

Stat 535 C - Statistical Computing & Monte Carlo Methods

Lecture 20 - 23rd March 2006

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1.1– Outline

- Nonlinear Non Gaussian Dynamic Models.
- Sequential Bayesian Inference.
- Sequential Importance Sampling.
- Sequential Importance Sampling Resampling.

2.1– What have we done so far?

- MCMC are iterative algorithms to sample from a fixed target distribution $\pi(x) \propto f(x)$ defined on \mathcal{X} .
- MCMC methods can also be used to estimate the normalizing constant $\int f(x) dx$ although there is no simple efficient method.
- MCMC methods are not adapted to sequential Bayesian inference where the posterior has to be recomputed each time a new observation is received.
- Generally speaking MCMC are not useful when the target distribution is “time-varying”; annealing is an exception but it requires target variations to decrease over time.

2.1– What have we done so far?

- Today we will present an alternative set of methods which allows us to estimate “time-varying” targets.
- These methods are non-iterative methods and rely on Importance sampling and resampling mechanisms.
- For sake of illustration, we will detail here an application to nonlinear non-Gaussian state-space models.
- We will show in the next lectures that the methodology is much more general.

3.1– Nonlinear non-Gaussian State-space models

- A nonlinear non-Gaussian state-space model is defined by a pair of stochastic processes $\{X_k\}_{k \geq 1}$ and $\{Y_k\}_{k \geq 1}$. $\{X_k\}_{k \geq 1}$ is an unobserved (hidden) Markov process defined by

$$X_1 \sim \mu, \quad X_k | (X_{k-1} = x_{k-1}) \sim f(\cdot | x_{k-1}).$$

The observations $\{Y_k\}_{k \geq 1}$ are conditionally independent given $\{X_k\}_{k \geq 1}$ and

$$Y_n | (X_k = x_k) \sim g(\cdot | x_k).$$

- The aim is to recover optimally (in a sense to precise) $\{X_k\}_{k \geq 1}$ given $\{Y_k\}_{k \geq 1}$.

3.1– Nonlinear non-Gaussian State-space models

3.1– Nonlinear non-Gaussian State-space models

- Remember that this class of models is extremely general and includes for example

$$X_k = \varphi(X_{k-1}, V_k) \text{ where } V_k \stackrel{\text{i.i.d.}}{\sim} f_V,$$

$$Y_k = \psi(X_k, W_k) \text{ where } W_k \stackrel{\text{i.i.d.}}{\sim} g_V.$$

- See Lecture 12 for numerous examples.

3.2– Some Examples

- *Stochastic Volatility model*

$$X_k = \phi X_{k-1} + \sigma V_k, \quad V_k \stackrel{\text{i.i.d.}}{\sim} \mathcal{N}(0, 1), \quad X_1 \sim \mathcal{N}\left(0, \frac{\sigma}{1 - \phi^2}\right)$$

$$Y_k = \beta \exp(X_k/2) W_k, \quad W_k \stackrel{\text{i.i.d.}}{\sim} \mathcal{N}(0, 1)$$

- *Bearings only tracking*

$$X_k = AX_{k-1} + BV_k, \quad V_k \stackrel{\text{i.i.d.}}{\sim} \mathcal{N}(0, \Sigma),$$

$$Y_k = \tan^{-1}\left(\frac{X_{k,3}}{X_{k,1}}\right) + \sigma W_k, \quad W_k \stackrel{\text{i.i.d.}}{\sim} \mathcal{N}(0, 1)$$

- In both cases, we have typically high-frequency data.

4.1– Bayesian model

- The evolution equation defines a prior for $X_{1:n} = (X_1, \dots, X_n)$

$$p(x_{1:n}) = \mu(x_1) \prod_{k=2}^n f(x_k | x_{k-1}).$$

- The observation equation defines a likelihood

$$p(y_{1:n} | x_{1:n}) = \prod_{k=1}^n g(y_k | x_k).$$

- We are “naturally” in a Bayesian framework.

4.2– Bayesian Inference

- Inference about $X_{1:n}$ given a realization of the observations $y_{1:n}$ is based on

$$p(x_{1:n} | y_{1:n}) = \frac{p(x_{1:n}) p(y_{1:n} | x_{1:n})}{\int p(x_{1:n}) p(y_{1:n} | x_{1:n}) dx_{1:n}} \propto p(x_{1:n}) p(y_{1:n} | x_{1:n}).$$

- We might also be interested in computing the marginal likelihood for model choice or ML parameter estimation

$$p(y_{1:n}) = \int p(x_{1:n}) p(y_{1:n} | x_{1:n}) dx_{1:n}$$

- Typically this posterior and the marginal likelihood does not admit a closed-form expression except in the (very) important cases where $\{X_k\}$ takes values in a finite state-space or $\{X_k\}$ & $\{Y_k\}$ follow linear Gaussian equations.

4.3– Bayesian Computation

- We have seen before how to estimate $p(x_{1:n} | y_{1:n})$ using MCMC.
- However, in many real-world applications, each time we receive a new observation say y_{n+1} at time $n + 1$, we want to update our knowledge, that is compute $p(x_{1:n+1} | y_{1:n+1})$ and in particular we are often interested in $p(x_{n+1} | y_{1:n+1})$.
- We could run a new MCMC of invariant $p(x_{1:n+1} | y_{1:n+1})$ but this is computationally expensive and the computational complexity would increase over time!
- We would like to have an algorithm whose computational complexity is independent of the time index n .

4.4– Recursion for the successive target distributions

- The basic idea consists of reusing the approximation of $p(x_{1:n} | y_{1:n})$ available at time n to generate an approximation of $p(x_{1:n+1} | y_{1:n+1})$.

- One has

$$\begin{aligned} p(x_{1:n+1} | y_{1:n+1}) &= \frac{p(y_{n+1} | x_{1:n+1}, y_{1:n}) p(x_{1:n+1} | y_{1:n})}{p(y_{n+1} | y_{1:n})} \\ &= \frac{p(y_{n+1} | x_{1:n+1}, y_{1:n}) p(x_{n+1} | x_{1:n}, y_{1:n}) p(x_{1:n} | y_{1:n})}{p(y_{n+1} | y_{1:n})} \\ &= \frac{g(y_{n+1} | x_{n+1}) f(x_{n+1} | x_n) p(x_{1:n} | y_{1:n})}{p(y_{n+1} | y_{1:n})}. \end{aligned}$$

4.4– Recursion for the successive target distributions

- An alternative way to derive the formula is as follows

$$\begin{aligned} p(x_{1:n+1} | y_{1:n+1}) &\propto p(x_{1:n+1}) p(y_{1:n+1} | x_{1:n+1}) \\ &\propto \mu(x_1) \prod_{k=2}^{n+1} f(x_k | x_{k-1}) \prod_{k=1}^{n+1} g(y_k | x_k) \\ &\propto f(x_{n+1} | x_n) g(y_{n+1} | x_{n+1}) p(x_{1:n}) p(y_{1:n} | x_{1:n}) \\ &\propto f(x_{n+1} | x_n) g(y_{n+1} | x_{n+1}) p(x_{1:n} | y_{1:n}) \end{aligned}$$

4.4– Recursion for the successive target distributions

- In most of the literature, you'll find the following recursion on the *marginal* distributions $\{p(x_n | y_{1:n})\}$

$$p(x_{n+1} | y_{1:n}) = \int f(x_{n+1} | x_n) p(x_n | y_{1:n}) dx_n,$$

$$p(x_{n+1} | y_{1:n+1}) = \frac{g(y_{n+1} | x_{n+1}) p(x_{n+1} | y_{1:n})}{p(y_{n+1} | y_{1:n})}$$

- This recursion yields the standard HMM filter and the Kalman filter for linear Gaussian models.
- In our case, this recursion will NOT be used and we will always deal with the joint distributions even if we are only interested in approximating $\{p(x_n | y_{1:n})\}$.

4.5– Building Sequentially Monte Carlo Approximations

- Assume that you are at time 1 and want to approximate $p(x_1|y_1)$ then, because the state is usually of reasonable dimension, you can use importance sampling.
- We select an importance distribution $q_1(x_1|y_1)$ and use the identity

$$p(x_1|y_1) = \frac{w_1(x_1, y_1) q_1(x_1|y_1)}{\int w_1(x_1, y_1) q_1(x_1|y_1) dx_1}$$

where

$$w_1(x_1, y_1) = \frac{p(x_1, y_1)}{q_1(x_1|y_1)}.$$

4.5– Building Sequentially Monte Carlo Approximations

- We sample N particles (random samples)

$$X_1^{(i)} \sim q_1(x_1 | y_1)$$

and obtain the approximation

$$p^N(x_1 | y_1) = \sum_{i=1}^N W_1^{(i)} \delta_{X_1^{(i)}}(x_1)$$

where

$$W_1^{(i)} = \frac{w_1(X_1^{(i)}, y_1)}{\sum_{j=1}^N w_1(X_1^{(j)}, y_1)}.$$

4.5– Building Sequentially Monte Carlo Approximations

- Now at time 2, we want to approximate $p(x_{1:2}|y_{1:2})$. We can also use IS to achieve that by selecting an importance distribution $q_2(x_{1:2}|y_{1:2})$, using the identity

$$p(x_{1:2}|y_{1:2}) = \frac{w_2(x_{1:2}, y_{1:2}) q_2(x_{1:2}|y_{1:2})}{\int w_2(x_{1:2}, y_{1:2}) q_2(x_{1:2}|y_{1:2}) dx_{1:2}},$$

$$w_2(x_{1:2}, y_{1:2}) = \frac{p(x_{1:2}, y_{1:2})}{q_2(x_{1:2}|y_{1:2})}$$

and sampling a large number N of particles

$$X_{1:2}^{(i)} \sim q_2(x_{1:2}|y_{1:2})$$

to obtain

$$p^N(x_{1:2}|y_{1:2}) = \sum_{i=1}^N W_2^{(i)} \delta_{X_{1:2}^{(i)}}(x_{1:2}) \text{ with } W_2^{(i)} \propto w_2(X_{1:2}^{(i)}, y_{1:2}).$$

4.5– Building Sequentially Monte Carlo Approximations

- We could repeat this method at each time step n . This would require designing an IS distribution $q_n(x_{1:n} | y_{1:n})$, sampling N paths $X_{1:n}^{(i)} \sim q_n(x_{1:n} | y_{1:n})$ and computing the associated weights

$$W_n^{(i)} \propto w_n \left(X_{1:n}^{(i)}, y_{1:n} \right) \text{ where } w_n \left(X_{1:n}^{(i)}, y_{1:n} \right) = \frac{p \left(X_{1:n}^{(i)}, y_{1:n} \right)}{q_n \left(X_{1:n}^{(i)} \mid y_{1:n} \right)}.$$

- In the general case this is NOT a sequential method because the computational complexity increases with the time index n .
- A very simple remark allows us to derive a sequential algorithm. We are going to limit the form of the IS distribution.

4.6– Sequential Importance Sampling

- At time n , we propose not to sample new paths $X_{1:n}^{(i)}$ but to keep the paths $X_{1:n-1}^{(i)}$ which are available at time $n-1$ and just add a component $X_n^{(i)}$.

Mathematically, it means that we set

$$\begin{aligned} q_n(x_{1:n} | y_{1:n}) &= \underbrace{q_{n-1}(x_{1:n-1} | y_{1:n-1})}_{\text{distribution of the paths } X_{1:n-1}^{(i)} \text{ at time } n-1} \\ &\times \underbrace{q_n(x_n | y_{1:n}, x_{1:n-1})}_{\text{conditional distribution of the new component } X_n^{(i)}} \\ &= q_1(x_1 | y_1) \prod_{k=2}^n q_k(x_k | y_{1:k}, x_{1:k-1}) \end{aligned}$$

4.6– Sequential Importance Sampling

- In practice, we will actually only use distributions of the form

$$q_n(x_n | y_{1:n}, x_{1:n-1}) = q_n(x_n | y_n, x_{n-1}).$$

This will be justified later but this should be intuitive. Given x_{n-1} , $y_{1:n-1}$ and $x_{1:n-2}$ do not bring any information about X_n .

- We don't have yet a recursive method as IS requires not only to sample the paths $X_{1:n}^{(i)}$ but also requires the computation of the weights

$$W_n^{(i)} \propto w_n(X_{1:n}^{(i)}, y_{1:n})$$

4.6– Sequential Importance Sampling

- The weights satisfy the following recursion

$$\begin{aligned}w_n(x_{1:n}, y_{1:n}) &= \frac{p(x_{1:n}, y_{1:n})}{q_n(x_{1:n} | y_{1:n})} \\ &= \frac{p(x_{1:n-1}, y_{1:n-1})}{q_{n-1}(x_{1:n-1} | y_{1:n-1})} \times \frac{f(x_n | x_{n-1}) g(y_n | x_n)}{q_n(x_n | y_n, x_{n-1})} \\ &= w_{n-1}(x_{1:n-1}, y_{1:n-1}) \times \frac{f(x_n | x_{n-1}) g(y_n | x_n)}{q_n(x_n | y_n, x_{n-1})}\end{aligned}$$

- This implies that

$$W_n^{(i)} \propto W_{n-1}^{(i)} \frac{f(X_n^{(i)} | X_{n-1}^{(i)}) g(y_n | X_n^{(i)})}{q_n(X_n^{(i)} | y_n, X_{n-1}^{(i)})}$$

- We have designed a SIS scheme of computational complexity $O(N)$ independent of the time index.

4.6– Sequential Importance Sampling

Given $\{X_{n-1}^{(i)}, W_{n-1}^{(i)}\}$ approximating $p(x_{1:n-1} | y_{1:n-1})$ at time $n-1$, the algorithm proceeds as follows at time n .

- At time n

- Sample $X_n^{(i)} \sim q_n(x_n | y_n, X_{n-1}^{(i)})$ for $i = 1, \dots, N$

- Compute the weights

$$W_n^{(i)} \propto W_{n-1}^{(i)} \frac{f(X_n^{(i)} | X_{n-1}^{(i)}) g(y_n | X_n^{(i)})}{q_n(X_n^{(i)} | y_n, X_{n-1}^{(i)})}$$

4.7– Selection of the Importance Distribution

- We know that it is crucial to select a good importance distribution for IS estimate to have reasonable performance.
- The optimal choice is obviously given by

$$q_n(x_{1:n} | y_{1:n}) = p(x_{1:n} | y_{1:n})$$

but this choice is impossible and we cannot even get a reasonable approximation of it (as in MCMC) because of the sequential design of the importance distribution. For example, remember that $X_1^{(i)} \sim q_1(x_1 | y_1)$ whereas at time n , we would love to have $X_1^{(i)} \sim p(x_1 | y_{1:n})!$

4.8– Suboptimal distributions

- A “locally” optimal choice consists of selecting the distribution $q_n(x_n | y_n, x_{n-1})$ minimizing the variance of

$$\begin{aligned} w_n(x_{1:n}, y_{1:n}) &= \frac{p(y_{1:n}) p(x_{1:n} | y_{1:n})}{q_{n-1}(x_{1:n-1} | y_{1:n-1}) q_n(x_n | y_n, x_{n-1})} \\ &= \frac{p(y_{1:n}) p(x_{1:n-1} | y_{1:n-1})}{q_{n-1}(x_{1:n-1} | y_{1:n-1})} \times \frac{p(x_n | y_n, x_{n-1})}{q_n(x_n | y_n, x_{n-1})} \end{aligned}$$

conditional upon $x_{1:n-1}$. This is given by

$$q_n(x_n | y_n, x_{n-1}) = p(x_n | y_n, x_{n-1}) = \frac{f(x_n | x_{n-1}) g(y_n | x_n)}{\int f(x_n | x_{n-1}) g(y_n | x_n) dx_n}$$

and

$$w_n(x_{1:n}, y_{1:n}) \propto w_n(x_{1:n-1}, y_{1:n-1}) \times \int f(x_n | x_{n-1}) g(y_n | x_n) dx_n.$$

4.8– Suboptimal distributions

- It is not always possible to use this choice but one can make some approximations.
- For example, one can use an Extended/Unscented Kalman filter to come up with a clever proposal.
- The key is once more that asymptotically (as $N \rightarrow \infty$), the Monte Carlo approximation will converge towards the true values.

4.8– Suboptimal distributions

- A simpler choice consists of selecting

$$q_n(x_{1:n} | y_{1:n}) = p(x_{1:n})$$

that is

$$q_n(x_1 | y_1) = \mu(x_1) \quad \text{and} \quad q_n(x_n | y_n, x_{n-1}) = f(x_n | x_{n-1})$$

and

$$w_n(x_{1:n}, y_{1:n}) = w_{n-1}(x_{1:n-1}, y_{1:n-1}) \times g(y_n | x_n).$$

- This choice will be extremely poor if the data are very informative and the prior is diffuse.

4.9– Application to Stochastic Volatility

- We present a simple application to SV where

$$f(x_k | x_{k-1}) = \mathcal{N}(x_k; \phi x, \sigma^2),$$

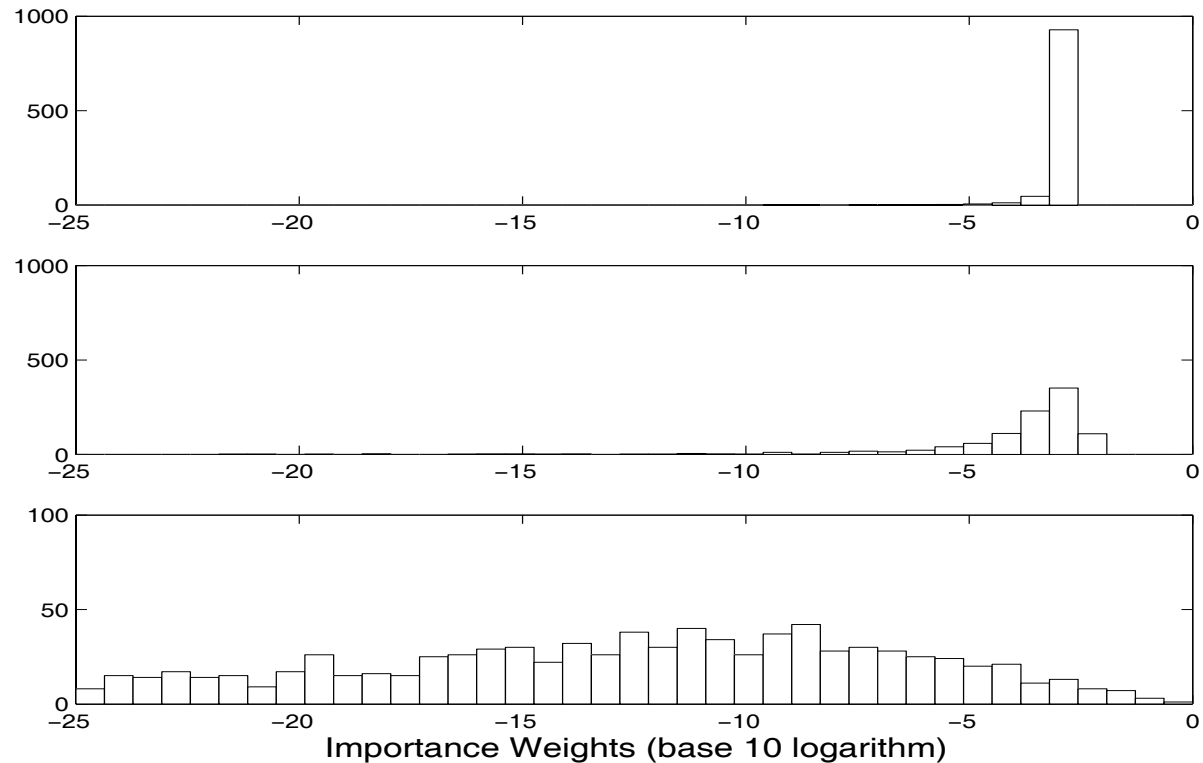
$$g(y_k | x_k) = \mathcal{N}(y_k; 0, \beta^2 \exp(x_k)).$$

- We cannot sample from $p(x_n | y_n, x_{n-1})$ but it is unimodal and we can compute numerically its mode $m_n(x_{n-1})$ and use a t -distribution with 5 degrees of freedom and scale set as the inverse of the negated second-order of $\log p(x_n | y_n, x_{n-1})$ evaluated at $m_n(x_{n-1})$ and given by

$$\sigma_n^2(x_{n-1}) = \left(\frac{1}{\sigma^2} + \frac{y_n^2}{2\beta^2} \exp(-m_n(x_{n-1})) \right)^{-1}.$$

4.10– Simulation Results

- The algorithm performs **EXTREMELY** poorly! After a few time steps, only a very small number of particles have non negligible weights.



Histograms of the base 10 logarithm of $W_n^{(i)}$ for $n = 1$ (top), $n = 50$ (middle) and $n = 100$ (bottom).

4.10– Simulation Results

- You should not be surprised! This algorithm is nothing but an implementation of IS where we severely restrict the structure of the importance distribution.
- As the dimension of the target $p(x_{1:n} | y_{1:n})$ increases over time, the problem is becoming increasingly difficult. In practice, the discrepancy between the target and the IS distribution $q_n(x_{1:n} | y_{1:n})$ can only also increase (on average).
- As n increases the variance of the weights increases (typically geometrically) and the IS approximation collapses.
- You can use any IS distribution you want (even the locally optimal one), the algorithm will collapse.

5.1– Resampling

- *Intuitive KEY idea:* When the variance of the weights $\{W_n^{(i)}\}$ is high, we would like to get rid of the particles with low weights (relative to $1/N$) and multiply the particles with high weights.
- The main reason is that if a particle at time n has a low weight then typically it will still have a low weight at time $n + 1$ (though I can easily give you a counterexample).
- You want to focus your computational efforts on the “promising” parts of the space.

5.1– Resampling

- To measure the variation of the weights, we can use the Effective Sample Size (ESS) or the coefficient of variation CV

$$ESS = \left(\sum_{i=1}^N \left(W_n^{(i)} \right)^2 \right)^{-1}, \quad CV = \left(\frac{1}{N} \sum_{i=1}^N \left(N W_n^{(i)} - 1 \right)^2 \right)^{1/2}$$

- We have $ESS = N$ and $CV = 0$ if $W_n^{(i)} = 1/N$ for any i .
- We have $ESS = 1$ and $CV = \sqrt{N-1}$ if $W_n^{(i)} = 1$ and $W_n^{(j)} = 1$ for $j \neq i$.

5.1– Resampling

- We can also use the entropy

$$Ent = - \sum_{i=1}^N W_n^{(i)} \log_2 \left(W_n^{(i)} \right)$$

- We have $Ent = \log_2 (N)$ if $W_n^{(i)} = 1/N$ for any i .
- We have $Ent = 0$ if $W_n^{(i)} = 1$ and $W_n^{(j)} = 0$ for $j \neq i$.

5.1– Resampling

- If the variation of the weights as measured by ESS, CV or Ent is too high, then we resample the particles.
- The simplest way to resample the particles consists of resampling N times from the current approximation

$$\overline{X}_{1:n}^{(i)} \sim p^N(x_{1:n} | y_{1:n})$$

where

$$p^N(x_{1:n} | y_{1:n}) = \sum_{i=1}^N W_n^{(i)} \delta_{X_{1:n}^{(i)}}(x_{1:n}).$$

5.1– Resampling

- This corresponds to perform an approximation of $p^N (x_{1:n} | y_{1:n})$

$$\sum_{i=1}^N \frac{N_n^{(i)}}{N} \delta_{X_{1:n}^{(i)}} (x_{1:n}) \simeq \sum_{i=1}^N W_n^{(i)} \delta_{X_{1:n}^{(i)}} (x_{1:n})$$

where $N_n^{(i)}$ is the number of offspring of the particle $X_{1:n}^{(i)}$ and $\sum_{i=1}^N N_n^{(i)} = N$.

- The previous scheme is equivalent to sample

$$\left(N_n^{(1)}, \dots, N_n^{(N)} \right) \sim \mathcal{M} \left(N; W_n^{(1)}, \dots, W_n^{(N)} \right)$$

which is such that $E \left(N_n^{(i)} \right) = N W_n^{(i)}$ but better schemes can be developed.

5.1– Resampling

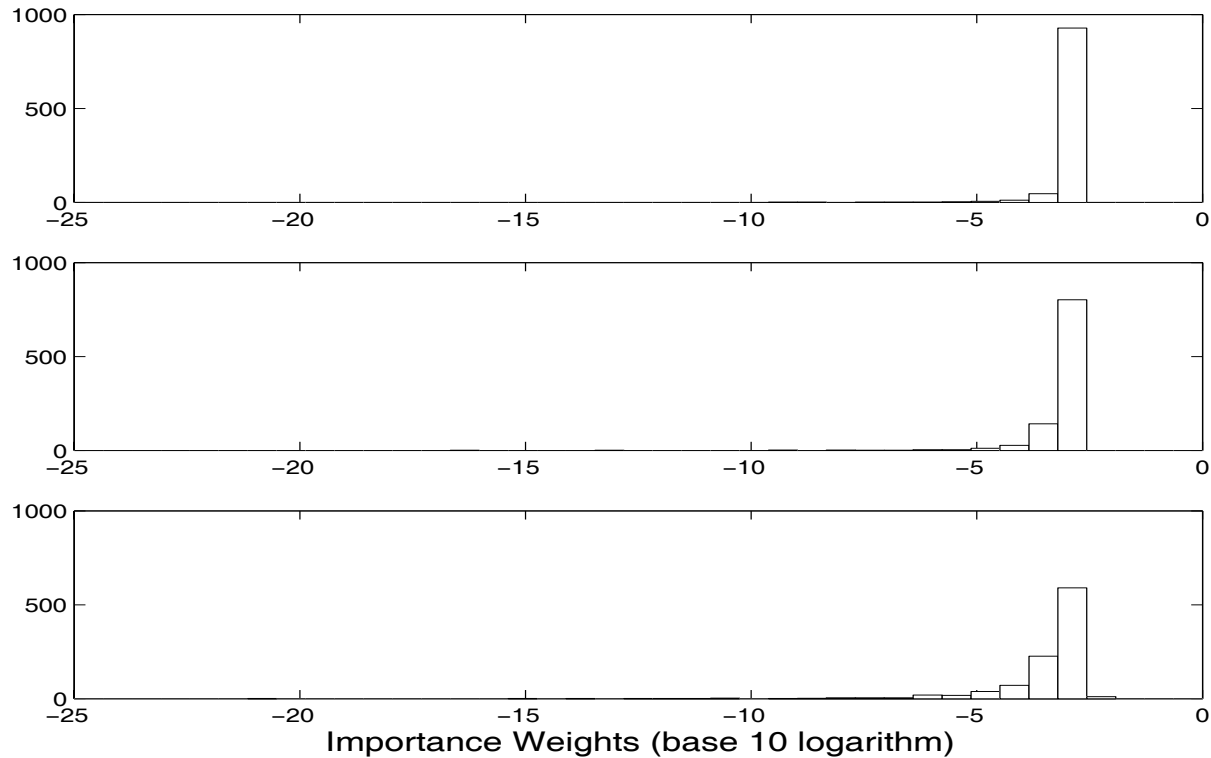
- At time n
 - Sample $X_n^{(i)} \sim q_n \left(x_n | y_n, X_{n-1}^{(i)} \right)$ for $i = 1, \dots, N$
 - Compute the weights

$$W_n^{(i)} \propto W_{n-1}^{(i)} \frac{f \left(X_n^{(i)} | X_{n-1}^{(i)} \right) g \left(y_n | X_n^{(i)} \right)}{q_n \left(X_n^{(i)} | y_n, X_{n-1}^{(i)} \right)}$$

- If the variation of the weights is high, resample the particles

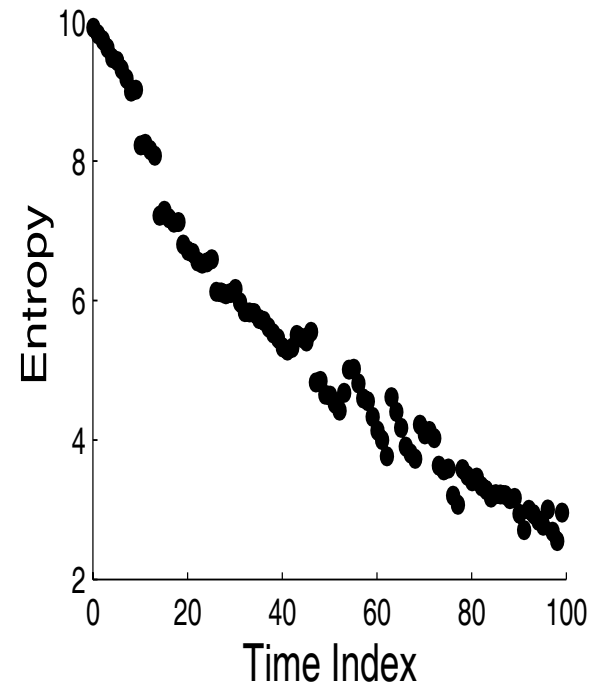
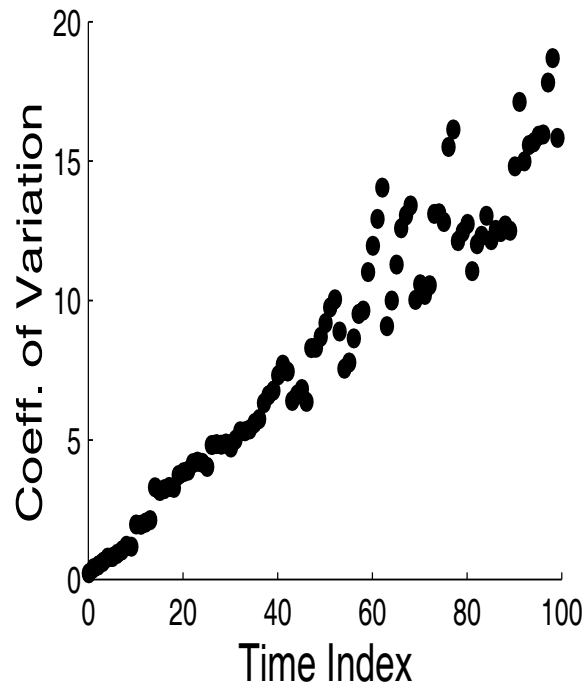
$\left\{ X_{1:n}^{(i)}, W_n^{(i)} \right\}$ to obtain a new population $\left\{ X_{1:n}^{(i)}, 1/N \right\}$.

5.1– Resampling



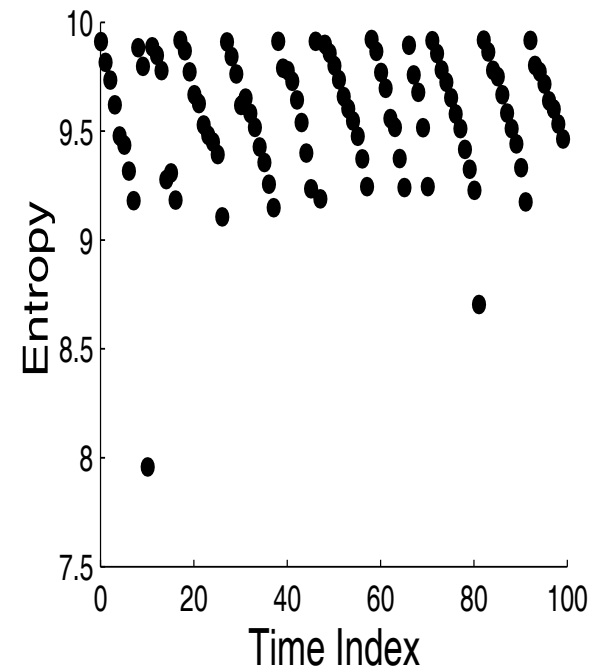
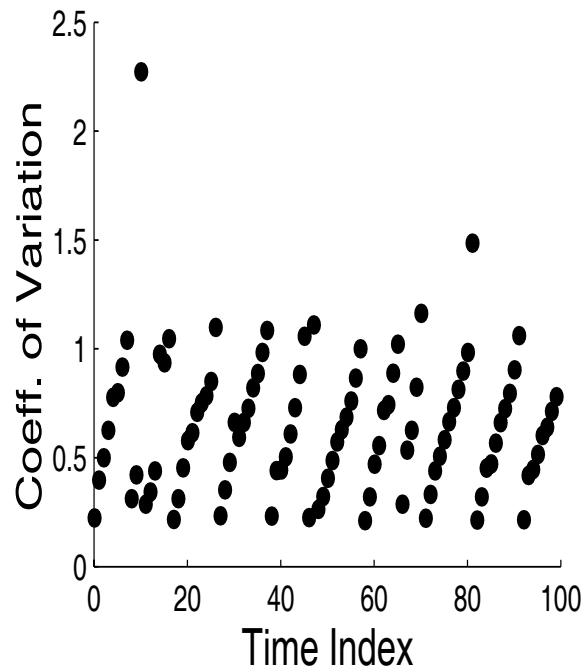
Histograms of the base 10 logarithm of $W_n^{(i)}$ for $n = 1$ (top), $n = 50$ (middle) and $n = 100$ (bottom).

5.1– Resampling



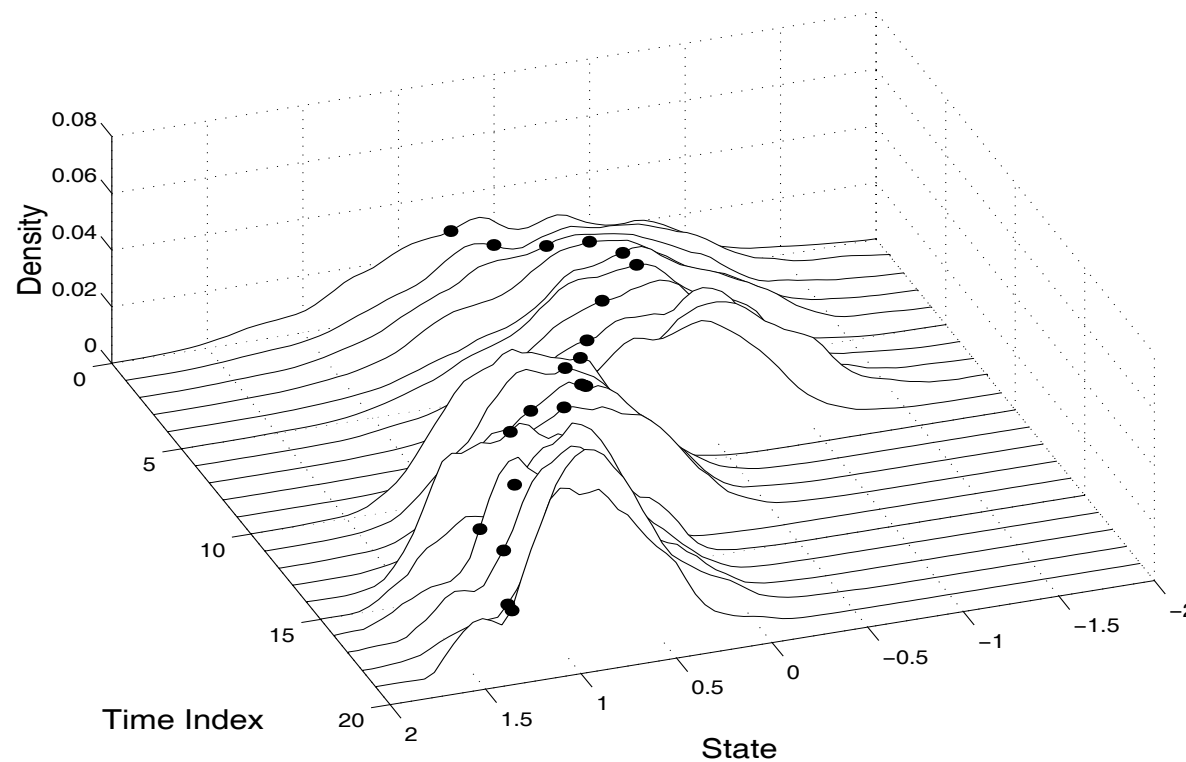
Coefficient of Variation and Entropy when NO resampling is used.

5.1– Resampling



Coefficient of Variation and Entropy when Resampling is used.

5.1– Resampling



Monte Carlo estimates of the marginal distributions $p(x_n | y_{1:n})$
and true values of $\{X_n\}$.

6.1– Summary

- Sequential Importance Sampling is inefficient.
- Resampling is a simple and effective mechanism which mitigates this problem.
- Next week, we will discuss the design of efficient SMC.