel chains needed. If the convergence properties of the chain are well understood then clearly a single chain suffices. Therefore, autocorrelation using single chain and multiple parallel ones are tried and their results then compared with each other in this study. And, the following question is answered from the two convergence results: Have the Markov chain realizations for source reconstruction achieved their target distribution? and which diagnostic is more suitable tool for convergence monitoring?

III. Results and Discussion

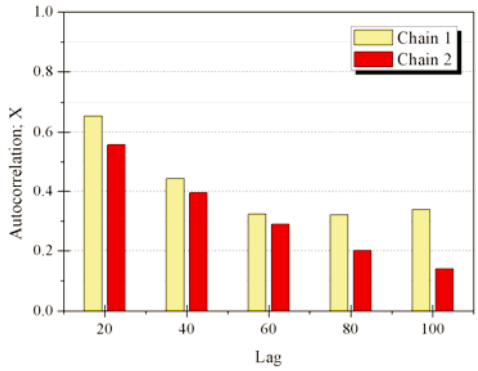
1. Summary of Autocorrelations

The autocorrelations for the realizations of the two Markov chains obtained have been depicted for the model parameters by lag in **Fig. 1**. The lags have been assumed as 20, 40, 60, 80 and 100. All figures show the autocorrelations to be decreased to low values approaching to zero with increase of the lag to 100, even though some variations of the autocorrelations are examined. In Markov chain 1 of x in **Fig. 1**, the autocorrelation shows some increase in lag 100, but this value is not much varied compared with that of lag 80. Therefore, the autocorrelation of x in chain 1 seems to be the optimal value in about 0.3 because of no its decrease. Through the summary of its autocorrelations in Markov chains 1 and 2, the posterior distribution of x has achieved its target one.

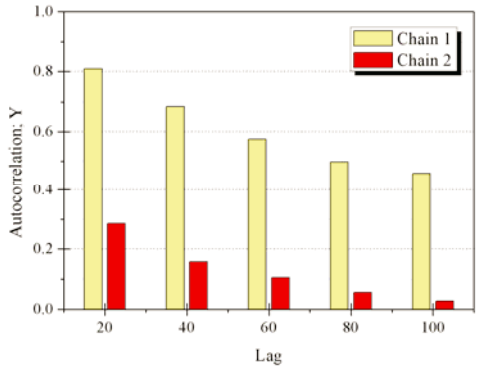
The converging velocities of y and Q in Markov chain 2 are especially faster than chain 1 due to rapidly approaching to low values with increase of the lag as shown in their figures. Through the summary of their autocorrelations in Markov chains 1 and 2, their posterior distributions have achieved its target ones as well. The dependency within two sequential realizations in each Markov chain by model parameter has been well examined from the results of the autocorrelations, and the decrease of the autocorrelations also means that the effect of the initial values on the realizations is being decreased to an insignificant level with increase of simulation.

2. Summary of PSRFs

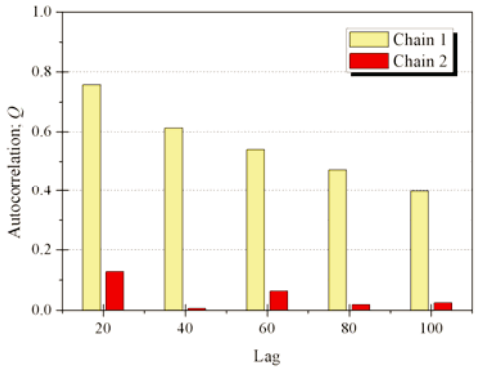
Fig. 2 shows the variation of PSRFs of model parameters vs. simulation. In early simulation stage, the PSRFs exceed 1.2 in all figures due to the effect of initial values on the Markov chains, but satisfy within 1.2 for all the model parameters immediately. From their figures, it is concluded that the Markov chains for x, y and Q have also achieved their target distributions and their convergences are then



(a) x



(b) y



(c) Release rate (Q)

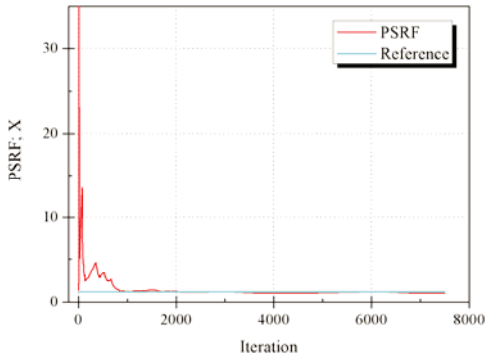
Fig. 1 Summary of autocorrelations

ensured.

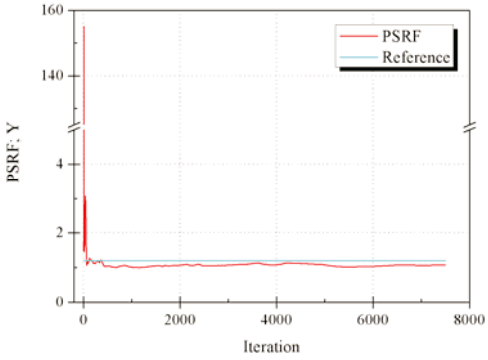
The optimal simulation number for this source reconstruction can be also recognized from PSRF. The optimal iteration for this source reconstruction may be about 8500 including the burn-in, which has been assumed as 7500 in another literature,[4] because of PSRFs satisfying within 1.2 near about simulations of 1000 for all parameters in **Fig. 2**. The reliable probabilistic answer has been, therefore, achieved within simulations of 15000 suggested in this study.

It is possible to selectively apply one of two diagnostics for a strategic purpose. Of course, a few of issues should be considered for selecting one of two diagnostics. First, the autocorrelation is considerably easy to diagnose a convergence of a Markov chains, but, the length of simulation should be much long for achieving the desired target distribution due to using a single Markov chain. A situation is occurred that the simulation approaching to the infinity may be expected for thoroughly exploring a posterior space for a model being estimated. It then means to require more time for simulation.

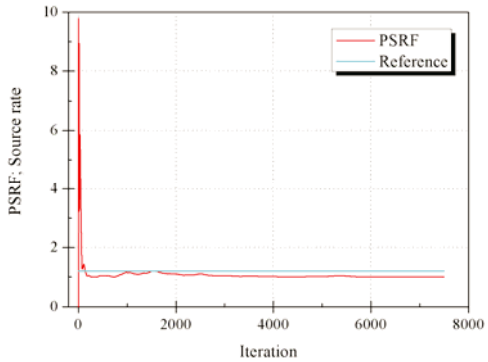
Second, the PSRF can be applied for shorter Markov chains than one required for the autocorrelation, because it is processed by employing multiple parallel chains for the convergence monitoring. But, the problem to be considered is how many chains are suitable for examining PSRF. It has been recommended that Markov chains within 10 be enough to estimate this PSRF according to the presenting studies[3]. But, this selection should not be randomly done without a detail review of the model to be estimated. Two Markov chains have been assumed for the source reconstruction in this study, but they are not always the best selection. The problem is whether the analysts can reasonably determine



(a) x



(b) y



(c) Release rate (Q)

Fig. 2 Summary of PSRFs

the number of Markov chains ensuring the objectivity or not.

Through reviewing the characteristics of the two diagnostics, PSRF is then recommended as more suitable diagnostic for source reconstruction based on MCMC method in this study. This is enables to examine the convergence within comparatively small simulation due to using multiple Markov chains generated. It, in turn, results in that the source reconstruction can be ensured by the small simulation and a more rapid decision would be provided for response under the emergency.

However, the autocorrelation is not inefficient convergence diagnostic for source reconstruction in atmospheric dispersion event. This is still the useful one for evaluating the degrees of two sequential dependencies by lag, which is difficult problem to be solved by PSRF. More meaningful results for the convergence can be obtained by harmoniously combining the two diagnostics.

V. Conclusion

The convergence monitoring is of great importance for validation of Markov chains of the generated model parameters having achieved their target distributions and for determination of the optimal simulation number for achieving them. All model parameters appear to meet the convergences through the autocorrelation and the potential scale reduction factor, and to achieve their target distributions with simulation number under 8500 including the burn-in. And, the approach for identifying optimal simulation number has been provided with PSRF. From these convergence diagnostics, the validation of Markov chains generated has been ensured and PSRF then suggested as the efficient tool for monitoring convergence in this source reconstruction.

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