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Sequential Monte Carlo samplers

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Summary. We propose a methodology to sample sequentially from a sequence of probability distributions that are defined on a common space, each distribution being known up to a normalizing constant. These probability distributions are approximated by a cloud of weighted random samples which are propagated over time by using sequential Monte Carlo methods. This methodology allows us to derive simple algorithms to make parallel Markov chain Monte Carlo algorithms interact to perform global optimization and sequential Bayesian estimation and to compute ratios of normalizing constants. We illustrate these algorithms for various integration tasks arising in the context of Bayesian inference.

Keywords: Importance sampling; Markov chain Monte Carlo methods; Ratio of normalizing constants; Resampling; Sequential Monte Carlo methods; Simulated annealing

1. Introduction

Consider a sequence of probability measures $\{\pi_n\}_{n\in\mathbb{T}}$ that are defined on a common measurable space $(E, \mathcal{E})$, where $\mathbb{T} = \{1, \ldots, p\}$. For ease of presentation, we shall assume that each $\pi_n(\mathrm{d}x)$ admits a density $\pi_n(x)$ with respect to a σ-finite dominating measure denoted $\mathrm{d}x$. We shall refer to n as the time index; this variable is simply a counter and need not have any relationship with 'real' time. We also denote, by E_n, the support of π_n, i.e. $E_n = \{x \in E : \pi_n(x) > 0\}$. In this paper, we are interested in sampling from the distributions $\{\pi_n\}_{n\in\mathbb{T}}$ *sequentially*, i.e. first sampling from π_1, then from π_2 and so on.

This problem arises in numerous applications. In the context of sequential Bayesian inference, π_n could be the posterior distribution of a parameter given the data collected until time n, e.g. $\pi_n(x) = p(x|y_1, \ldots, y_n)$. In a batch set-up where a fixed set of observations $y_1, \ldots, y_p$ is available, we could also consider the sequence of distributions $p(x|y_1, \ldots, y_n)$ for $n \leqslant p$ for the following two reasons. First, for large data sets, standard simulation methods such as Markov chain Monte Carlo (MCMC) methods require a complete 'browsing' of the observations; in contrast, a sequential strategy may have reduced computational complexity. Second, by including the observations one at a time, the posterior distributions exhibit a beneficial tempering effect (Chopin, 2002). Alternatively, we may want to move from a tractable (easy-to-sample)

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distribution π_1 to a distribution of interest, π_p, through a sequence of artificial intermediate distributions (Neal, 2001). In the context of optimization, and in a manner that is similar to simulated annealing, we could also consider the sequence of distributions $\pi_n(x) \propto \pi(x)^{\phi_n}$ for an increasing schedule $\{\phi_n\}_{n\in\mathbb{T}}$.

The tools that are favoured by statisticians, to sample from complex distributions, are MCMC methods (see, for example, Robert and Casella (2004)). To sample from π_n, MCMC methods consist of building an ergodic Markov kernel K_n with invariant distribution π_n by using Metropolis–Hastings (MH) steps and Gibbs moves. MCMC algorithms have been successfully applied to many problems in statistics (e.g. mixture modelling (Richardson and Green, 1997) and changepoint analysis (Green, 1995)). However, in general, there are two major drawbacks with MCMC methods. It is difficult to assess when the Markov chain has reached its stationary regime and it can easily become trapped in local modes. Moreover, MCMC methods cannot be used in a sequential Bayesian estimation context.

In this paper, we propose a different approach to sample from $\{\pi_n\}_{n\in\mathbb{T}}$ that is based on sequential Monte Carlo (SMC) methods (Del Moral, 2004; Doucet *et al.*, 2001; Liu, 2001). Henceforth, the resulting algorithms will be called SMC samplers. More precisely, this is a complementary approach to MCMC sampling, as MCMC kernels will often be ingredients of the methods proposed. SMC methods have been recently studied and used extensively in the context of sequential Bayesian inference. At a given time n, the basic idea is to obtain a large collection of N weighted random samples $\{W_n^{(i)}, X_n^{(i)}\}$ $(i = 1, \ldots, N, W_n^{(i)} > 0; \Sigma_{i=1}^N W_n^{(i)} = 1)$ named particles whose empirical distribution converges asymptotically $(N \to \infty)$ to π_n, i.e. for any π_n-integrable function $\varphi : E \to \mathbb{R}$

$$\sum_{i=1}^{N} W_n^{(i)} \varphi(X_n^{(i)}) \to \mathbb{E}_{\pi_n}(\varphi) \qquad \text{almost surely}$$

where

$$\mathbb{E}_{\pi_n}(\varphi) = \int_E \varphi(x)\, \pi_n(x)\, \mathrm{d}x. \tag{1}$$

These particles are carried forward over time by using a combination of sequential importance sampling (IS) and resampling ideas.

Standard SMC algorithms in the literature do not apply to the problems that were described above. This is because these algorithms deal with the case where the target distribution of interest, at time n, is defined on S_n with $\dim(S_{n-1}) < \dim(S_n)$, e.g. $S_n = E^n$. Conversely, we are interested in the case where the distributions $\{\pi_n\}_{n\in\mathbb{T}}$ are all defined on a common space E. Our approach has some connections with adaptive IS methods (West, 1993; Oh and Berger, 1993; Givens and Raftery, 1996), resample–move (RM) strategies (Chopin, 2002; Gilks and Berzuini, 2001), Annealed IS (AIS) (Neal, 2001) and population Monte Carlo methods (Cappé *et al.*, 2004) which are detailed in Section 3. However, the generic framework that we present here is more flexible. It allows us to define general moves and can be used in scenarios where previously developed methodologies do not apply (see Section 5). Additionally, we can develop new algorithms to make parallel MCMC runs interact in a simple way, to perform global optimization or to solve sequential Bayesian estimation problems. It is also possible to estimate ratios of normalizing constants as a by-product of the algorithm. As for MCMC sampling, the performance of these algorithms is highly dependent on the target distributions $\{\pi_n\}_{n\in\mathbb{T}}$ and proposal distributions that are used to explore the space.

This paper focuses on the algorithmic aspects of SMC samplers. However, it is worth noting that our algorithms can be interpreted as interacting particle approximations of a Feynman–Kac

flow in distribution space. Many general convergence results are available for these approximations and, consequently, for SMC samplers (Del Moral, 2004). Nevertheless, the SMC samplers that are developed here are such that many known estimates on the asymptotic behaviour of these general processes can be greatly improved. Several of these results can be found in Del Moral and Doucet (2003). In this paper we provide the expressions for the asymptotic variances that are associated with central limit theorems.

The rest of the paper is organized as follows. In Section 2, we present a generic sequential IS (SIS) algorithm to sample from a sequence of distributions $\{\pi_n\}_{n\in\mathbb{T}}$. We outline the limitations of this approach which severely restricts the way that we can move the particles around the space. In Section 3, we provide a method to circumvent this problem by building an artificial sequence of joint distributions which admits fixed marginals. We provide guidelines for the design of efficient algorithms. Some extensions and connections with previous work are outlined. The remaining sections describe how to apply the SMC sampler methodology to two important special cases. Section 4 presents a generic approach to convert an MCMC sampler into an SMC sampler to sample from a fixed target distribution. This is illustrated on a Bayesian analysis of finite mixture distributions. Finally, Section 5 presents an application of SMC samplers to a sequential, transdimensional Bayesian inference problem. The proofs of the results in Section 3 can be found in Appendix A.

2. Sequential importance sampling

In this section, we describe a generic iterative SIS method to sample from a sequence of distributions $\{\pi_n\}_{n\in\mathbb{T}}$. We provide a review of the standard IS method; then we outline its limitations and describe a sequential version of the algorithm.

2.1. Importance sampling

Let π_n be a target density on E such that

$$\pi_n(x) = \gamma_n(x)/Z_n$$

where $\gamma_n : E \to \mathbb{R}^+$ is known pointwise and the normalizing constant Z_n is unknown. Let $\eta_n(x)$ be a positive density with respect to $\mathrm{d}x$, referred to as the importance distribution. IS is based on the identities

$$\mathbb{E}_{\pi_n}(\varphi) = Z_n^{-1} \int_E \varphi(x)\, w_n(x)\, \eta_n(x)\, \mathrm{d}x, \tag{2}$$

$$Z_n = \int_E w_n(x)\, \eta_n(x)\, \mathrm{d}x, \tag{3}$$

where the unnormalized importance weight function is equal to

$$w_n(x) = \gamma_n(x)/\eta_n(x). \tag{4}$$

By sampling N particles $\{X_n^{(i)}\}$ from η_n and substituting the Monte Carlo approximation

$$\eta_n^N(\mathrm{d}x) = \frac{1}{N}\sum_{i=1}^{N} \delta_{X_n^{(i)}}(\mathrm{d}x)$$

(with δ denoting Dirac measure) of this distribution into equations (2) and (3), we obtain an approximation for $\mathbb{E}_{\pi_n}(\varphi)$ and Z_n.

In statistics applications, we are typically interested in estimating equation (1) for a large range of test functions φ. In these cases, we are usually trying to select η_n 'close' to π_n as the variance is approximately proportional to $1 + \mathrm{var}_{\eta_n}\{w_n(X_n)\}$ (see Liu (2001), pages 35–36). Unfortunately, selecting such an importance distribution is very difficult when π_n is a non-standard high dimensional distribution. As a result, despite its relative simplicity, IS is almost never used when MCMC methods can be applied.

2.2. Sequential importance sampling

To obtain better importance distributions, we propose the following sequential method. At time $n = 1$, we start with a target distribution π_1 which is assumed to be easy to approximate efficiently by using IS, i.e. η_1 can be selected such that the variance of the importance weights (4) is small. In the simplest case, $\eta_1 = \pi_1$. Then, at time $n = 2$, we consider the new target distribution π_2. To build the associated IS distribution η_2, we use the particles sampled at time $n = 1$, say $\{X_1^{(i)}\}$. The rationale is that, if π_1 and π_2 are not too different from one another, then it should be possible to move the particles $\{X_1^{(i)}\}$ in the regions of high probability density of π_2 in a sensible way.

At time $n-1$ we have N particles $\{X_{n-1}^{(i)}\}$ distributed according to η_{n-1}. We propose to move these particles by using a Markov kernel $K_n : E \times \mathcal{E} \to [0, 1]$, with associated density denoted $K_n(x, x')$. The particles $\{X_n^{(i)}\}$ that are obtained this way are marginally distributed according to

$$\eta_n(x') = \int_E \eta_{n-1}(x)\, K_n(x, x')\, \mathrm{d}x. \tag{5}$$

If η_n *can be computed pointwise*, then it is possible to use the standard IS estimates of π_n and Z_n.

2.3. Algorithm settings

This SIS strategy is very general. There are many potential choices for $\{\pi_n\}_{n\in\mathbb{T}}$ leading to various integration and optimization algorithms.

2.3.1. Sequence of distributions $\{\pi_n\}$

(a) In the context of Bayesian inference for static parameters, where p observations $(y_1, \ldots, y_p)$ are available, we can consider

$$\pi_n(x) = p(x|y_1, \ldots, y_n). \tag{6}$$

See Chopin (2002) for such applications.

(b) It can be of interest to consider an inhomogeneous sequence of distributions to move 'smoothly' from a tractable distribution $\pi_1 = \mu_1$ to a target distribution π through a sequence of intermediate distributions. For example, we could select a geometric path (Gelman and Meng, 1998; Neal, 2001)

$$\pi_n(x) \propto \pi(x)^{\phi_n} \mu_1(x)^{1-\phi_n} \tag{7}$$

with $0 \leqslant \phi_1 < \ldots < \phi_p = 1$.

Alternatively, we could simply consider the case where $\pi_n = \pi$ for all $n \in \mathbb{T}$. This has been proposed numerous times in the literature. However, if π is a complex distribution, it is difficult to build a sensible initial importance distribution. In particular, such algo-

rithms may fail when the target is multimodal with well-separated narrow modes. Indeed, in this case, the probability of obtaining samples in all the modes of the target is very small and an importance distribution that is based on these initial particles is likely to be inefficient. Therefore, for difficult scenarios, it is unlikely that such approaches will be robust.

(c) For global optimization, as in simulated annealing, we can select

$$\pi_n(x) \propto \pi(x)^{\phi_n} \tag{8}$$

where $\{\phi_n\}_{n\in\mathbb{T}}$ is an increasing sequence such that $\phi_p \to \infty$ for large p.

(d) Assume that we are interested in estimating the probability of a rare event, $A \in \mathcal{E}$, under a probability measure π ($\pi(A) \approx 0$). In most of these applications, π is typically easy to sample from and the normalizing constant of its density is known. We can consider the sequence of distributions

$$\pi_n(x) \propto \pi(x)\, \mathbb{I}_{E_n}(x)$$

where $E_n \in \mathcal{E}\ \forall n \in \mathbb{T}$, $\mathbb{I}_A(x)$ is the indicator function for $A \in \mathcal{E}$ and $E_1 \supset E_2 \supset \ldots \supset E_{p-1} \supset E_p$, $E_1 = E$ and $E_p = A$. An estimate of $\pi(A)$ is given by an estimate of the normalizing constant Z_p.

2.3.2. *Sequence of transition kernels $\{K_n\}$*

It is easily seen that the optimal proposal, in the sense of minimizing the variance of the importance weights, is $K_n(x, x') = \pi_n(x')$. As this choice is impossible, we must formulate sensible alternatives.

2.3.2.1. Independent proposals. It is possible to select $K_n(x, x') = K_n(x')$ where $K_n(\cdot)$ is a standard distribution (e.g. Gaussian or multinomial) whose parameters can be determined by using some statistics based on η_{n-1}^N. This approach is standard in the literature, e.g. West (1993). However, independent proposals appear overly restrictive and it seems sensible to design local moves in high dimensional spaces.

2.3.2.2. Local random-walk moves. A standard alternative consists of using for $K_n(x, x')$ a random-walk kernel. This idea has appeared several times in the literature where $K_n(x, x')$ is selected as a standard smoothing kernel (e.g. Gaussian or Epanechikov), e.g. Givens and Raftery (1996). However, this approach is problematic. Firstly, the choice of the kernel bandwidth is difficult. Standard rules to determine kernel bandwidths may indeed not be appropriate here, because we are not trying to obtain a kernel density estimate $\eta_{n-1}^N K_n(x')$ of $\eta_{n-1}(x')$ but to design an importance distribution to approximate $\pi_n(x')$. Secondly, no information about π_n is typically used to build $K_n(x, x')$.

Two alternative classes of local moves exploiting the structure of π_n are now proposed.

2.3.2.3. Markov chain Monte Carlo moves. It is natural to set K_n as an MCMC kernel of invariant distribution π_n. In particular, this approach is justified if either K_n is fast mixing and/or π_n is slowly evolving so that we can expect η_n to be reasonably close to the target distribution. In this case, the resulting algorithm is an IS technique which would allow us to correct for the fact that the N inhomogeneous Markov chains $\{X_n^{(i)}\}$ are such that $\eta_n \neq \pi_n$. This is an attractive

strategy: we can use the vast literature on the design of efficient MCMC algorithms to build 'good' importance distributions.

2.3.2.4. Approximate Gibbs moves. When it is impossible to sample from the full conditional distributions that are required by a Gibbs kernel of invariant distribution π_n, an approximation to these distributions can be used to build K_n. This strategy is very popular in the SMC literature for optimal filtering where the so-called optimal proposal (Doucet *et al*. (2000), page 199, and Liu (2001), page 47) corresponds to a Gibbs step but can rarely be implemented and is approximated.

2.4. Limitations of sequential importance sampling

For any probability density ν, we use the notation

$$\nu K_{i:j}(x_j) \triangleq \int \nu(x_{i-1}) \prod_{k=i}^{j} K_k(x_{k-1}, x_k)\, \mathrm{d}x_{i-1:j-1}$$

where $x_{i:j}$, $i \leqslant j$, and $X_{i:j}$ respectively denote $(x_i, \ldots, x_j)$ and $(X_i, \ldots, X_j)$.

The algorithm that was discussed above suffers from a major drawback. In most cases, it is impossible to compute the importance distribution $\eta_n(x_n)$ that is given by

$$\eta_n(x_n) = \eta_1 K_{2:n}(x_n) \tag{9}$$

and hence impossible to compute the importance weights. An important exception is when we use independent proposal distributions and, in our opinion, this explains why this approach is often used in the literature. However, whenever local moves are used, η_n does not admit a closed form expression in most cases.

A potential solution is to attempt to approximate η_n pointwise by

$$\eta_{n-1}^N K_n(x_n) = \frac{1}{N} \sum_{i=1}^{N} K_n(X_{n-1}^{(i)}, x_n).$$

This approximation has been used in the literature for local random-walk moves. However, this approach suffers from two major problems. First, the computational complexity of the resulting algorithm would be in $O(N^2)$, which is prohibitive. Second, it is impossible to compute $K_n(x_{n-1}, x_n)$ pointwise in important scenarios. For example, consider the case where $E = \mathbb{R}$, K_n is an MH kernel and $\mathrm{d}x$ is Lebesgue measure: we cannot, typically, compute the rejection probability of the MH kernel analytically.

3. Sequential Monte Carlo samplers

In this section, we show how it is possible to use any local move—including MCMC moves—in the SIS framework while circumventing the calculation of distribution (9). The algorithm preserves complexity of $O(N)$ and provides asymptotically consistent estimates.

3.1. Methodology and algorithm

As noted above, the importance weight can be computed exactly at time 1. At time $n > 1$, it is typically impossible to compute $\eta_n(x_n)$ pointwise as it requires an integration with respect to $x_{1:n-1}$. Instead, we propose an auxiliary variable technique and introduce artificial backward (in time) Markov kernels $L_{n-1} : E \times \mathcal{E} \to [0, 1]$ with density $L_{n-1}(x_n, x_{n-1})$. We then perform

IS between the joint importance distribution $\eta_n(x_{1:n})$ and the artificial joint target distribution defined by

$$\tilde{\pi}_n(x_{1:n}) = \tilde{\gamma}_n(x_{1:n})/Z_n$$

where

$$\tilde{\gamma}_n(x_{1:n}) = \gamma_n(x_n) \prod_{k=1}^{n-1} L_k(x_{k+1}, x_k).$$

As $\tilde{\pi}_n(x_{1:n})$ admits $\pi_n(x_n)$ as a marginal by construction, IS provides an estimate of this distribution and its normalizing constant. By proceeding thus, we have defined a sequence of probability distributions $\{\tilde{\pi}_n\}$ whose dimension is increasing over time; i.e. $\tilde{\pi}_n$ is defined on E^n. We are then back to the 'standard' SMC framework that was described, for example, in Del Moral (2004), Doucet *et al.* (2001) and Liu (2001). We now describe a generic SMC algorithm to sample from this sequence of distributions based on SIS resampling methodology.

At time $n-1$, assume that a set of weighted particles $\{W_{n-1}^{(i)}, X_{1:n-1}^{(i)}\}$ $(i = 1, \ldots, N)$ approximating $\tilde{\pi}_{n-1}$ is available,

$$\tilde{\pi}_{n-1}^N(\mathrm{d}x_{1:n-1}) = \sum_{i=1}^N W_{n-1}^{(i)} \delta_{X_{1:n-1}^{(i)}}(\mathrm{d}x_{1:n-1}), \tag{10}$$

$$W_{n-1}^{(i)} = w_{n-1}(X_{1:n-1}^{(i)}) \Big/ \sum_{j=1}^N w_{n-1}(X_{1:n-1}^{(j)}).$$

At time n, we extend the path of each particle with a Markov kernel $K_n(x_{n-1}, x_n)$. IS is then used to correct for the discrepancy between the sampling distribution $\eta_n(x_{1:n})$ and $\tilde{\pi}_n(x_{1:n})$. In this case the new expression for the unnormalized importance weights is given by

$$\begin{aligned} w_n(x_{1:n}) &= \tilde{\gamma}_n(x_{1:n})/\eta_n(x_{1:n}) \\ &= w_{n-1}(x_{1:n-1})\, \tilde{w}_n(x_{n-1}, x_n) \end{aligned} \tag{11}$$

where the so-called (unnormalized) incremental weight $\tilde{w}_n(x_{n-1}, x_n)$ is equal to

$$\tilde{w}_n(x_{n-1}, x_n) = \frac{\gamma_n(x_n) L_{n-1}(x_n, x_{n-1})}{\gamma_{n-1}(x_{n-1}) K_n(x_{n-1}, x_n)}. \tag{12}$$

As the discrepancy between η_n and $\tilde{\pi}_n$ tends to increase with n, the variance of the unnormalized importance weights tends to increase, resulting in a potential degeneracy of the particle approximation. This degeneracy is routinely measured by using the effective sample size (ESS) criterion $\{\Sigma_{i=1}^N (W_n^{(i)})^2\}^{-1}$ (Liu and Chen, 1998). The ESS takes values between 1 and N. If the degeneracy is too high, i.e. the ESS is below a prespecified threshold, say $N/2$, then each particle $X_{1:n}^{(i)}$ is copied $N_n^{(i)}$ times under the constraint $\Sigma_{i=1}^N N_n^{(i)} = N$, the expectation of $N_n^{(i)}$ being equal to $NW_n^{(i)}$ such that particles with high weights are copied multiple times whereas particles with low weights are discarded. Finally, all resampled particles are assigned equal weights. The simplest way to perform resampling consists of sampling the N new particles from the weighted distribution $\tilde{\pi}_n^N$; the resulting $\{N_n^{(i)}\}$ are distributed according to a multinomial distribution of parameters $\{W_n^{(i)}\}$. Stratified resampling (Kitagawa, 1996) and residual resampling can also be used and all of these reduce the variance of $N_n^{(i)}$ relatively to that of the multinomial scheme.

A summary of the algorithm is described in the next subsection. The complexity of this algorithm is in $O(N)$ and it can be parallelized easily.

3.1.1. Algorithm: sequential Monte Carlo sampler

Step 1: initialization—
set $n=1$;
for $i=1,\ldots,N$ draw $X_1^{(i)}\sim\eta_1$;
evaluate $\{w_1(X_1^{(i)})\}$ by using equation (4) and normalize these weights to obtain $\{W_1^{(i)}\}$.
Iterate steps 2 and 3.
Step 2: resampling—
if ESS $<T$ (for some threshold T), resample the particles and set $W_n^{(i)}=1/N$.
Step 3: sampling—
set $n=n+1$; if $n=p+1$ stop;
for $i=1,\ldots,N$ draw $X_n^{(i)}\sim K_n(X_{n-1}^{(i)},\cdot)$;
evaluate $\{\tilde{w}_n(X_{n-1:n}^{(i)})\}$ by using equation (12) and normalize the weights

$$W_n^{(i)}=W_{n-1}^{(i)}\,\tilde{w}_n(X_{n-1:n}^{(i)})\Big/\sum_{j=1}^{N}W_{n-1}^{(j)}\,\tilde{w}_n(X_{n-1:n}^{(j)}).$$

Remark 1. If the weights $\{W_n^{(i)}\}$ are independent of $\{X_n^{(i)}\}$, then the particles $\{X_n^{(i)}\}$ should be sampled after the weights $\{W_n^{(i)}\}$ have been computed and after the particle approximation $\{W_n^{(i)},X_{n-1}^{(i)}\}$ of $\pi_n(x_{n-1})$ has possibly been resampled. This scenario appears when $\{L_n\}$ is given by equation (30) in Section 3.3.2.3.

Remark 2. It is also possible to derive an auxiliary version of algorithm 1 in the spirit of Pitt and Shephard (1999).

3.2. Notes on algorithm

3.2.1. Estimates of target distributions and normalizing constants

At time n, we obtain after the sampling step a particle approximation $\{W_n^{(i)},X_{1:n}^{(i)}\}$ of $\tilde{\pi}_n(x_{1:n})$. As the target $\pi_n(x_n)$ is a marginal of $\tilde{\pi}_n(x_{1:n})$ by construction, an approximation of it is given by

$$\pi_n^N(\mathrm{d}x)=\sum_{i=1}^{N}W_n^{(i)}\,\delta_{X_n^{(i)}}(\mathrm{d}x). \tag{13}$$

The particle approximation $\{W_{n-1}^{(i)},X_{n-1:n}^{(i)}\}$ of $\pi_{n-1}(x_{n-1})\,K_n(x_{n-1},x_n)$ that is obtained after the sampling step also allows us to approximate

$$\frac{Z_n}{Z_{n-1}}=\frac{\int\gamma_n(x_n)\,\mathrm{d}x_n}{\int\gamma_{n-1}(x_{n-1})\,\mathrm{d}x_{n-1}}$$

by

$$\widehat{\frac{Z_n}{Z_{n-1}}}=\sum_{i=1}^{N}W_{n-1}^{(i)}\tilde{w}_n(X_{n-1:n}^{(i)}). \tag{14}$$

To estimate Z_n/Z_1, we can use the product of estimates of the form (14) from time $k=2$ to $k=n$. However, if we do not resample at each iteration, a simpler alternative is given by

$$\widehat{\frac{Z_n}{Z_1}} = \prod_{j=1}^{r_{n-1}+1} \widehat{\frac{Z_{k_j}}{Z_{k_{j-1}}}},$$

with

$$\widehat{\frac{Z_{k_j}}{Z_{k_{j-1}}}} = \sum_{i=1}^{N} W_{k_{j-1}}^{(i)} \prod_{m=k_{j-1}+1}^{k_j} \tilde{w}_m(X_{m-1:m}^{(i)}) \tag{15}$$

where $k_0 = 1$, k_j is the jth time index at which we resample for $j > 1$. The number of resampling steps between 1 and $n-1$ is denoted r_{n-1} and we set $k_{r_{n-1}+1} = n$.

There is a potential alternative estimate for ratios of normalizing constants that is based on path sampling (Gelman and Meng, 1998). Indeed, consider a continuous path of distributions

$$\pi_{\theta(t)} = \gamma_{\theta(t)} / Z_{\theta(t)}$$

where $t \in [0, 1]$, $\theta(0) = 0$ and $\theta(1) = 1$. Then, under regularity assumptions, we have the path sampling identity

$$\log\left(\frac{Z_1}{Z_0}\right) = \int_0^1 \frac{\mathrm{d}\theta(t)}{\mathrm{d}t} \int \frac{\mathrm{d}[\log\{\gamma_{\theta(t)}(x)\}]}{\mathrm{d}t} \pi_{\theta(t)}(\mathrm{d}x)\, \mathrm{d}t.$$

In the SMC samplers context, if we consider a sequence of $p+1$ intermediate distributions denoted here $\pi_{\theta(k/P)}$, $k = 0, \ldots, p$, to move from π_0 to π_1 then the above equation can be approximated by using a trapezoidal integration scheme and substituting $\hat{\pi}^N_{\theta(k/P)}(\mathrm{d}x)$ for $\pi_{\theta(k/P)}(\mathrm{d}x)$. Some applications of this identity in an SMC framework are detailed in Johansen *et al.* (2005) and Rousset and Stoltz (2005).

3.2.2. Mixture of Markov kernels

The algorithm that is described in this section must be interpreted as the basic element of more complex algorithms. It is to SMC sampling what the MH algorithm is to MCMC sampling. For complex MCMC problems, one typically uses a combination of MH steps where the J components of x say $(x_1, \ldots, x_J)$ are updated in subblocks. Similarly, to sample from high dimensional distributions, a practical SMC sampler can update the components of x via subblocks and a mixture of transition kernels can be used at each time n.

Let us assume that $K_n(x_{n-1}, x_n)$ is of the form

$$K_n(x_{n-1}, x_n) = \sum_{m=1}^{M} \alpha_{n,m}(x_{n-1})\, K_{n,m}(x_{n-1}, x_n) \tag{16}$$

where $\alpha_{n,m}(x_{n-1}) \geqslant 0$, $\Sigma_{m=1}^{M} \alpha_{n,m}(x_{n-1}) = 1$ and $\{K_{n,m}\}$ is a collection of transition kernels. In this case, the incremental weights can be computed by the standard formula (12). However, this could be too expensive if M is large. An alternative, valid, approach consists of considering a backward Markov kernel of the form

$$L_{n-1}(x_n, x_{n-1}) = \sum_{m=1}^{M} \beta_{n-1,m}(x_n)\, L_{n-1,m}(x_n, x_{n-1}) \tag{17}$$

where $\beta_{n-1,m}(x_n) \geqslant 0$, $\Sigma_{m=1}^{M} \beta_{n-1,m}(x_n) = 1$ and $\{L_{n-1,m}\}$ is a collection of backward transition kernels. We now introduce, explicitly, a discrete latent variable M_n taking values in $\mathcal{M} = \{1, \ldots, M\}$ such that $\mathbb{P}(M_n = m) = \alpha_{n,m}(x_{n-1})$ and perform IS on the extended space $E \times E \times \mathcal{M}$.

This yields an incremental importance weight that is equal to

$$\tilde{w}_n(x_{n-1}, x_n, m_n) = \frac{\gamma_n(x_n)\,\beta_{n-1,m_n}(x_n)\,L_{n-1,m_n}(x_n, x_{n-1})}{\gamma_{n-1}(x_{n-1})\,\alpha_{n,m_n}(x_{n-1})\,K_{n,m_n}(x_{n-1}, x_n)}. \tag{18}$$

The variance of equation (18) will always be superior or equal to the variance of equation (12).

3.3. Algorithm settings

3.3.1. Optimal backward kernels

In standard applications of SMC methods, only the proposal kernels $\{K_n\}$ have to be selected as the joint distributions $\{\tilde{\pi}_n\}$ are given by the problem at hand. In the framework that is considered here, $\{L_n\}$ is arbitrary. However, in practice, $\{L_n\}$ should be optimized with respect to $\{K_n\}$ to obtain good performance. Recall that $\{L_n\}$ has been introduced because it was impossible to compute the marginal importance distribution $\{\eta_n\}$ pointwise.

The marginal distribution of the particles $\{X_n^{(i)}\}$ at time n is given by

$$\eta_n(x_n) = \eta_1 K_{2:n}(x_n) \tag{19}$$

if the particles have not been resampled before time n and approximately

$$\eta_n(x_n) = \pi_l K_{l+1:n}(x_n) \tag{20}$$

if the last time that the particles were resampled was l. To simplify the discussion, we consider here the case (19). The more general case (20) can be handled similarly.

The introduction of the auxiliary kernels $\{L_n\}$ means that we need not compute $\eta_n(x_n)$. This comes at the price of extending the integration domain from E to E^n and increasing the variance (if it exists) of the importance weights. The following proposition establishes the expression of the sequence of optimal backward Markov kernels.

Proposition 1. The sequence of kernels $\{L_k^{\text{opt}}\}$ $(k = 1, \ldots, n)$ minimizing the variance of the unnormalized importance weight $w_n(x_{1:n})$ is given for any k and n by

$$L_{k-1}^{\text{opt}}(x_k, x_{k-1}) = \frac{\eta_{k-1}(x_{k-1})\,K_k(x_{k-1}, x_k)}{\eta_k(x_k)} \tag{21}$$

and in this case

$$w_n(x_{1:n}) = \gamma_n(x_n)/\eta_n(x_n).$$

Remark 3. This proposition is intuitive and simply states that the optimal backward Markov kernels take us back to the case where we perform IS on E instead of on E^n. The result can also be intuitively understood through the following forward–backward formula for Markov processes:

$$\eta_1(x_1) \prod_{k=2}^{n} K_k(x_{k-1}, x_k) = \eta_n(x_n) \prod_{k=2}^{n} L_{k-1}^{\text{opt}}(x_k, x_{k-1}). \tag{22}$$

In the context of a mixture of kernels (16), we can use proposition 1 to establish that the optimal backward kernel is of the form (17) with

$$\beta_{n-1,m}^{\text{opt}}(x_n) \propto \int \alpha_{n,m}(x_{n-1})\,\eta_{n-1}(x_{n-1})\,K_n(x_{n-1}, x_n)\,\mathrm{d}x_{n-1}, \tag{23}$$

$$L_{n-1,m}^{\text{opt}}(x_n, x_{n-1}) = \frac{\alpha_{n,m}(x_{n-1})\,\eta_{n-1}(x_{n-1})\,K_n(x_{n-1}, x_n)}{\displaystyle\int \alpha_{n,m}(x_{n-1})\,\eta_{n-1}(x_{n-1})\,K_n(x_{n-1}, x_n)\,\mathrm{d}x_{n-1}}. \tag{24}$$

3.3.2. Suboptimal backward kernels

It is typically impossible, in practice, to use the optimal kernels as they themselves rely on marginal distributions which do not admit any closed form expression. However, this suggests that we should select $\{L_k\}$ to approximate equation (21). The key point is that, even if $\{L_k\}$ is different from expression (21), the algorithm will still provide asymptotically consistent estimates. Some approximations are now discussed.

3.3.2.1. Substituting π_{n-1} for η_{n-1}. One point that is used recurrently is that equation (12) suggests that a sensible, suboptimal, strategy consists of using an L_n which is an approximation of the optimal kernel (21) where we have substituted π_{n-1} for η_{n-1}, i.e.

$$L_{n-1}(x_n, x_{n-1}) = \frac{\pi_{n-1}(x_{n-1})\, K_n(x_{n-1}, x_n)}{\pi_{n-1}\, K_n(x_n)} \tag{25}$$

which yields

$$\tilde{w}_n(x_{n-1}, x_n) = \frac{\gamma_n(x_n)}{\displaystyle\int_E \gamma_{n-1}(x_{n-1})\, K_n(x_{n-1}, x_n)\, \mathrm{d}x_{n-1}}. \tag{26}$$

It is often more convenient to use equation (26) than equation (21) as $\{\gamma_n\}$ is known analytically, whereas $\{\eta_n\}$ is not. If particles have been resampled at time $n-1$, then η_{n-1} is indeed approximately equal to π_{n-1} and thus equation (21) is equal to equation (25).

3.3.2.2. Gibbs-type updates. Consider the case where $x = (x_1, \ldots, x_J)$ and we only want to update the kth ($k \in \{1, \ldots, J\}$) component x_k of x, denoted $x_{n,k}$, at time n. It is straightforward to establish that the proposal distribution minimizing the variance of equation (26) conditional on x_{n-1} is a Gibbs update, i.e.

$$K_n(x_{n-1}, \mathrm{d}x_n) = \delta_{x_{n-1,-k}}(\mathrm{d}x_{n,-k})\, \pi_n(\mathrm{d}x_{n,k} | x_{n,-k}) \tag{27}$$

where $x_{n,-k} = (x_{n,1}, \ldots, x_{n,k-1}, x_{n,k+1}, \ldots, x_{n,J})$. In this case equations (25) and (26) are given by

$$L_{n-1}(x_n, \mathrm{d}x_{n-1}) = \delta_{x_{n,-k}}(\mathrm{d}x_{n-1,-k})\, \pi_{n-1}(\mathrm{d}x_{n-1,k} | x_{n-1,-k}),$$

$$\tilde{w}_n(x_{n-1}, x_n) = \frac{\gamma_n(x_{n-1,-k}, x_{n,k})}{\gamma_{n-1}(x_{n-1,-k})\, \pi_n(x_{n,k} | x_{n-1,-k})}.$$

When it is not possible to sample from $\pi_n(x_{n,k} | x_{n-1,-k})$ and/or to compute

$$\gamma_{n-1}(x_{n-1,-k}) = \int \gamma_{n-1}(x_{n-1})\, \mathrm{d}x_{n-1,k}$$

analytically, this suggests using an approximation $\hat{\pi}_n(x_{n,k} | x_{n-1,-k})$ to $\pi_n(x_{n,k} | x_{n-1,-k})$ to sample the particles and another approximation $\hat{\pi}_{n-1}(x_{n-1,k} | x_{n-1,-k})$ to $\pi_{n-1}(x_{n-1,k} | x_{n-1,-k})$ to obtain

$$L_{n-1}(x_n, \mathrm{d}x_{n-1}) = \delta_{x_{n,-k}}(\mathrm{d}x_{n-1,-k})\, \hat{\pi}_{n-1}(\mathrm{d}x_{n-1,k} | x_{n-1,-k}), \tag{28}$$

$$\tilde{w}_n(x_{n-1}, x_n) = \frac{\gamma_n(x_{n-1,-k}, x_{n,k})\, \hat{\pi}_{n-1}(x_{n-1,k} | x_{n-1,-k})}{\gamma_{n-1}(x_{n-1})\, \hat{\pi}_n(x_{n,k} | x_{n-1,-k})}. \tag{29}$$

3.3.2.3. Markov chain Monte Carlo kernels. A generic alternative approximation to equation (25) can also be made when K_n is an MCMC kernel of invariant distribution π_n. It is given by

$$L_{n-1}(x_n, x_{n-1}) = \frac{\pi_n(x_{n-1})\, K_n(x_{n-1}, x_n)}{\pi_n(x_n)} \tag{30}$$

and will be a good approximation to equation (25) if $\pi_{n-1} \approx \pi_n$; note that equation (30) is the reversed Markov kernel that is associated with K_n. In this case, we have unnormalized incremental weight

$$\tilde{w}_n(x_{n-1}, x_n) = \gamma_n(x_{n-1})/\gamma_{n-1}(x_{n-1}). \tag{31}$$

Contrary to equation (25), this approach does not apply in scenarios where $E_{n-1} \subset E_n$ and $E_n \in \mathcal{E}\ \forall n \in \mathbb{T}$ as discussed in Section 5. Indeed, in this case

$$L_{n-1}(x_n, x_{n-1}) = \frac{\pi_n(x_{n-1})\, K_n(x_{n-1}, x_n)}{\displaystyle\int_{E_{n-1}} \pi_n(x_{n-1})\, K_n(x_{n-1}, x_n)\, \mathrm{d}x_{n-1}} \tag{32}$$

but the denominator of this expression is different from $\pi_n(x_n)$ as the integration is over E_{n-1} and not over E_n.

3.3.2.4. Mixtures of kernels. Practically, we cannot typically compute expressions (23) and (24) in closed form and so approximations are also necessary. As discussed previously, one suboptimal choice consists of replacing η_{n-1} with π_{n-1} in expressions (23) and (24) or using further approximations like equation (30).

3.3.3. Summarizing remarks

To conclude this subsection, we emphasize that selecting $\{L_n\}$ as close as possible to $\{L_n^{\mathrm{opt}}\}$ is crucial for this method to be efficient. It could be tempting to select $\{L_n\}$ in a different way. For example, if we select $L_{n-1} = K_n$ then the incremental importance weight looks like an MH ratio. However, this 'aesthetic' choice will be inefficient in most cases, resulting in importance weights with a very large or infinite variance.

3.4. Convergence results

Using equation (13), the SMC algorithm yields estimates of expectations (1) via

$$\mathbb{E}_{\pi_n^N}(\varphi) = \int_E \varphi(x)\, \pi_n^N(\mathrm{d}x). \tag{33}$$

Using equation (14), we can also obtain an estimate of $\log(Z_n/Z_1)$:

$$\log\left(\frac{\widehat{Z_n}}{Z_1}\right) = \sum_{k=2}^{n} \log\left(\frac{\widehat{Z_k}}{Z_{k-1}}\right). \tag{34}$$

We now present a central limit theorem, giving the asymptotic variance of these estimates in two 'extreme' cases: when we never resample and when we resample at each iteration. For simplicity, we have considered only the case where multinomial resampling is used (see Chopin (2004a) for analysis using residual resampling and also Künsch (2005) for results in the context of filtering). The asymptotic variance expressions (33) and (34) for general SMC algorithms have previously

been established in the literature. However, we propose here a new representation which clarifies the influence of the kernels $\{L_n\}$.

In the following proposition, we denote by $\mathcal{N}(\mu, \sigma^2)$ the normal distribution with mean μ and variance σ^2, convergence in distribution by '$\Rightarrow$', $\int \tilde{\pi}_n(x_{1:n})\,\mathrm{d}x_{1:k-1}\,\mathrm{d}x_{k+1:n}$ by $\tilde{\pi}_n(x_k)$ and $\int \tilde{\pi}_n(x_{1:n})\,\mathrm{d}x_{1:k-1}\,\mathrm{d}x_{k+1:n-1}/\tilde{\pi}_n(x_k)$ by $\tilde{\pi}_n(x_n|x_k)$.

Proposition 2. Under the weak integrability conditions that were given in Chopin (2004a), theorem 1, or Del Moral (2004), section 9.4, pages 300–306, we obtain the following results. When no resampling is performed, we have

$$N^{1/2}\{\mathbb{E}_{\pi_n^N}(\varphi) - \mathbb{E}_{\pi_n}(\varphi)\} \Rightarrow \mathcal{N}\{0, \sigma^2_{\mathrm{IS},n}(\varphi)\}$$

with

$$\sigma^2_{\mathrm{IS},n}(\varphi) = \int \frac{\tilde{\pi}_n(x_{1:n})^2}{\eta_n(x_{1:n})}\{\varphi(x_n) - \mathbb{E}_{\pi_n}(\varphi)\}^2\,\mathrm{d}x_{1:n} \tag{35}$$

where the joint importance distribution η_n is given by

$$\eta_n(x_{1:n}) = \eta_1(x_1)\prod_{k=2}^{n} K_k(x_{k-1}, x_k).$$

We also have

$$N^{1/2}\left\{\log\left(\frac{\widehat{Z_n}}{Z_1}\right) - \log\left(\frac{Z_n}{Z_1}\right)\right\} \Rightarrow \mathcal{N}(0, \sigma^2_{\mathrm{IS},n})$$

with

$$\sigma^2_{\mathrm{IS},n} = \int \frac{\tilde{\pi}_n(x_{1:n})^2}{\eta_n(x_{1:n})}\mathrm{d}x_{1:n} - 1. \tag{36}$$

When multinomial resampling is used at each iteration, we have

$$N^{1/2}\{\mathbb{E}_{\pi_n^N}(\varphi) - \mathbb{E}_{\pi_n}(\varphi)\} \Rightarrow \mathcal{N}\{0, \sigma^2_{\mathrm{SMC},n}(\varphi)\}$$

where, for $n \geqslant 2$,

$$\begin{aligned}\sigma^2_{\mathrm{SMC},n}(\varphi) = {} & \int \frac{\tilde{\pi}_n(x_1)^2}{\eta_1(x_1)}\left\{\int \varphi(x_n)\,\tilde{\pi}_n(x_n|x_1)\,\mathrm{d}x_n - \mathbb{E}_{\pi_n}(\varphi)\right\}^2 \mathrm{d}x_1 \\ & + \sum_{k=2}^{n-1}\int \frac{\{\tilde{\pi}_n(x_k)L_{k-1}(x_k, x_{k-1})\}^2}{\pi_{k-1}(x_{k-1})\,K_k(x_{k-1}, x_k)}\left\{\int \varphi(x_n)\,\tilde{\pi}_n(x_n|x_k)\,\mathrm{d}x_n - \mathbb{E}_{\pi_n}(\varphi)\right\}^2 \mathrm{d}x_{k-1:k} \\ & + \int \frac{\{\pi_n(x_n)\,L_{n-1}(x_n, x_{n-1})\}^2}{\pi_{n-1}(x_{n-1})\,K_n(x_{n-1}, x_n)}\{\varphi(x_n) - \mathbb{E}_{\pi_n}(\varphi)\}^2\,\mathrm{d}x_{n-1:n}\end{aligned} \tag{37}$$

and

$$N^{1/2}\left\{\log\left(\frac{\widehat{Z_n}}{Z_1}\right) - \log\left(\frac{Z_n}{Z_1}\right)\right\} \Rightarrow \mathcal{N}(0, \sigma^2_{\mathrm{SMC},n})$$

where

$$\begin{aligned}\sigma^2_{\mathrm{SMC},n} = {} & \int \frac{\tilde{\pi}_n(x_1)^2}{\eta_1(x_1)}\,\mathrm{d}x_1 - 1 + \sum_{k=2}^{n-1}\left[\int \frac{\{\tilde{\pi}_n(x_k)\,L_{k-1}(x_k, x_{k-1})\}^2}{\pi_{k-1}(x_{k-1})\,K_k(x_{k-1}, x_k)}\mathrm{d}x_{k-1:k} - 1\right] \\ & + \int \frac{\{\pi_n(x_n)\,L_{n-1}(x_n, x_{n-1})\}^2}{\pi_{n-1}(x_{n-1})\,K_n(x_{n-1}, x_n)}\mathrm{d}x_{n-1:n} - 1.\end{aligned} \tag{38}$$

Remark 4. In the general case, we cannot claim that $\sigma^2_{\mathrm{SMC},n}(\varphi) < \sigma^2_{\mathrm{IS},n}(\varphi)$ or $\sigma^2_{\mathrm{SMC},n} < \sigma^2_{\mathrm{IS},n}$. This is because, if the importance weights do not have a large variance, resampling is typically wasteful as any resampling scheme introduces some variance. However, resampling is beneficial in cases where successive distributions can vary significantly. This has been established theoretically in the filtering case in Chopin (2004a), theorem 5: under mixing assumptions, the variance is shown to be upper bounded uniformly in time with resampling and to go to ∞ without it. The proof may be adapted to the class of problems that is considered here, and it can be shown that for expression (8)—under mixing assumptions on $\{K_n\}$ and using equations (25) or (30) for $\{L_n\}$—the variance $\sigma^2_{\mathrm{SMC},n}(\varphi)$ is upper bounded uniformly in time for a logarithmic schedule $\{\phi_n\}$ whereas $\sigma^2_{\mathrm{IS},n}(\varphi)$ goes to ∞ with n. Similar results hold for residual resampling. Finally we note that, although the resampling step appears somewhat artificial in discrete time, it appears naturally in the continuous time version of these algorithms (Del Moral, 2004; Rousset and Stoltz, 2005).

3.5. Connections with other work

To illustrate the connections with, and differences from, other published work, let us consider the case where we sample from $\{\pi_n\}$ using MCMC kernels $\{K_n\}$ where K_n is π_n invariant.

Suppose that, at time $n-1$, we have the particle approximation $\{W^{(i)}_{n-1}, X^{(i)}_{n-1}\}$ of π_{n-1}. Several recent algorithms are based on the implicit or explicit use of the backward kernel (30). In the case that is addressed here, where all the target distributions are defined on the same space, it was used for example in Chopin (2002), Jarzynski (1997) and Neal (2001). In the case where the dimension of the target distributions increases over time, it was used in Gilks and Berzuini (2001) and MacEachern *et al.* (1999).

For the algorithms that are listed above, the associated backward kernels lead to the incremental weights

$$\tilde{w}_n(X^{(i)}_{n-1}, X^{(i)}_n) \propto \pi_n(X^{(i)}_{n-1}) / \pi_{n-1}(X^{(i)}_{n-1}). \tag{39}$$

The potential problem with expression (39) is that these weights are independent of $\{X^{(i)}_n\}$ where $X^{(i)}_n \sim K_n(X^{(i)}_{n-1}, \cdot)$. In particular, the variance of expression (39) will typically be high if the discrepancy between π_{n-1} and π_n is large even if the kernel K_n mixes very well. This result is counter-intuitive. In the context of AIS (Neal, 2001) where the sequence of p target distributions (7) is supposed to satisfy $\pi_{n-1} \approx \pi_n$, this is not a problem. However, if successive distributions vary significantly, as in sequential Bayesian estimation, this can become a significant problem. For example, in the limiting case where $K_n(x_{n-1}, x_n) = \pi_n(x_n)$, we would end up with a particle approximation $\{W^{(i)}_n, X^{(i)}_n\}$ of π_n where the weights $\{W^{(i)}_n\}$ have a high variance whereas $\{X^{(i)}_n\}$ are independent and identically distributed samples from π_n; this is clearly suboptimal.

To deal with this problem, RM strategies were used by (among others) Chopin (2002) and Gilks and Berzuini (2001). RM corresponds to the SMC algorithm that is described in Section 3 using the backward kernel (30). RM resamples the particle approximation $\{W^{(i)}_n, X^{(i)}_{n-1}\}$ of $\tilde{\pi}_n(x_{n-1})$ if the variance (that is measured approximately through the ESS) is high and only then do we sample $\{X^{(i)}_n\}$ to obtain a particle approximation $\{N^{-1}, X^{(i)}_n\}$ of π_n, i.e. all particles have an equal weight. This can be expected to improve over not resampling if consecutive targets differ significantly and the kernels $\{K_n\}$ mix reasonably well; we demonstrate this in Section 4.

Proposition 1 suggests that a better choice (than equation (30)) of backward kernels is given by equation (25) for which the incremental weights are given by

$$\tilde{w}_n(X_{n-1}^{(i)}, X_n^{(i)}) \propto \frac{\pi_n(X_n^{(i)})}{\pi_{n-1}K_n(X_n^{(i)})}. \tag{40}$$

Expression (40) is much more intuitive than expression (39). It depends on K_n and thus the expression of the weights (40) reflects the mixing properties of the kernel K_n. In particular, the variance of expression (40) decreases as the mixing properties of the kernel increases.

To illustrate the difference between SMC sampling using expression (40) instead of expression (39), consider the case where $x = (x_1, \ldots, x_J)$ and we use the Gibbs kernel (27) to update the component x_k so that expression (40) is given by

$$\tilde{w}_n(X_{n-1}^{(i)}, X_n^{(i)}) \propto \pi_n(X_{n-1,-k}^{(i)})/\pi_{n-1}(X_{n-1,-k}^{(i)}). \tag{41}$$

By a simple Rao–Blackwell argument, the variance of expression (41) is always smaller than the variance of expression (39). The difference will be particularly significant in scenarios where the marginals $\pi_{n-1}(x_{-k})$ and $\pi_n(x_{-k})$ are close to each other but the full conditional distributions $\pi_n(x_k|x_{-k})$ and $\pi_{n-1}(x_k|x_{-k})$ differ significantly. In such cases, SMC sampling using expression (39) resamples many more times than SMC sampling using expression (41). Such scenarios appear for example in sequential Bayesian inference as described in Section 5 where each new observation only modifies the distribution of a subset of the variables significantly.

It is, unfortunately, not always possible to use equation (25) instead of equation (30) as an integral appears in expression (40). However, if the full conditional distributions of π_{n-1} and π_n can be approximated analytically, it is possible to use equations (28) and (29) instead.

Recent work of Cappé *et al.* (2004) is another special case of the framework proposed. They considered the homogeneous case where $\pi_n = \pi$ and $L_n(x, x') = \pi(x')$. Their algorithm corresponds to the case where $K_n(x, x') = K_n(x')$ and the parameters of $K_n(x')$ are determined by using statistics over the entire population of particles at time $n-1$. Extensions of this work for missing data problems are presented in Celeux *et al.* (2006).

Finally Liang (2002) presented a related algorithm where $\pi_n = \pi$ and $K_n(x, x') = L_n(x, x') = K(x, x')$.

4. From Markov chain Monte Carlo to sequential Monte Carlo samplers

4.1. Methodology

We now summarize how it is possible to obtain an SMC algorithm to sample from a fixed target distribution π, using MCMC kernels or approximate Gibbs steps to move the particles around the space. The procedure is

(a) build a sequence of distributions $\{\pi_n\}$, $n = 1, \ldots, p$, such that π_1 is easy to sample from or to approximate and $\pi_p = \pi$,
(b) build a sequence of MCMC transition kernels $\{K_n\}$ such that K_n is π_n invariant or K_n is an approximate Gibbs move of invariant distribution π_n,
(c) on the basis of $\{\pi_n\}$ and $\{K_n\}$, build a sequence of artificial backward Markov kernels $\{L_n\}$ approximating $\{L_n^{\text{opt}}\}$ (two generic choices are equations (25) and (30); for approximate Gibbs moves, we can use equation (28)) and
(d) use the SMC algorithm that was described in the previous section to approximate $\{\pi_n\}$ and to estimate $\{Z_n\}$.

4.2. Bayesian analysis of finite mixture distributions

In the following example, we consider a mixture modelling problem. Our objective is to illustrate the potential benefits of resampling in the SMC methodology.

4.2.1. Model

Mixture models are typically used to model heterogeneous data, or as a simple means of density estimation; see Richardson and Green (1997) and the references therein for an overview. Bayesian analysis of mixtures has been fairly recent and there is often substantial difficulty in simulation from posterior distributions for such models; see Jasra *et al*. (2005b) for example.

We use the model of Richardson and Green (1997), which is as follows; data $y_1, \ldots, y_c$ are independent and identically distributed with distribution

$$y_i|\theta_r \sim \sum_{j=1}^{r} \omega_j \mathcal{N}(\mu_j, \lambda_j^{-1})$$

where $\theta_r = (\mu_{1:r}, \lambda_{1:r}, \omega_{1:r})$, $2 \leqslant r < \infty$ and r known. The parameter space is $E = \mathbb{R}^r \times (\mathbb{R}^+)^r \times \mathcal{S}_r$ for the r-component mixture model where $\mathcal{S}_r = \{\omega_{1:r} : 0 \leqslant \omega_j \leqslant 1 \cap \Sigma_{j=1}^r \omega_j = 1\}$. The priors, which are the same for each component $j = 1, \ldots, r$, are taken to be $\mu_j \sim \mathcal{N}(\xi, \kappa^{-1})$, $\lambda_j \sim \mathrm{Ga}(\nu, \chi)$, $\omega_{1:r-1} \sim \mathcal{D}(\rho)$, where $\mathcal{D}(\rho)$ is the Dirichlet distribution with parameter ρ and $\mathrm{Ga}(\nu, \chi)$ is the gamma distribution with shape ν and scale χ. We set the priors in an identical manner to those in Richardson and Green (1997), with the χ-parameter set as the mean of the hyperprior that they assigned that parameter.

One particular aspect of this model, which makes it an appropriate test example, is the feature of label switching. As noted above, the priors on each component are exchangeable, and consequently, in the posterior, the marginal distribution of μ_1 is the same as μ_2, i.e. the marginal posterior is equivalent for each component-specific quantity. This provides us with a diagnostic to establish the effectiveness of the simulation procedure. For more discussion see, for example, Jasra *et al*. (2005b). It should be noted that very long runs of an MCMC sampler targeting π_p could not explore all the modes of this distribution and failed to produce correct estimates (see Jasra *et al*. (2005b)).

4.2.2. Sequential Monte Carlo sampler

We shall consider AIS and SMC samplers. Both algorithms use the same MCMC kernels K_n with invariant distribution π_n and the same backward kernels (30). The MCMC kernel is a composition of the following update steps.

(a) Update $\mu_{1:r}$ via an MH kernel with an additive normal random-walk proposal.
(b) Update $\lambda_{1:r}$ via an MH kernel with a multiplicative log-normal random-walk proposal.
(c) Update $\omega_{1:r}$ via an MH kernel with an additive normal random-walk proposal on the logit scale.

For some of the runs of the algorithm, we shall allow more than one iteration of the above Markov kernel per time step. Finally, the sequence of densities is taken as

$$\pi_n(\theta_r) \propto l(y_{1:c}; \theta_r)^{\phi_n} f(\theta_r)$$

where $0 \leqslant \phi_1 < \ldots < \phi_p = 1$ are tempering parameters and we have denoted the prior density as f and likelihood function as l.

4.2.3. Illustration

4.2.3.1. Data and simulation parameters. For the comparison, we used the simulated data from Jasra *et al*. (2005b): 100 simulated data points from an equally weighted mixture of four (i.e. $r = 4$) normal densities with means at $(-3,0,3,6)$ and standard deviations 0.55. We ran SMC samplers and AIS with MCMC kernels with invariant distribution π_n for 50, 100, 200, 500 and

1000 time steps with 1 and 10 MCMC iterations per time step. The proposal variances for the MH steps were the same for both procedures and were dynamically falling to produce an average acceptance rate in $(0.15, 0.6)$. The initial importance distribution was the prior. The C^{++} code and the data are available at `http://www.cs.ubc.ca/~arnaud/smcsamplers.html`.

We ran the SMC algorithm with $N = 1000$ particles and we ran AIS for a similar central processor unit time. The absence of a resampling step allows AIS to run for a few more iterations than SMC sampling. We ran each sampler 10 times (i.e. for each time specification and iteration number, each time with 1000 particles). For this demonstration, the resampling threshold was 500 particles. We use systematic resampling. The results with residual resampling are very similar.

We selected a piecewise linear cooling schedule $\{\phi_n\}$. Over 1000 time steps, the sequence increased uniformly from 0 to 15/100 for the first 200 time points, then from 15/100 to 40/100 for the next 400 and finally from 40/100 to 1 for the last 400 time points. The other time specifications had the same proportion of time attributed to the tempering parameter setting. The choice was made to allow an initially slow evolution of the densities and then to allow more complex densities to appear at a faster rate. We note that other cooling schedules may be implemented (such as logarithmic or quadratic) but we did not find significant improvement with such approaches.

4.2.3.2. Results. Table 1 gives the average of the (unnormalized) log-posterior values of the particles at time p (averaged over 10 runs), the average number of times that resampling occurred for SMC sampling and the averaged estimates of the log-normalizing constant (or log-marginal likelihood).

Table 1 displays the following: the particles that are generated by the SMC samplers have on average much higher log-posterior values. The standard deviation of these values (which is not given here) is also significantly smaller than for AIS. However, the estimates of the normalizing constant that were obtained via SMC sampling are not improved compared with AIS. For a low number of time steps p, the estimates for both algorithms are particularly poor and improve similarly as p increases. Therefore, if we are interested in estimating normalizing constants, it appears that it is preferable to use only one iterate of the kernel and more time steps. In addition, and as expected, the number of resampling steps decreases when p increases. This is because the discrepancy between consecutive densities falls, and this leads to reduced weight degeneracy. As the number of iterations per time step increases, this further reduces the number of resampling steps, which we attribute to the fact that the kernels mix faster, allowing us a better coverage of the space.

We now turn to Table 2 which displays estimates of the posterior means for $\{\mu_r\}$ for both algorithms. Owing to the non-identifiability of the mixture components, we expect the estimated means (for each component) to be all equal and approximately 1.5. In this case, SMC sampling provides more accurate estimates of these quantities than AIS. This is particularly significant when p is moderate ($p = 100$ and $p = 200$) and when the kernel is mixing reasonably well (i.e. the number of iterations is 10). This underlines that the resampling step can improve the sampler substantially, with little extra coding effort. This is consistent with the discussion in Section 3.5.

These experimental results can also be partially explained via the expressions of the asymptotic variances (38) and (37). (We do not use multinomial resampling in our experiments and we do not resample at each iteration but the variance expressions behave similarly for more complex resampling schemes). For the estimates of the normalizing constants, when the kernel

Table 1. Results from the mixture comparison for SMC sampling and AIS†

Sampler details	*Results for the following iterations per time step:*	
	1	*10*
SMC (50 time steps)		
Average log-posterior	−155.22	−152.03
Average times resampled	7.70	10.90
Average log-normalizing constant	−245.86	−240.90
AIS (50 time steps)		
Average log-posterior	−191.07	−166.73
Average log-normalizing constant	−249.04	−242.07
SMC (100 time steps)		
Average log-posterior	−153.08	−152.97
Average times resampled	8.20	5.10
Average log-normalizing constant	−245.43	−244.18
AIS (100 time steps)		
Average log-posterior	−180.76	−162.37
Average log-normalizing constant	−250.22	−244.17
SMC (200 time steps)		
Average log-posterior	−152.62	−152.99
Average times resampled	8.30	4.20
Average log-normalizing constant	−246.22	−245.84
AIS (200 time steps)		
Average log-posterior	−174.40	−160.00
Average log-normalizing constant	−247.45	−245.92
SMC (500 time steps)		
Average log-posterior	−152.31	−151.90
Average times resampled	7.00	3.00
Average log-normalizing constant	−247.08	−247.01
AIS (500 time steps)		
Average log-posterior	−167.67	−157.06
Average log-normalizing constant	−247.30	−247.94
SMC (1000 time steps)		
Average log-posterior	−152.12	−151.94
Average times resampled	5.70	2.00
Average log-normalizing constant	−247.40	−247.40
AIS (1000 time steps)		
Average log-posterior	−163.14	−155.31
Average log-normalizing constant	−247.50	−247.36

†We ran each sampler 10 times with 1000 particles. For AIS the number of time steps is slightly higher than stated, as it corresponds to the same central processor unit time as the SMC sampler.

Table 2. Estimates of means from mixture comparison for SMC sampling and AIS†

Sampler details	*Estimates for the following components:*			
	1	*2*	*3*	*4*
SMC (50 steps, 1 iteration)	0.38	0.83	1.76	2.69
AIS (50 steps, 1 iteration)	0.03	0.75	1.68	2.28
SMC (50 steps, 10 iterations)	1.06	1.39	1.62	1.70
AIS (50 steps, 10 iterations)	0.26	0.96	1.61	2.85
SMC (100 steps, 1 iteration)	0.68	0.91	2.02	2.14
AIS (100 steps, 1 iteration)	0.61	0.75	1.46	2.72
SMC (100 steps, 10 iterations)	1.34	1.44	1.44	1.54
AIS (100 steps, 10 iterations)	0.88	1.06	1.59	2.25
SMC (200 steps, 1 iteration)	1.11	1.29	1.39	1.98
AIS (200 steps, 1 iteration)	0.89	1.23	1.72	1.96
SMC (200 steps, 10 iterations)	1.34	1.37	1.53	1.53
AIS (200 steps, 10 iterations)	1.26	1.34	1.45	1.74
SMC (500 steps, 1 iteration)	0.98	1.38	1.54	1.87
AIS (500 steps, 1 iteration)	0.87	1.31	1.47	2.12
SMC (500 steps, 10 iterations)	1.40	1.44	1.42	1.50
AIS (500 steps, 10 iterations)	1.36	1.38	1.48	1.57
SMC (1000 steps, 1 iteration)	1.10	1.48	1.50	1.69
AIS (1000 steps, 1 iteration)	1.17	1.36	1.57	1.60
SMC (1000 steps, 10 iterations)	1.39	1.39	1.41	1.51
AIS (1000 steps, 10 iterations)	1.39	1.41	1.41	1.53

†We ran each sampler 10 times with 1000 particles. For AIS the number of time steps is slightly higher than stated, as it corresponds to the same central processor unit time as the SMC sampler. The estimates are presented in increasing order, for clarity.

mixes perfectly (i.e. $K_k(x_{k-1}, x_k) = \pi_k(x_k)$) the terms appearing in the variance expression are of the form

$$\int \frac{\{\tilde{\pi}_n(x_k)\, L_{k-1}(x_k, x_{k-1})\}^2}{\pi_{k-1}(x_{k-1})\, K_k(x_{k-1}, x_k)}\, \mathrm{d}x_{k-1:k} - 1 = \int \frac{\{\pi_k(x_{k-1})\, \pi_{k+1}(x_k)\}^2}{\pi_{k-1}(x_{k-1})\, \pi_k(x_k)}\, \mathrm{d}x_{k-1:k} - 1$$

when L_{k-1} is given by equation (30). These terms will remain high if the discrepancy between successive target distributions is large. For estimates of conditional expectations, the terms appearing in the variance expression are of the form

$$\int \frac{\{\tilde{\pi}_n(x_k)\, L_{k-1}(x_k, x_{k-1})\}^2}{\pi_{k-1}(x_{k-1})\, K_k(x_{k-1}, x_k)} \left\{ \int \varphi(x_n)\, \tilde{\pi}_n(x_n|x_k)\, \mathrm{d}x_n - \mathbb{E}_{\pi_n}(\varphi) \right\}^2 \mathrm{d}x_{k-1:k}.$$

These terms go to 0 as the mixing properties of K_k improve as in such cases $\tilde{\pi}_n(x_n|x_k) \approx \pi_n(x_n)$.

4.2.4. Summarizing remarks

In this example we have provided a comparison of SMC sampling and AIS. For normalizing constants, SMC sampling does not seem to improve estimation over AIS. However, for posterior expectations, it can provide a substantial gain when p is moderate and the kernels mix well. This is of importance in more complicated applications. For example, in many modern statistics problems (e.g. the population genetics example in Jasra *et al.* (2005a)), the computational cost of applying many iterations of an MCMC kernel (and thus good performance of AIS) is prohibitive

and thus the usage of the resampling step can enhance the performance of the algorithm.

In the situations for which the kernels mix quickly but p is small (i.e. where SMC sampling outperforms AIS for the same N) we might improve AIS by reducing N and increasing p to obtain similar computational cost and performance. The drawback of this approach is that it often takes a significant amount of investigation to determine an appropriate trade-off between N and p for satisfactory results, i.e. SMC sampling is often easier to calibrate (to specify simulation parameters) than AIS.

For more complex problems, say if $r \geqslant 5$, it is unlikely that SMC sampling will explore all the $r!$ modes for a reasonable number of particles. However, in such contexts, the method could provide a good indication of the properties of the target density and could be used as an exploratory technique.

5. Sequential Bayesian estimation

In the following example we present an application of SMC samplers to a sequential, transdimensional inference problem. In particular, we demonstrate our methodology in a case where the supports of the target distributions are nested, i.e. $E_{n-1} \subset E_n$. Such scenarios also appear in numerous counting problems in theoretical computer science, e.g. Jerrum and Sinclair (1996).

5.1. Model

We consider the Bayesian estimation of the rate of an inhomogeneous Poisson process, sequentially in time. In the static case, a similar problem was addressed in Green (1995). In the sequential case, related problems were discussed in Chopin (2004b), Fearnhead and Clifford (2003), Godsill and Vermaak (2005) and Maskell (2004).

We suppose that we record data $y_1, \ldots, y_{c_n}$ up to some time t_n with associated likelihood

$$l_n[y_{1:c_n} | \{\lambda(u)\}_{u \leqslant t_n}] \propto \left\{ \prod_{j=1}^{c_n} \lambda(y_j) \right\} \exp\left\{ - \int_0^{t_n} \lambda(u) \, \mathrm{d}u \right\}.$$

To model the intensity function, we follow Green (1995) and adopt a piecewise constant function, defined for $u \leqslant t_n$:

$$\lambda(u) = \sum_{j=0}^{k} \lambda_j \, \mathbb{I}_{[\tau_j, \tau_{j+1})}(u)$$

where $\tau_0 = 0$, $\tau_{k+1} = t_n$ and the changepoints (or knots) $\tau_{1:k}$ of the regression function follow a Poisson process of intensity ν whereas for any $k > 0$

$$f(\lambda_{0:k}) = f(\lambda_0) \prod_{j=1}^{k} f(\lambda_j | \lambda_{j-1})$$

with $\lambda_0 \sim \mathrm{Ga}(\mu, \upsilon)$ and $\lambda_j | \lambda_{j-1} \sim \mathrm{Ga}(\lambda_{j-1}^2/\chi, \lambda_{j-1}/\chi)$.

At time t_n we restrict ourselves to the estimation of $\lambda(u)$ on the interval $[0, t_n)$. Over this interval the prior on the number k of changepoints follows a Poisson distribution of parameter νt_n,

$$f_n(k) = \exp(-\nu t_n) \frac{(\nu t_n)^k}{k!},$$

and, conditionally on k, we have

$$f_n(\tau_{1:k}) = \frac{k!}{t_n^k} \mathbb{I}_{\Theta_{n,k}}(\tau_1, \ldots, \tau_k)$$

where $\Theta_{n,k} = \{\tau_{1:k} : 0 < \tau_1 < \ldots < \tau_k < t_n\}$. Thus at time t_n we have the density

$$\pi_n(\lambda_{0:k}, \tau_{1:k}, k) \propto l_n[y_{1:c_n} | \{\lambda(u)\}_{u \leqslant t_n}] \, f(\lambda_0) \left\{ \prod_{j=1}^{k} f(\lambda_j | \lambda_{j-1}) \right\} f_n(\tau_{1:k}) \, f_n(k).$$

5.2. Sequential Monte Carlo sampler

We shall consider a sequence of strictly increasing times $\{t_n\}$. For the problem that was considered above, we have defined a sequence of distributions on spaces:

$$E_n = \bigcup_{k \in \mathbb{N}_0} [\{k\} \times (\mathbb{R}^+)^{k+1} \times \Theta_{n,k}],$$

i.e. our densities are defined on a sequence of *nested* transdimensional spaces, $E_{n-1} \subset E_n$. As noted in Section 3.3.2, previously developed methodologies such as AIS and RM cannot be applied in such scenarios. Additionally, we must be careful, as in Green (1995), to construct incremental weights which are indeed well-defined Radon–Nikodym derivatives.

As noted in the transdimensional MCMC and SMC literatures (e.g. Green (2003), Carpenter *et al*. (1999), Doucet *et al*. (2000) and Pitt and Shephard (1999)) and in Section 3.3.2, a potentially good way to generate proposals in new dimensional spaces is to use the full conditional density. We shall use a similar idea to generate the new changepoints.

5.2.1. Extend move

In the extend move, we modify the location of the last changepoint, i.e. we use the Markov kernel

$$K_n(x, \mathrm{d}x') = \delta_{\tau_{1:k-1}, \lambda_{0:k}, k}\{d(\tau'_{1:k-1}, \lambda'_{0:k}, k')\} \, \pi_n(\mathrm{d}\tau'_k | \tau_{1:k-1}, \lambda_{0:k}, k).$$

The backward kernel (25) is used.

In the context of the present problem, the full conditional density is given by

$$\pi_n(\tau'_k | \tau_{1:k-1}, \lambda_{0:k}, k) \propto \lambda_{k-1}^{n_{[\tau_{k-1}, \tau'_k)}} \lambda_k^{n_{[\tau'_k, t_n)}} \exp\{-\tau'_k(\lambda_{k-1} - \lambda_k)\} \, \mathbb{I}_{[\tau_{k-1}, t_n)}(\tau'_k)$$

where $n_{[a,b)} = \sum_{j=1}^{c_n} \mathbb{I}_{[a,b)}(y_j)$. It is possible to sample exactly from this distribution through composition. It is also possible to compute in closed form its normalizing constant, which is required for the incremental weight (26).

5.2.2. Birth move

We also adopt a birth move which is simulated as follows. We generate a new changepoint τ'_{k+1} from a uniform distribution on $[\tau_k, t_n)$ and conditionally on this generate a new intensity according to its full conditional:

$$\pi_n(\lambda'_{k+1} | \tau'_{k+1}, \lambda_k) \propto \lambda'^{\, n_{[\tau'_{k+1}, t_n)} + \lambda_k^2/\chi - 1}_{k+1} \exp\{-\lambda'_{k+1}(t_n - \tau'_{k+1}) + \lambda_k/\chi\}.$$

All other parameters are kept the same. This leads to incremental weight

$$\frac{\pi_n(k+1, \tau'_{1:k+1}, \lambda'_{0:k+1})(t_n - \tau_k)}{\pi_{n-1}(k, \tau_{1:k+1}, \lambda_{0:k+1}) \, \pi_n(\lambda'_{k+1} | \tau'_{k+1}, \lambda_k)}.$$

5.2.3. The sampler

We thus adopt the following SMC sampler.

(a) At time n make a random choice between the extend move (chosen with probability $\alpha_n(x)$) or birth move. Clearly no extend move is possible if $k=0$.
(b) Perform the selected move.
(c) Choose whether or not to resample and do so.
(d) Perform an MCMC sweep of the moves that were described in Green (1995), i.e. we retain the same target density and thus the incremental weight is 1, owing to the invariance of the MCMC kernel.

5.3. Illustration

To illustrate the approach that was outlined above we use the popular coal-mining disaster data set that was analysed in (among others) Green (1995). The data consist of the times of coal-mining disasters in the UK, between 1851 and 1962. We assume that inference is of interest annually and so we define 112 densities (i.e. the nth density is defined up to time $t_n=n$). For illustration we take prior parameters as $\mu=4.5$, $\upsilon=1.5$, $\chi=0.1$ and $\nu=20/112$. For this example, the extend move performed better than the birth move; thus we let $\alpha_n(x)$ equal 1 if $k\geqslant 1$ and 0 otherwise. The backward probability is taken as equal to $\alpha_n(x)$ when $k\geqslant 1$ (as this is the only state that it is evaluated in).

We ran our SMC sampler with 10000 particles and resampling threshold 3000 particles, using the systematic resampling approach. The initial (importance) distribution was the prior. The C^{++} code and the data are available at `http://www.cs.ubc.ca/~arnaud/smcsamplers.html`.

Fig. 1(a) demonstrates the performance of our algorithm with respect to weight degeneracy. Here we see that, after the initial difficulty of the sampler (due to the initialization from the prior, and the targets' dynamic nature—we found that using more MCMC sweeps did not improve the performance) the ESS never drops below 25% of its previous value. Additionally, we resample, on average, every 8.33 time steps. These statements are not meaningless when using resampling. This is because we found, for less efficient forward and backward kernels, that the ESS would drop to 1 or 2 if consecutive densities had regions of high probability mass in different areas of the support. Thus the plot indicates that we can indeed extend the space in an efficient manner.

Fig. 1(c) shows the intensity function for the final density (full curve) in the sequence, the filtered density at each time point (i.e. $\mathbb{E}\{\lambda(t_n)|y_{1:c_n}\}$, the crosses) and the smoothed estimate, up to lag 10 ($\mathbb{E}\{\lambda(t_n)|y_{1:c_{n+10}}\}$, the pluses). We can see, as expected, that the smoothed intensity approaches the final density, with the filtered intensity displaying more variability. We found that the final rate was exactly the same as Green's (1995) transdimensional MCMC sampler for our target density.

Figs 1(b) and 1(d) illustrate the performance when we only allow the MCMC steps to operate on the last five knot points. This will reduce the amount of central processor unit time that is devoted to sampling the particles and will allow us to consider a truly realistic on-line implementation. This is of interest for large data sets. Here, we see (in Fig. 1(b)) a similar number of resampling steps to those in Fig. 1(a). In Fig. 1(d), we observe that the estimate of the intensity function suffers (slightly), with a more elongated structure at later times (in comparison with Fig. 1(c)), reflecting the fact that we cannot update the values of early knots in light of new data.

5.4. Summarizing remarks

In this example we have presented an application of SMC samplers to a transdimensional, sequential inference problem in Bayesian statistics. We successfully applied our methodology to the coal-mining disaster data set.

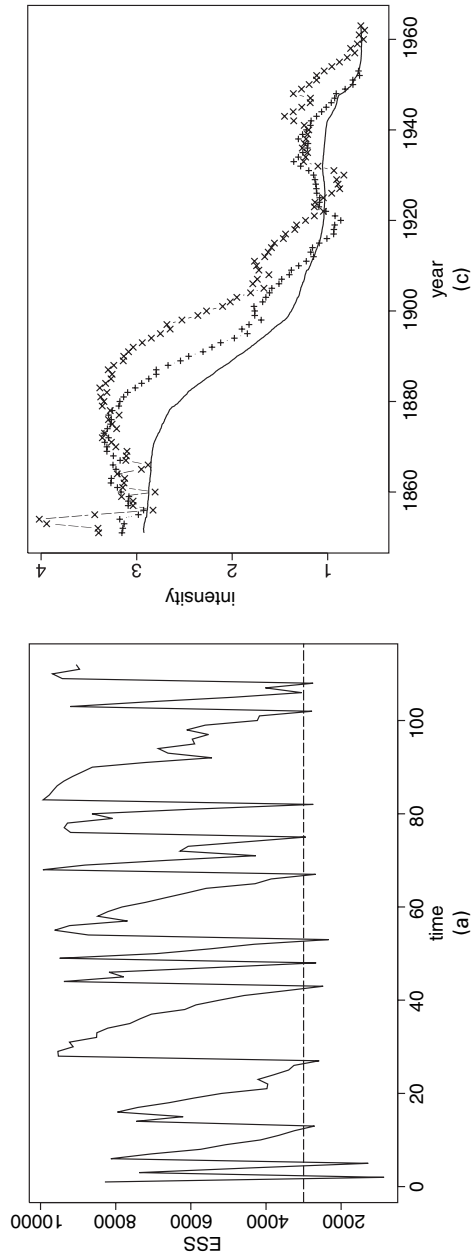

Fig. 1. (a), (b) Effective sample size plots and (c), (d) intensity functions for the coal-mining disaster data (we ran 10 000 particles for 112 densities and resampling threshold (------ in (a) and (b)) 3000 particles; in (c) and (d), ———, estimated intensity given the entire data, ×, filtered density at each time, +, smoothed estimate (lag 10)): (a), (c) results when the MCMC steps operate on the entire state space; (b), (d) results when the MCMC steps operate only on the last five, or fewer, knot points

One point of interest is the performance of the algorithm if we cannot use the backward kernel (25) in the extend step for alternative likelihood functions. We found that not performing the integration and using the approximation idea in equations (28) and (29) could still lead to good performance; this idea is also useful for alternative problems such as optimal filtering for non-linear, non-Gaussian state space models (Doucet *et al.*, 2006).

6. Conclusion

SMC algorithms are a class of flexible and general methods to sample from distributions and to estimate their normalizing constants. Simulations demonstrate that this set of methods is potentially powerful. However, the performances of these methods are highly dependent on the sequence of targets $\{\pi_n\}$, forward kernels $\{K_n\}$ and backward kernels $\{L_n\}$.

In cases where we want to use SMC methods to sample from a fixed target π, it would be interesting—in the spirit of path sampling (Gelman and Meng, 1998)—to obtain the optimal path (in the sense of minimizing the variance of the estimate of the ratio of normalizing constants) for moving from an easy-to-sample distribution π_1 to $\pi_p = \pi$. This is a very difficult problem. Given a parameterized family $\{\pi_{\theta(t)}\}_{t\in(0,1)}$ such that $\pi_{\theta(0)}$ is easy to sample and $\pi_{\theta(1)} = \pi$, a more practical approach consists of monitoring the ESS to move adaptively on the path $\theta(t)$; see Johansen *et al.* (2005) for details.

Finally, we have restricted ourselves here to Markov kernels $\{K_n\}$ to sample the particles. However, it is possible to design kernels whose parameters are a function of the whole set of current particles as suggested in Crisan and Doucet (2000), Cappé *et al.* (2004), Chopin (2002) or West (1993). This allows the algorithm to scale a proposal distribution automatically. This idea is developed in Jasra *et al.* (2005a).

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Appendix A

A.1. Proof of proposition 1

The result follows easily from the variance decomposition formula

$$\operatorname{var}\{w_n(X_{1:n})\} = \mathbb{E}[\operatorname{var}\{w_n(X_{1:n})|X_n\}] + \operatorname{var}[\mathbb{E}\{w_n(X_{1:n})|X_n\}]. \tag{42}$$

The second term on the right-hand side of equation (42) is independent of the backward Markov kernels $\{L_k\}$ as

$$\mathbb{E}\{w_n(X_{1:n})|X_n\} = \gamma_n(X_n)/\eta_n(X_n)$$

whereas $\operatorname{var}\{w(X_{1:n})|X_n\}$ is equal to 0 if we use equation (21).

A.2. Proof of proposition 2

Expression (35) follows from the delta method. Expression (37) follows from a convenient rewriting of the variance expression that was established in Del Moral (2004), proposition 9.4.2, page 302; see also Chopin (2004a), theorem 1, for an alternative derivation. The variance is given by

$$\sigma^2_{\mathrm{SMC},n}(\varphi) = \mathbb{E}_{\eta_1}[\bar{w}_1^2\, Q_{2:n}\{\varphi - \mathbb{E}_{\pi_n}(\varphi)\}^2] + \sum_{k=2}^{n} \mathbb{E}_{\pi_{k-1}K_k}[\bar{w}_k^2\, Q_{k+1:n}\{\varphi - \mathbb{E}_{\pi_n}(\varphi)\}^2] \tag{43}$$

where the semigroup Q is defined as $Q_{n+1:n}(\varphi) = \varphi$,

$$Q_{k+1:n}(\varphi) = Q_{k+1} \circ \ldots \circ Q_n(\varphi)$$

and

$$Q_n(\varphi)(x_{n-1}) = \mathbb{E}_{K_n(x_{n-1},\cdot)}\{\bar{w}_n(x_{n-1}, X_n)\, \varphi(X_n)\}$$

where

$$\begin{aligned}\bar{w}_n(x_{n-1}, x_n) &= \frac{\pi_n(x_n)\, L_{n-1}(x_n, x_{n-1})}{\pi_{n-1}(x_{n-1})\, K_n(x_{n-1}, x_n)} \\ &= \frac{Z_{n-1}}{Z_n} \tilde{w}_n(x_{n-1}, x_n).\end{aligned}$$

Expression (43) is difficult to interpret. It is conveniently rearranged here. The key is to note that

$$\begin{aligned}Q_n(\varphi)(x_{n-1}) &= \mathbb{E}_{K_n(x_{n-1},\cdot)}\{\bar{w}_n(x_{n-1}, X_n)\, \varphi(X_n)\} \\ &= \int K_n(x_{n-1}, x_n) \frac{\pi_n(x_n)\, L_{n-1}(x_n, x_{n-1})}{\pi_{n-1}(x_{n-1})\, K_n(x_{n-1}, x_n)} \varphi(x_n)\, \mathrm{d}x_n \\ &= \frac{1}{\pi_{n-1}(x_{n-1})} \int \varphi(x_n)\, \pi_n(x_n)\, L_{n-1}(x_n, x_{n-1})\, \mathrm{d}x_n \\ &= \frac{\tilde{\pi}_n(x_{n-1})}{\pi_{n-1}(x_{n-1})} \int \varphi(x_n)\, \tilde{\pi}_n(x_n|x_{n-1})\, \mathrm{d}x_n.\end{aligned}$$

Similarly, we obtain

$$\begin{aligned}Q_{n-1:n}(\varphi) &= Q_{n-1}\{Q_n(\varphi)\}(x_{n-1}) \\ &= \mathbb{E}_{K_{n-1}(x_{n-2},\cdot)}\{w_{n-1}(x_{n-2:n-1})\, Q_n(\varphi)(x_{n-1})\} \\ &= \frac{1}{\pi_{n-2}(x_{n-2})} \int \left\{ \frac{1}{\pi_{n-1}(x_{n-1})} \int \varphi(x_n)\, \pi_n(x_n)\, L_{n-1}(x_n, x_{n-1})\, \mathrm{d}x_n \right\} \pi_{n-1}(x_{n-1})\, L_{n-2}(x_{n-1}, x_{n-2})\, \mathrm{d}x_{n-1} \\ &= \frac{1}{\pi_{n-2}(x_{n-2})} \int \left\{ \int \varphi(x_n)\, \tilde{\pi}_n(x_{n-1:n}|x_{n-2})\, \mathrm{d}x_{n-1:n} \right\} \tilde{\pi}_{n-2}(x_{n-2})\, \mathrm{d}x_{n-1} \\ &= \frac{\tilde{\pi}_{n-1}(x_{n-2})}{\pi_{n-2}(x_{n-2})} \int \varphi(x_n)\, \tilde{\pi}_n(x_n|x_{n-2})\, \mathrm{d}x_n\end{aligned}$$

and, by induction, we obtain

$$\begin{aligned}Q_{k+1:n}(\varphi) &= \frac{1}{\pi_k(x_k)} \int \cdots \int \varphi(x_n)\, \pi_n(x_n) \prod_{i=k}^{n-1} L_i(x_i, x_{i-1})\, \mathrm{d}x_{k+1:n} \\ &= \frac{\tilde{\pi}_n(x_k)}{\pi_k(x_k)} \int \varphi(x_n)\, \tilde{\pi}_n(x_n|x_k)\, \mathrm{d}x_n.\end{aligned} \tag{44}$$

The expression of $\sigma^2_{\mathrm{SMC},n}(\varphi)$ that is given in equation (37) follows now directly from equations (44) and (43). Similarly we can rewrite the variance expression that was established in Del Moral (2004), proposition 9.4.1, page 301, and use the delta method to establish equation (38).

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