짱뚱어 자료로 살펴본 장기 시계열 자료의 순차적 몬테 칼로 추론

최일수*

A Sequential Monte Carlo inference for longitudinal data with luespotted mud hopper data

Ilsu Choi

이 논문은 2004년도 여수대학교 연구비를 지원 받았음

요 약

비선형이고 정규분포에 따르지 않는 state-space모형분석에서 순차적 몬테 칼로(SMC)는 유용한 도구 중의 하나이다. 모수와 시그널을 동시에 추정하기 위해 Monte Carlo particle filters를 사용할 수가 있다. 그러나 SMC는 여러단계의 반복을 요구하는 특별한 particle filtering 기법을 필요로 하게 된다. 본 논문은 particle filering과 순차적 hybrid Monte Carlo(SHMC)을 결합하는 방법을 제시하고자 한다. 실험을 위해 짱뚱어 자료를 사용하였다.

ABSTRACT

Sequential Monte Carlo techniques are a set of powerful and versatile simulation-based methods to perform optimal state estimation in nonlinear non-Gaussian state-space models. We can use Monte Carlo particle filters adaptively, i.e. so that they simultaneously estimate the parameters and the signal.

However, Sequential Monte Carlo techniques require the use of special particle filtering techniques which suffer from several drawbacks. We consider here an alternative approach combining particle filtering and Sequential Hybrid Monte Carlo. We give some examples of applications in fisheries(luespotted mud hopper data).

키워드

Sequential Hybrid Monte Carlo, state-space model

Ⅰ. INTRODUCTION

A state-space model is a stochastic process (X_t, Y_t) in which $\{X_t\}$ is an unobservable Markov process with transition probability density function $f(\cdot|\cdot)$ with respect to some measure ν on the state space, and given $\{X_t\}$, the observable random variable Y_t are conditionally independent such that Y_s has density function $g(\cdot|X_s)$ with respect to some measure[3]. Such models have wide discussions of methods in time

* 여수대학교 응용수학과

접수일자 : 2005. 3. 21

series applications and have applications in signal processing, bioinformatics and time series modelling[1,2]. The particle filtering have been suggested in above model. Much of the particle filtering literature has been concerned with filtering for nonlinear models in tracking applications[5,7,8]. There are many other important contexts in which sequential methods are needed. In this paper, we develop sequential Monte Carlo methodology with Hybrid Monte Carlo(HMC) for longitudinal data.

Hybrid Monte Carlo (HMC) which can be very effective means for exploring complex posterior distribution[4]. Hybrid Monte Carlo(HMC) as a Markov chain Monte Carlo(MCMC) technique built upon the basic principle of Hamiltonian mechanics. Its applications in molecular simulation have attracted much interest from researchers. Thus we are to propose that the Sequential Hybrid Monte Carlo(SHMC) within Markov chain Monte Carlo(MCMC), dealing with any nonlinear and non-Gaussian state-space model in a Bayesian framework. We apply Gaussian state-space model in Shephard and Pitt[6] as daily catched data of luespotted mud hopper. We show in this paper that SHMC can very effective means for Bayesian estimation of state-space model. In our initial discussions we will assume the standard

Markovian state-space model

$$x_t \sim f(x_t|x_{t-1}) \text{ [State evolution density]}$$

$$y_t \sim g(y_t|x_t) \text{ [Observation density]}$$

where $\{x_t\}$ are unobserved states of the system and $\{y_t\}$ are observations made over some time interval $t \in \{1, 2, \cdots, T\}$. The initial state has density $p(x_1)$.

Ⅱ. SEQUENTIAL HYBRID MONTE CARLO

We formulate the sequential hybrid Monte Carlo method in terms of updates to the smoothing density. Once we have samples drawn from the smoothing density, it is straightforward to discard those that are not required if filtering is main objective. At time t, we draw $\{x_{j|1:t}, j = 1, 2, \cdots, t\}$ from the smoothing density $p(x_{1:t}|y_{1:t})$ and can represent the SHMC following formula with auxiliary momenta variables $p = (p_1, \cdots, p_t)$ and the related Hamiltonian function $H(x, p)$.

$$H(x,p) = U(x_1, \cdots, x_t) + \frac{1}{2}\sum_{i=1}^{t} p_i^2 = U(x) + \frac{p^2}{2}$$

$$P(x,p) \propto e^{(-H(x,p))} = e^{(-U(x))} e^{(-\frac{p^2}{2})}$$

The method deduce that, form the statistical point of view, the momenta p are nothing but a set of independent, Gaussian distributed, random variables of zero mean and variance equal to the system. There is no simple closed form for the proposal probability $k(x^* \mid x)$, and the proposal change x of x^* is done in the following way: first, a set of initial values for the momenta p are generated by using the Gaussian distribution $e^{(-\frac{p^2}{2})}$, next Hamilton's equation of motion, $\dot{x}_{j|1:t} = p_{j|1:t}$, $\dot{p}_{j|1:t} = F_{j|1:t}$ where $F_{j|1:t}(x) = -\partial U(x)/\partial x_{j|1:t}$ is the force acting on the variable x_i, are integrated numerically using the leap-flog algorithm with a time step δt.

$$x^*_{j|1:t} = x_{j|1:t} + \delta t p_{j|1:t} + \frac{\delta t^2}{2} F_{j|1:t}(x)$$

$$p^*_{j|1:t} = p_{j|1:t} + \frac{\delta t}{2}(F_{j|1:t}(x) + F_{j|1:t}(x^*)),$$
$$j = 1, 2, \cdots, t$$

The proposal x^* is obtained after n iterations of the previous basic integration step. In other words, by numerical integration of Hamilton's equations during a time $n\delta t$. The value x^* must now be accepted with a probability given by

$$h(x^* \mid x) = min\{1, e^{-(H(x^*, p^*) - H(x,p))}\}$$

Ⅲ. BAYESIAN FORMULA VIA SHMC IN STATE-SPACE MODEL

We consider a nonlinear and nonnormal state-space model in the following general form

$x_t = f(x_{t-1}, \eta_t, \delta)$ [Transition Equation]

$y_t = g(x_t, \epsilon_t, \lambda)$ [Measurement Equation]

for $t = 1, 2, \cdots, T$, where T denotes the sample size. Suppose we observe only $y_{1:t} = (y_1, y_2, \cdots, y_t)$ and the functional forms of both $g(\cdot)$ and $f(\cdot)$ are known, whereas $x_{1:t} = (x_1, x_2, \cdots, x_t)$ is not directly observed. Since the analytical computation of the likelihood function of λ is generally infeasible, the standard maximum likelihood estimation method cannot be applied. We overcome this difficulty by contaminated error ϵ_t. Treating the problem as a missing data problem, we write the pseudo posterior distribution of λ and δ as follows,

$$P(x_{1:t}, \lambda \mid Y_{1:t}) \propto P(Y_{1:t} \mid x_{1:t}, \lambda) P(x_{1:t} \mid \lambda) P(\lambda)$$

It can be shown that under mild conditions, the pseudo posterior of λ converges to its true posterior almost surely as $\sigma^2 \rightarrow 0$. Under the setup, the density of x_t and Y_t given λ and δ is written as,

$$P(x_{1:t}, Y_{1:t} \mid \lambda, \delta) = P(x_{1:t} \mid \delta) P(Y_{1:t} \mid x_{1:t}, \lambda)$$

where the two densities in the right hand side are represented by

$$P(x_{1:t} \mid \delta) = P(x_0) \prod_{j=1}^{t} P(x_{1:j} \mid x_{1:j-1}, \delta)$$

$$P(Y_{1:t} \mid x_{1:t}, \lambda) = \prod_{j=1}^{t} P(y_j \mid x_j, \lambda)$$

where $P(x_0 \mid \delta)$ denotes the initial density of x_0 when x_0 is assumed to be a random variable. From the Bayes theorem, the conditional distribution of $x_{\{1:t\}}$ given $Y_{\{1:t\}}$, and δ is obtained as follows

$$P(x_{1:t} \mid Y_{1:t}, \lambda, \delta) = \frac{P(x_{1:t}, Y_{1:t} \mid \lambda, \delta)}{\int P(x_{1:t}, Y_{1:t} \mid \lambda, \delta) dx_{1:t}}$$

Hence Bayesian smoothing random draws via SHMC in State-space model are generated as follows

(STEP)

1. Take appropriate values for λ, δ and $x_{\{1:t\}}$, $t = 1, 2, \cdots, t$

2. Generate a random draw of $x_{\{1:t\}}$ from $P(x_j \mid \cdot)$ for $j = 1, 2, \cdots, t$

 2-1 Generate a new momentum vector x_j from Gaussian distribution $\pi(p_j) \propto \exp\{-K(p_j)\}$

 2-2 Run the leapfrog algorithm for L steps to reach a new configuration in the phase space $(x_j^{(L)}, p_j^{(L)})$

 2-3 Let $(x_{(j,n)}, p_{(j,n)}) = (x_j^{(L)}, p_j^{(L)})$ with probability

$$min[1, \exp(-H(x_j^{(L)}, -p_t^{(L)}) + H(x_{j-1}, -p_t))]$$

where $H(\cdot, \cdot)$ is Hamiltonian.

3. Generate a random draw of λ from $P(\lambda \mid \cdot)$

4. Generate a random draw of δ from $P(\delta \mid \cdot)$

5. Repeat 2)-4) N times to obtain random draws of $x_{\{1:t\}}$, δ and λ.

Ⅳ. APPLICATION

Consider the following Gaussian state-space model in Shephard and Pitt[6]

$$y_t = \mu + x_t + \epsilon_t \qquad \epsilon_t \sim N(0, \sigma_\epsilon^2)$$

$$x_t = \phi x_{t-1} + \eta_t \qquad \eta_t \sim N(0, \sigma_\eta^2)$$

$$x_1 \sim N(0, \sigma_\eta^2/(1-\pi^2))$$

where one observes y and is interested in sampling from the posterior distribution of x and μ. Our dataset consist of daily catched data of luespotted mud hopper from 3/15/2003 to 11/30/2004 (a total of T=480 observations).

Let $x_{1:t} = (x_1, x_2, \cdots, x_t)$ and $y_{1:t} = (y_1, y_2, \cdots, y_t)$, and let the priors of parameters follow

$$\sigma_\eta^2 \sim Inv - \chi^2(\alpha_1, \beta_1)$$
$$\mu \sim N(0, \sigma_\mu^2)$$
$$\sigma_\epsilon^2 \sim Inv - \chi^2(\alpha_2, \beta_2)$$
$$(\phi + 1)/2 \sim Beta(\alpha_3, \beta_3)$$

Then the following conditional distributions can be easily sampled from

$$\sigma_\eta^2 \mid \phi, x_{1:t} \sim Inv - \chi^2(t + \alpha_1, V)$$

$$\phi \mid \sigma_\eta^2, x_{1:t}$$
$$\propto exp\left(- \frac{x_1^2(1-\phi^2) + \sum_{j=1}^{t-1} (x_{j+1} - \phi x_j^2)}{2\sigma_\eta^2} \right)$$
$$(1+\phi)^{\alpha_3 - 0.5}(1-\phi)^{\beta_3 - 0.5}$$

$$\sigma_\epsilon^2 | x_{1:t}, y_{1:t}, \mu$$
$$\sim Inv - \chi^2\left(\alpha_2 + t, \frac{1}{\alpha_2 + T}\left(\alpha_2\beta_2 + \sum_{j=1}^{t} (y_j - \mu - x_t)^2\right)\right)$$

$$\mu \mid x_{1:t}, y_{1:t} \sim \left(\frac{\sigma_\mu^2 \sum_{j=1}^{t} (y_j - \dot{x}_j)}{2(t\sigma_\mu^2 + \sigma_\epsilon^2)}, \frac{\sigma_\epsilon^2 \sigma_\mu^2}{t\sigma_\mu^2 + \sigma_\epsilon^2} \right)$$

where

$$V = \frac{1}{t + \alpha_1}\left(\alpha_1\beta_1 + x_1^2(1-\phi^2) + \sum_{j=2}^{t} (x_j - \phi x_{j-1})^2\right)$$

Once the parameter values are given, the negative log density is

$$U(x_{1:t}) = \sum_{j=1}^{t} \frac{(y_j - \mu - x_j)^2}{2} + \frac{x_1^2(1-\phi^2)}{2\sigma_\eta^2} + \sum_{j=1}^{t-1} \frac{(x_{j+1} - \phi x_j)^2}{2\sigma_\eta^2}$$

The posterior density of $x_{1:t}$, given the parameter values, is proportional to $e(-U(x_{1:t}))$.

V. RESULTS AND CONCLUSION

We implemented the following iterative sampling algorithm: Given ,we drew the parameters , and from the above conditional distributions; whereas given the realized values of the parameters, we drew the state variable by the SHMC. This SHMC within Gibbssampler were run for 110,000 iterations and the results from the last 100,000 iterations are reported in table 1.

table 1. Bayes estimates of the parameters.

variables	mean	sd	MC error	2.5%	median	97.5%
β_2	0.5009	0.2882	9.422E-4	0.0249	0.502	0.9744
ϕ	0.9993	0.00058	2.735E-6	0.9978	0.999	0.9999
σ^2	0.0017	0.00024	8.064E-7	0.0013	0.001	0.0023

We have the result that is the density estimator of the parameters in figure 1-3. Especially σ^2 is a important measure of volatility. SHMC is stable since the density estimator of this paper is so stable. The state-space models that they used are quite restricted to some functional forms, because they studied the special state-space models such that it is easy to generate random draws from the underlying assumptions or they considered the case where rejection method works well. We have shown the SHMC within Gibbs sampler.

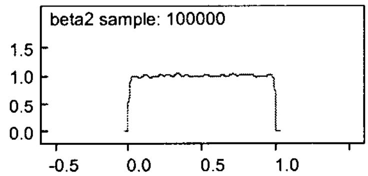

Figure 1. Bayesian density estimator of β_2

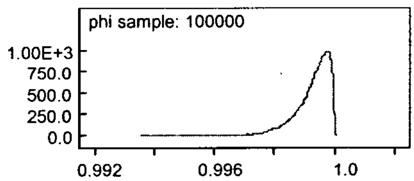

Figure 2. Bayesian density estimator of ϕ

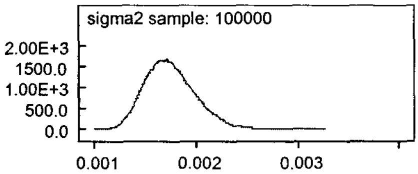

Figure 3. Bayesian density estimator of σ^2

References

[1] B. P. Carlin, N. G. Polson and D. S. Stoffer,A Monte Carlo Approach to Nonnormal and nonlinear State Space Modeling, Journal of American Statistical Association, vol 87, pp. 493-500, 1992.

[2] C. K. Carter and R. Kohn, On Gibbs sampling for state space models, Biometrika, vol 81-3, pp. 541-553, 1994.

[3] C. K. Carter and R. Kohn, Markov Chain Monte Carlo in Conditionally Gaussian State space models, Biometrika, vol 83-3, pp. 589-601, 1996.

[4] S. Duane, A. D. Kennedy, B. Pendleton, B and D. Roweth, Hybrid Monte Carlo , Physics Letters B, vol 195, pp. 216-222, 1984.

[5] J. Geweke and H. Tanizaki, Bayesian Estimation of State-Space Models Using the Metropolis-Hastings Algorithm within Gibbs Sampling, Unpublished manuscript, 1999.

[6] N. Shephard and M. K. Pitt, Likelihood analysis of non-Gaussian measurement time series. Biometrika vol 84, pp. 653-667, 1997.

[7] H. Tanizaki, Nonlinear Filters: Estimation and Applications (Second, rivesed and enlarged edition), Springer-Verlag, 1996.

[8] H. Tanizaki, On the Nonlinear and nonnormal filter using rejection sampling, IEEE transactions on automatic control, vol 44, pp 314-319, 1999.

저자약력

최일수(Ilsu Choi)

1997년 9월～현재 여수대학교 응용수학과 부교수

※ 관심분야 : 베이지안 통계학, 자원생물 통계학