Sequential Monte Carlo Samplers

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Abstract

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1 Introduction

Assume we want to sample from a sequence of probability distributions \( \{ \pi_n \}_{n \in \mathcal{N}} \) defined on a common measurable space \( E \) where \( \mathcal{N} = \{0, 1, \ldots, p\} \) or \( \mathcal{N} = \mathbb{N} \). As a special case, one can set \( \pi_n = \pi \) for all \( n \in \mathcal{N} \). Alternatively the distribution can vary across \( \mathcal{N} \).

Similarly to simulated annealing, one could be interested in the sequence of distributions \( \pi_n(dx) \propto \pi^{\gamma_n}(x) dx \) for an increasing schedule \( \{\gamma_n\}_{n \in \mathcal{N}} \) so as to maximize \( \pi \) or \( \pi_n \) could be the posterior distribution of a parameter given the data collected till time \( n \). In this paper, we are interested in sampling this sequence of distributions sequentially; that is first sampling from \( \pi_0 \) then \( \pi_1 \) and so on. We will further on refer to \( n \) as the time index.

The tools favoured by statisticians to achieve this are Markov Chain Monte Carlo (MCMC) methods; see for example (Robert and Casella, 1999). To sample from \( \pi_n \), MCMC methods consists of building an ergodic Markov kernel \( K_n \) with invariant distribution \( \pi_n \) using Metropolis-Hastings (MH) steps, Gibbs steps etc. MCMC have been successfully used in many applications in statistics and physics. When the distribution to sample is multimodal, MCMC samplers can be easily stucked in one mode. A standard approach to improve mixing consists of using interacting parallel MCMC/tempering mechanisms where one runs a MCMC chain on an extended space \( E^N \) with a specified joint invariant distribution admitting \( \pi_n \) as a marginal (Geyer and Thompson, 1995). However, MCMC are not well adapted to sequential simulation. At index \( n \), one needs to wait for the Markov chain with kernel \( K_n \) to reach its stationary distribution \( \pi_n \).

We propose here a different approach to sample from \( \{ \pi_n \}_{n \in \mathcal{N}} \). Our approach is based on Sequential Monte Carlo (SMC) methods (Doucet et al., 2001; Liu, 2001). Henceforth the resulting algorithms will be called SMC samplers. SMC methods have been recently studied and used extensively in the context of sequential Bayesian inference and physics (Doucet et al., 2001; Iba, 2001; Liu, 2001). At a given time \( n \), the basic idea is to obtain a large collection of \( N \) (\( N \gg 1 \)) random samples \( \{X_n^{(1)}\}_{i=1,\ldots,N} \) named particles
whose marginal distribution is asymptotically \( N \to \infty \) equal to \( \pi_n \). These particles are carried forward over time using a combination of Sequential Importance Sampling (SIS) and resampling ideas. This approach is very different from parallel MCMC algorithms where one builds a Markov kernel with a specified joint invariant distribution on \( E^n \).

Standard SMC algorithms available in the literature do not apply to our problem. Indeed, these algorithms deal with the case where each target distribution of interest \( \pi_n \) is defined on \( E_n \) with \( E_{n-1} \subset E_n \). In (Chopin, 2002), a SMC algorithm is proposed to deal with the case \( E_n = E \). However, this approach restricts severely the way particles can explore the space. The idea in this paper is different and consists of building an artificial sequence of distributions \( \{\tilde{\pi}_n\}_{n \in \mathbb{N}} \) defined on \( E_n = E^{n+1} \) with \( \tilde{\pi}_n \) admitting a marginal \( \pi_n \). We are then back to the standard SMC framework. More precisely, \( \tilde{\pi}_n \) is defined on \( E^{n+1} \) by \( \tilde{\pi}_0(dx_0) = \pi_0(dx_0) \) and

\[
\tilde{\pi}_n(d(x_0, \ldots, x_n)) = \pi_n(dx_n) \prod_{k=1}^{n} L_k(x_k, dx_{k-1})
\]

(1)

where \( \{L_n\}_{n \in \mathbb{N} \setminus \{0\}} \) is a sequence of auxiliary Markov transition kernels.

Our approach has some connections with Annealed Importance Sampling (AIS) (Neal, 2001) and the algorithm recently proposed in (Cappé et al., 2002) which are detailed in Section 2. However, the framework we present here is more general and allows to derive a whole class of principled integration and genetic-type optimization algorithms based on interacting particle systems. Similarly to MCMC, the efficiency of the algorithms is dependent on the target distributions, the proposal and auxiliary kernels. Nevertheless, generally speaking, one can expect that SMC samplers will outperform MCMC when the distributions to sample are multimodal with well-separated modes. Moreover SMC samplers can be used for sequential Bayesian inference problems with static parameters like those addressed by Chopin (2002).

This paper focuses on the algorithmic aspects of SMC samplers. However, it is worth noting that our algorithms can be interpreted as an interacting particle approximating
model of a nonlinear Feynman–Kac flow in distribution space. Under additional assumptions, we provide a nonlinear Markov interpretation of the measure-valued dynamic system associated to the flow \( \{ \pi_n \}_{n \in \mathbb{N}} \). We show that this interpretation is a natural nonlinear version of the MH algorithm. Many convergence results are available for Feynman–Kac flows and their interacting particle approximations (Del Moral and Miclo, 2000; Del Moral and Miclo, 2001) and, consequently, for SMC samplers. However, the Feynman–Kac flow associated to SMC samplers is such that many known estimates on the asymptotic behaviour of these interacting processes can be greatly improved. Several of these results can be found in (Del Moral and Doucet, 2003).

The rest of the paper is organized as follows. In Section 2, we review a generic SMC algorithm to sample from the sequence of distributions \( \{ \pi_n \}_{n \in \mathbb{N}} \). Various settings for this algorithm are presented, some extensions and the connections with previous work are outlined. Section 3 describes the distribution flow associated to our interacting particle approximating model and also presents an original nonlinear Markovian interpretation of this flow. Section 4 applies this class of algorithms to a nonlinear regression problem. Finally, we discuss briefly a few open methodological and theoretical problems in Section 5.

2 Sequential Monte Carlo Sampling

2.1 A Generic Algorithm

We describe here a generic SMC algorithm to sample from the sequence of distributions \( \{ \pi_n \}_{n \in \mathbb{N}} \) defined in (1) based on a Sampling Importance Resampling strategy; see (Doucet et al., 2001) for a booklength survey of the SMC literature. Alternative SMC algorithms such as the Auxiliary Particle method of Pitt and Shephard (1999) could also be used.

Further on we will use the notation \( X_{0:k} \) to denote \( (X_0, \ldots, X_k) \). At time \( n-1 \), assume a set of particles \( \{ X_{0:n-1}^{(i)} \} (i = 1, \ldots, N) \) distributed approximately according to \( \tilde{\pi}_{n-1} \) is
available, i.e. the empirical measure
\[ \hat{\pi}_{n-1} \left( dx_{0:n-1} \right) = \frac{1}{N} \sum_{i=1}^{N} \delta_{X_{n-1}^{(i)}} \left( dx_{0:n-1} \right) \]
is an approximation of \( \tilde{\pi}_{n-1} \). At time \( n \), we extend the path of each particle according to a Markov kernel \( M_n \left( x_{n-1}, dx_n \right) \). The resulting path is thus approximately distributed according to \( \tilde{\pi}_{n-1} \left( dx_{0:n-1} \right) M_n \left( x_{n-1}, dx_n \right) \). Importance sampling can then be used to correct for the discrepancy between the sampling distribution and \( \tilde{\pi}_n \left( dx_{0:n} \right) \), with the importance weight satisfying
\[ G_n \left( x_{n-1}, x_n \right) = \frac{\hat{\pi}_n \left( dx_{0:n} \right)}{\tilde{\pi}_{n-1} \left( dx_{0:n-1} \right) M_n \left( x_{n-1}, dx_n \right)} \]
and being assumed well-defined. Finally, the particles are resampled according to their importance weights; particles with low weights are discarded whereas particles with high weights are multiplied. The resampled particles are given an equal weight. To sum up, the algorithm proceeds as follows.

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**Sequential Monte Carlo Sampler**

**Initialization;** \( n = 0 \).

**Sampling step**

- For \( i = 1, ..., N \), sample \( \tilde{X}_0^{(i)} \sim v_0 \). ⬤
- For \( i = 1, ..., N \), evaluate the normalized weights \( W_0^{(i)} \)
  \[ W_0^{(i)} \propto G_0 \left( \tilde{X}_0^{(i)} \right) = \frac{\pi_0 \left( d\tilde{X}_0^{(i)} \right)}{v_0 \left( d\tilde{X}_0^{(i)} \right)} \sum_{i=1}^{N} W_0^{(i)} = 1. \]

**Resampling step**

- Multiply/Discard particles \( \left\{ \tilde{X}_0^{(i)} \right\} \) with respect to high/low weights \( \left\{ W_0^{(i)} \right\} \) to obtain \( N \) particles \( \left\{ X_0^{(i)} \right\} \).

\(^1\)The Markov assumption could be relaxed.
Iteration \( n; n \in \mathbb{N}\setminus\{0\}. \\

\textbf{Sampling step} \\

- For \( i = 1, ..., N \), set \( \bar{X}_0^{(i)} = X_0^{(i)} \) and sample \( \bar{X}_n^{(i)} \sim M_n \left( \bar{X}_{n-1}, \cdot \right) \).

- For \( i = 1, ..., N \), evaluate the normalized weights \( W_n^{(i)} \)

\[ W_n^{(i)} \propto G_n \left( \bar{X}_n^{(i)}, \bar{X}_0^{(i)} \right), \quad \sum_{i=1}^{N} W_n^{(i)} = 1. \]

\textbf{Resampling step} \\

- Multiply/Discard particles \( \{\bar{X}_{0:n}^{(i)}\} \) with respect to high/lows weights \( \{W_n^{(i)}\} \) to obtain \( N \) particles \( \{X_{0:n}^{(i)}\} \).

In this algorithm, \( v_0 \) is the initial importance distribution. The resampling step can be done using a standard procedure such as multinomial resampling (Gordon \textit{et al.}, 1993), stratified resampling (Kitagawa, 1996) or minimum entropy resampling (Crisan, 2001). All these resampling schemes are unbiased; that is the number of times \( N_i \) the particle \( \bar{X}_0^{(i)} \) is copied satisfies \( E(N_i) = NW_n^{(i)} \). MCMC steps with invariant distribution \( \bar{\pi}_n \) can also be included after the resampling step (Gilks and Berzuini, 1999).

The complexity of this algorithm is in \( O(N) \) and it can be parallelized easily. In practice, the memory requirements are in \( O(N) \) too and do not increase over time as one does not need to keep in memory at time \( n \) the whole paths \( \{X_{0:n}^{(i)}\} \) but only \( \{X_n^{(i)}\} \).

The algorithm can be interpreted as an adaptive importance sampling strategy. Initially, \( v_0 \) is used and the particles with the highest importance weights are multiplied whereas the ones with small weights are discarded. At time \( n \), new “candidate” particles are sampled according to a proposal distribution kernel \( M_n \). If \( M_n \) is a random walk, then the new particles can be interpreted as a local exploration of the distribution. The crucial point is that these candidates are weighted by (3) so as to ensure that after the resampling step their distribution is approximately \( \bar{\pi}_n \). The introduction of the auxiliary
kernel $L_n$ allows the use of importance sampling without having to compute the marginal distribution $\int \pi_{n-1}(du) M_n(u, dx)$ of the particles $\{\tilde{X}_n^{(i)}\}$. Indeed, this marginal importance distribution does not typically admit an analytical expression except when $M_n$ is a MCMC kernel of invariant distribution $\pi_{n-1}$. A similar idea is the basis of the conditional Monte Carlo method described by Hammersley (1956).

2.2 Particle Estimates

At time $n$, we have the following empirical approximations of $\pi_n$ before the resampling step

$$\hat{\pi}_{n,1}(dx) = \sum_{i=1}^{N} W^{(i)}_n \delta_{\tilde{X}_n^{(i)}}(dx).$$

and after the resampling step it is equal to

$$\hat{\pi}_{n,2}(dx) = \frac{1}{N} \sum_{i=1}^{N} \delta_{X_n^{(i)}}(dx).$$

For any measure $\mu$ and function $f$, we will denote $\mu(f) = \int f(x) \mu(dx)$. An estimate of $\pi_n(f)$ is given by

$$\int f(x) \hat{\pi}_{n,1}(dx) = \sum_{i=1}^{N} W^{(i)}_n f(\tilde{X}_n^{(i)}).$$

or alternatively $\int f(x) \hat{\pi}_{n,2}(dx) = \frac{1}{N} \sum_{i=1}^{N} f(X_n^{(i)})$ which has higher variance. If $\pi_n = \pi$, then the following estimate can be also used

$$\frac{1}{n} \sum_{k=1}^{n} \sum_{i=1}^{N} W^{(i)}_k f(\tilde{X}_k^{(i)}).$$

(3)

Though the particles are statistically dependent, one can show under assumptions given in (Del Moral and Miclo, 2000) that this estimate is consistent as $N \to \infty$.

The algorithm described above can also be used to compute the ratio of normalizing constants. Indeed, typically the sequence of distributions $\pi_n(dx)$ is only known up to a normalizing constant, i.e. say $\pi_n(dx) \propto f_n(x) dx$. In this case, the unnormalized importance weights one computes are equal to

$$\tilde{W}^{(i)}_n = \frac{f_n(\tilde{X}_n^{(i)}) L_n(\tilde{X}_n^{(i)}, d\tilde{X}_n^{(i)})}{f_{n-1}(\tilde{X}_{n-1}^{(i)}) M_n(\tilde{X}_{n-1}^{(i)}, d\tilde{X}_n^{(i)})} \propto W^{(i)}_n.$$
at time \( n \). It is possible to obtain an estimate of the ratio of the normalizing constants

\[
\frac{Z_n}{Z_{n-1}} = \frac{\int f_n(x) \, dx}{\int f_{n-1}(x) \, dx}
\]

using

\[
\frac{\tilde{Z}_n}{Z_{n-1}} = \frac{1}{N} \sum_{i=1}^{N} \tilde{W}_n^{(i)}.
\] (4)

Thus an estimate of \( \log \left( \frac{Z_n}{Z_0} \right) \) is given by

\[
\log \left( \frac{\tilde{Z}_n}{Z_0} \right) = \sum_{k=1}^{n} \log \left( \frac{\tilde{Z}_k}{Z_{k-1}} \right) = \sum_{k=1}^{n} \log \left( \sum_{i=1}^{N} \tilde{W}_k^{(i)} \right) - n \log N.
\]

If the resampling scheme used is unbiased, then (4) is also unbiased (Del Moral and Miclo, 2000).

2.3 Algorithm Settings

The algorithm presented in the previous subsection is very general. There are many potential choices for \( \{\pi_n, M_n, L_n\}_{n \in \mathbb{N}} \) leading to various integration and optimization algorithms.

**Homogeneous sequences.** A simple choice consists of setting \( \pi_n = \pi, M_n = M \) and \( L_n = L \). In this case, the importance weight (2) is the following generalized MH ratio

\[
G(x, x') = \frac{\pi(dx')}{\pi(dx)} \frac{L(x', dx)}{M(x, dx')},
\] (5)

the standard MH ratio corresponds to \( M = L \). In this simple case, the particles evolve independently according to a proposal distribution \( M \), their generalized MH ratio is computed and normalized. The particles are then multiplied or discarded with respect to the value of their normalized MH ratio.

**Sequence of distributions \( \pi_n \).** It might be of interest to consider non homogeneous sequence of distributions either to move “smoothly” from \( \pi_0 = \nu_0 \) to a target distribution \( \pi \) through a sequence of intermediate distributions or for the sake of optimization. In the case of integration as suggested by Neal (2001), one can select

\[
\pi_n(dx) \propto \pi^{\gamma_n}(x) \pi_0^{1-\gamma_n}(x) \, dx
\]
with $\mathcal{N} = \{0, \ldots, p\}$, $\gamma_0 = 0$ and $\gamma_p = 1$. For the case of optimization, one can select

$$
\pi_n (dx) \propto \pi^{\gamma_n} (x) dx
$$

where $\mathcal{N} = \mathbb{N}$, $\{\gamma_n\}_{n \geq 0}$ is an increasing sequence such that $\gamma_n \to \infty$. In this case, the resulting algorithm is a genetic algorithm where the sampling step is the “mutation” step and the resampling step is the selection step (Goldberg, 1989). However, there is a significant difference with standard genetic algorithms as we know the asymptotic ($N \to \infty$) distribution of the particles. This makes the analysis of the resulting algorithm easier than in cases where this distribution is unknown such as in (Del Moral and Miclo, 2003). Convergence properties of the algorithm are currently under study.

Finally, another application of this algorithm consists of estimating the sequence of posterior distributions $\pi_n (dx) = \pi_n (dx | y_1, \ldots, y_n)$ where $y_n$ is an observation available at time $n$. As briefly discussed in the introduction, SMC algorithms have been recently proposed in this framework by Chopin (2002) but the SIS framework used is somehow restricted: it only allows $M_n$ to be a MCMC kernel of invariant distribution $\pi_{n-1}$.

**Sequence of proposal kernels $M_n$ and auxiliary kernels $L_n$.** Any couple of kernels can be used as long as the ratio (5) is well defined. However, one can only expect good properties of the algorithm if this ratio admits a reasonable variance and also if $L_n$ is mixing. Indeed, loosely speaking, the faster $L_n$ mixes, the faster the SMC algorithm forgets Monte Carlo errors (Del Moral and Doucet, 2003).

In SMC algorithms (Doucet *et al.*, 2001), it is known that the importance sampling distribution minimizing the conditional variance of the weights at time $n$, i.e. $\{X_{0:n-1}^{(i)}\}$ fixed, is given by

$$
M_n (x, dx') = \frac{\pi_n (dx') L_n (x', dx)}{\int \pi_n (du) L_n (u, dx)}. \tag{6}
$$

In this case, the importance weight $G_n (x, x')$ is given by

$$
G_n (x) = \frac{\int \pi_n (du) L_n (u, dx)}{\pi_{n-1} (dx)}. \tag{7}
$$
and is independent of $x'$. This allows the resampling step to be performed before the sampling step.

In standard applications of SMC algorithms, the kernel $L_n$ is usually given by the problem at hand whereas in our setup this kernel is arbitrary and can be optimized for a given proposal distribution $M_n$. One can alternatively select the kernel $L_n$ so as to be able to compute (8): e.g. a MCMC kernel of invariant distribution $\pi_n$, and then sample the particles according to (6).

For a fixed $M_n$, an alternative natural choice\textsuperscript{2} consists of choosing

$$L_n (x, dx') = \frac{\pi_{n-1} (dx') M_n (x', dx)}{\int \pi_{n-1} (du) M_n (u, dx)}.$$  \hfill (8)

In this case, the associated importance weight $G_n (x, x')$ is given by

$$G_n (x') = \frac{\pi_n (dx')}{\int \pi_{n-1} (du) M_n (u, dx')}.$$  \hfill (9)

If $M_n$ is a MCMC kernel of invariant distribution $\pi_{n-1}$, then the weight (9) can be computed easily. If not, numerical integration using the current set of particles can be used to approximate it but the resulting algorithms would be of complexity $O(N^2)$.

2.4 Connections to previous work and Extensions

Connections to previous work. AIS is a method proposed recently by Neal (2001). Reversing the time index in (Neal, 2001) to be consistent with our notation, AIS corresponds to the case where one considers a finite sequence of distributions, $M_n$ is a MCMC kernel of invariant distribution $\pi_n$ and

$$L_n (x, dx') = M_n (x', dx) \frac{\pi_n (dx')}{\pi_n (dx)}.$$  \hfill (10)

For a given $M_n$, one can check that this choice of $L_n$ ensures that (9) is satisfied. In this case, one obtains by combining (9) and (10)

$$G_n (x, x') = G_n (x) = \frac{\pi_n (dx)}{\pi_{n-1} (dx)}.$$

\textsuperscript{2}thanks to C. Andrieu
The resampling step is not included in the AIS algorithm. In our framework, we point out that this is a crucial step to include to make the method efficient as established theoretically in (Del Moral and Miclo, 2000) and practically in our simulations. Otherwise the method is just a special instance of SIS and collapses if $n$ is too large. In (Godsill and Clapp, 2001), the authors used the AIS algorithm in combination with resampling in the context of optimal filtering.

A more recent work (Cappé et al., 2002) contemporary of (Del Moral and Doucet, 2003) and developed independently is another special case of our framework. In (Cappé et al., 2002), the authors consider the homogeneous case. Their algorithm corresponds to the case where $M$ is an MCMC kernel of invariant distribution $\pi$ (namely a Gibbs sampler) and $L(x,dx') = \pi(dx')$, it follows that

$$G(x,x') = \frac{\pi(dx')}{M(x,dx')}.$$  

This particular case has limited applications as $G(x,x')$ would not be defined in most applications; e.g. $\pi(dx') = \pi(x')dx'$ and $M$ is an MH kernel.

**Extensions.** The algorithm described in this section must be interpreted as the basic element of more complex algorithms. It is what the MH algorithm is to MCMC. For complex MCMC problems, one typically uses a combination of MH steps where the $n_x$ components of $x$ say ($x_1, \ldots, x_{n_x}$) are updated by subblocks (Robert and Casella, 1999). Similarly, to sample from high dimensional distributions, a practical SMC sampler can update the components of $x$ via subblocks. There are also numerous potential extensions:

- It is straightforward to develop a version of the algorithm so as to sample distributions defined on an union of subspaces of different dimensions. However, contrary to reversible jump MCMC algorithms (Green, 1995), no reversibility condition is needed.

- As suggested in (Crisan and Doucet, 2000), one can use a proposal kernel whose
parameters are a function of the whole set of current particles. This allows the algorithm to automatically scale the proposal distribution based on the previous importance weights.

• In the general case, the sequence of probability distributions \( \{ \pi_n \}_{n \in \mathbb{N}} \) of interest is such that \( \pi_n \) is defined on \( E_n \) and not on \( E \). We can generalize the algorithm described in this section to this case. We introduce an auxiliary kernel \( L_n \) from \( E_n \) to \( E_{n-1} \) and a proposal kernel \( M_n \) from \( E_{n-1} \) to \( E_n \). At time \( n-1 \), \( N \) particles \( \{ X_{n-1}^{(i)} \} \) approximately distributed according to \( \pi_{n-1} \) are available. At time \( N \) new particles \( \{ X_n^{(i)} \} \) are sampled according to \( X_n^{(i)} \sim M_n \left( X_{n-1}^{(i)}, \cdot \right) \) and the following importance weights are computed

\[
W_n^{(i)} \propto \frac{\pi_n \left( dX_n^{(i)} \right) L_n \left( X_n^{(i)}, dX_{n-1}^{(i)} \right)}{\pi_{n-1} \left( dX_{n-1}^{(i)} \right) M_n \left( X_{n-1}^{(i)}, dX_n^{(i)} \right)}.
\]

Then the particles are resampled.

3 Feynman-Kac Representation and Particle Interpretations

In this Section, we show that the algorithm presented in Section 2 corresponds to an interacting particle approximation model of a nonlinear Feynman-Kac flow in distribution space. We provide an alternative nonlinear Markovian representation of this flow and its interacting particle approximation. Here the Feynman-Kac flow corresponds to the special case where the so-called potential function is given by the generalized Metropolis ratio (3). The abstract description and the analysis of general Feynman-Kac flows and their particle approximations have been investigated in several recent research articles. Many asymptotic (\( n \to \infty \) and/or \( N \to \infty \)) results are available in this field including empirical process convergence, central limit theorems, large deviation principles as well as increasing propagation of chaos estimates and uniform convergence estimates with respect to the time parameter; all of which can be used for SMC samplers. The interested reader is referred to the survey article (Del Moral and Miclo, 2000) and the more recent
studies (Del Moral and Miclo, 2001; Del Moral and Miclo, 2003). As mentioned in the introduction, the particular choice of the potential function simplifies the analysis and many known estimates on the asymptotic behaviour of these interacting processes can be greatly improved. Several of these results can be found in (Del Moral and Doucet, 2003).

3.1 Feynman-Kac Representation

Define the following distributions on $E^2 = E \times E$

$$(\pi_n \times L_n) (d(x, x')) = \pi_n (dx') L_n (x', dx).$$

Using (3) and (4), it is clear that the sequence of distributions $\{\pi_n \times L_n\}_{n \in \mathbb{N}}$ (with the convention $\pi_0 \times L_0 = \pi_0 \times \pi_0$) admits the following so-called Feynman-Kac representation

$$(\pi_n \times L_n) (f) = \lambda_n (f) / \lambda_n (1),$$

with

$$\lambda_n (f) = \mathbb{E}_{v_0, \{M_k\}} \left( f (X_{n-1}, X_n) G_0 (X_0) \prod_{k=1}^n G_k (X_{k-1}, X_k) \right),$$

where $\mathbb{E}_{v_0, \{M_k\}}$ denotes the expectation with respect to

$$v_0 (dx_0) \prod_{k=1}^n M_k (x_{k-1}, dx_k).$$

This representation is at the core of the results given in (Del Moral and Miclo, 2000).

We give now two “operator-like” interpretations of the sequence $\{\pi_n \times L_n\}_{n \in \mathbb{N}}$. For a measure $\mu$ and a Markov kernel $K$, we use the standard notation

$$\mu K (A) = \int_A \mu (dz) K (z, dz').$$

Let $\mathcal{P} (E^2)$ be the set of probability measures on $E^2$. The mapping $\Psi_n : \mathcal{P} (E^2) \rightarrow \mathcal{P} (E^2)$ is defined as

$$\pi_n \times L_n = \Psi_n \left( (\pi_{n-1} \times L_{n-1}) \tilde{M}_n \right)$$

(11)

where

$$\Psi_n (\mu) (d(u, v)) = \frac{\mu (d(u, v)) G_n (u, v)}{\mu (G_n)}$$

(12)
\( \tilde{M}_n \) is a Markov kernel on \( \mathbb{E}^2 \) defined as
\[
\tilde{M}_n \left( (u, v), d(u', v') \right) = \delta_v \left( du' \right) M_n \left( u', dv' \right).
\]

Assuming that \( G_n \) can be upper bounded over \( \mathbb{E}^2 \), one can easily check that an alternative representation is given by
\[
(\pi_n \times L_n) = (\pi_{n-1} \times L_{n-1}) \tilde{M}_n S_n, \quad \left(\pi_{n-1} \times L_{n-1}\right) \tilde{M}_n
\]
where
\[
S_{n,\mu} \left( (u, v), d(u', v') \right) = \epsilon G_n \left( u, v \right) \delta_{(u,v)} \left( d(u', v') \right) + (1 - \epsilon G_n \left( u, v \right)) \Psi_n \left( \mu \right) \left( d(u', v') \right),
\]
\( \epsilon \) being chosen such that \( \epsilon G_n \left( u, v \right) \leq 1 \) over \( \mathbb{E}^2 \).

The kernel \( \tilde{M}_n S_n, \left(\pi_{n-1} \times L_{n-1}\right) \tilde{M}_n \) is a so-called nonlinear Markov kernel; i.e. the transition kernel is dependent not only on the current state but also on its distribution. A generic nonlinear Markov chain \( \{Z_n\}_{n \geq 0} \) satisfies
\[
Z_n \sim K_{n, \text{Law}(Z_{n-1})} (Z_{n-1}, \cdot).
\]

It is typically impossible to simulate a realization from such a Markov chain as the distribution of the state is not available. However, a particle approximation of it can be used. Consider a Markov chain \( \{Z_n\}_{n \geq 0} \) taking values in \( \mathbb{E}^2 \) with transition kernel \( \tilde{M}_n S_n, \left(\pi_{n-1} \times L_{n-1}\right) \tilde{M}_n \). This kernel can be interpreted as follows. Given \( Z_{n-1} = (U_{n-1}, V_{n-1}) \sim (\pi_{n-1} \times L_{n-1}) \), one first sample a candidate \( Z^*_n = (U^*_n, V^*_n) = (V_{n-1}, V^*_n) \) where \( V^*_n \sim M_n \left( U^*_n, \cdot \right) \). With probability \( \epsilon G_n \left( U^*_n, V^*_n \right) \), one sets \( Z_n = (U^*_n, V^*_n) \), otherwise \( Z_n \sim \Psi_n \left( (\pi_{n-1} \times L_{n-1}) \tilde{M}_n \right) \). By construction, one has \( Z_n \sim (\pi_n \times L_n) \). This algorithm can be interpreted as a nonlinear version of the MH algorithm. The main difference being that, when a candidate is rejected, the chain does not stay where it is a new state is proposed according to \( \Psi_n \left( (\pi_{n-1} \times L_{n-1}) \tilde{M}_n \right) \).
3.2 Particle Interpretations

The first particle interpretation of the flow follows (11)-(12). It corresponds to the standard algorithm which has been described in Section 2. The second alternative algorithm corresponds to a particle interpretation of the flow corresponding to (13). It proceeds as follows.

**Iteration** \( n; n \in \mathbb{N} \setminus \{0\} \).

**Sampling step**

- For \( i = 1, ..., N \), set \( X_0^{(i)} = X_0^{(i)} \) and sample \( X_n^{(i)} \sim M_n \left( X_{n-1}^{(i)}, \cdot \right) \).  

- For \( i = 1, ..., N \), evaluate the normalized weights \( W_n^{(i)} \)

\[
W_n^{(i)} \propto G_n \left( X_{n-1}^{(i)}, X_n^{(i)} \right), \quad \sum_{i=1}^{N} W_n^{(i)} = 1. \tag{15}
\]

**Resampling step**

- \( J = \emptyset \).

- For \( i = 1, ..., N \), with probability \( \epsilon G_n \left( X_{n-1}^{(i)}, X_n^{(i)} \right) \), set \( X_{0:n}^{(i)} = X_{0:n}^{(i)} \) otherwise set \( J = J \cup \{i\} \).

- Multiply/Discard particles \( \left\{ X_{0:n}^{(i)} \right\} \) with respect to high/low weights \( \left\{ W_n^{(i)} \right\} \) to obtain \( \left\{ X_{0:n}^{(i)} \right\}_{i \in J} \).

4 Simulation Results

4.1 Model

We consider the following harmonic regression model (Andrieu and Doucet, 1999)

\[
Y = D(\omega) \beta + n,
\]
where \( Y = (y_0, \ldots, y_{m-1})^T \), \( \beta = (\beta_1, \ldots, \beta_{2k})^T \), \( n = (n_0, \ldots, n_{m-1})^T \), \( \omega = (\omega_1, \ldots, \omega_k)^T \in (0, \pi)^k \) and \( D(\omega) \) is a \( m \times 2k \) matrix where for \( i = 0, \ldots, m-1, j = 1, \ldots, k \).

\[
[D(\omega)]_{i+1,2j-1} = \cos(\omega_j i), \quad [D(\omega)]_{i+1,2j} = \sin(\omega_j i).
\]

We assume that \( n|\sigma^2 \sim \mathcal{N}(0, \sigma^2 I_p) \) and we use the following prior \( p(\sigma^2, \beta, \omega) = p(\omega) p(\beta|\sigma^2) p(\sigma^2) \) with

\[
\sigma^2 \sim IG\left(\frac{v_0}{2}, \frac{\gamma_0}{2}\right), \quad \beta|\sigma^2 \sim \mathcal{N}(0, \sigma^2 \Sigma_0),
\]

where \( \Sigma_0^{-1} = \delta^{-2} D(\omega)^T D(\omega) \) (\( \delta^2 = 25 \)), \( v_0 = \gamma_0 = 1 \); \( p(\omega) \) is uniform on \( \Omega = \{\omega \in (0, \pi)^k; 0 < \omega_1 < \ldots < \omega_k < \pi\} \). The posterior density satisfies on \( \Omega \)

\[
p(\omega|Y) \propto (\gamma_0 + Y^T P Y)^{-\frac{p+k}{2}}
\]

with

\[
M^{-1} = (1 + \delta^{-2}) D(\omega)^T D(\omega),
\]

\[
m = MD(\omega)^T Y,
\]

\[
P = I_p - D(\omega) M D(\omega)^T.
\]

We simulate a realization of \( m = 100 \) observations with \( k = 6, \sigma^2 = 5 \),

\[
\omega = (0.08, 0.13, 0.21, 0.29, 0.35, 0.42)^T,
\]

\[
\beta = (1.24, 0.00, 1.23, 0.43, 0.67, 1.00, 1.11, 0.39, 1.31, 0.16, 1.28, 0.13)^T.
\]

The posterior density is multimodal with well-separated modes.

4.2 Algorithms

To sample from \( \pi(\omega) = p(\omega|Y) \), we use an homogeneous SMC sampler with \( N = 1000 \) particles where the \( k \) components are updated one-at-a-time using a simple Gaussian random walk proposal \( M \) of standard deviation \( \sigma_{RW} \). We select \( L \) to be equal to \( M \) and use the stratified resampling procedure. We compare our algorithm with a MCMC algorithm. The MCMC algorithm updates the component one-at-a-time using a MH
step with the proposal kernel $M$. In both case, the initial distribution is the uniform distribution on $\Omega$.

We consider the case where $\sigma_{RW} = 0.1$. Obviously one could come up with a better proposal kernel. We want to emphasize here that the SMC approach is more robust to a poor scaling of the proposal. A similar remark was made in (Cappé et al., 2002). In Figure 1, we present the marginal posterior distributions of $\omega_1$ and $\omega_2$ obtained using the SMC sampler with 100 iterations. We then run 12000 iterations of the MCMC algorithm so as the computational complexity to be roughly the same for the two algorithms. The MCMC algorithm is more sensitive to the initialization. On 50 realizations of the SMC and the MCMC algorithm, the SMC always explores the main mode whereas the MCMC algorithm converges towards it only 36 times.

We also use an inhomogeneous version of the SMC sampler so as to optimize $p(\omega|Y)$. In this case the target density at time $n$ is $\pi_n(\omega) \propto p^{\gamma_n}(\omega|Y)$ with $\gamma_n = n$ and we use 50 iterations. We compare this algorithm to a simulated annealing version of the MH algorithm with 60000 iterations with $\gamma_n = n/1200$. In Table 1, we display the mean and standard deviations of the log-posterior density of the posterior mode estimate; the posterior mode estimate being chosen as the sample generated during the simulation maximizing the posterior density. Contrary to the simulated annealing algorithm, the SMC algorithm converges consistently towards the same mode.

| Algorithm                  | SMC     | MCMC    |
|----------------------------|---------|---------|
| Mean of the log-posterior values | -326.12 | -328.87 |
| Standard deviation of the log-posterior values | 0.12    | 1.48    |

Table 1: Performance of SMC and MCMC algorithm obtained over 50 simulations
Figure 1: Histograms of the simulated values of $(\omega_1, \omega_2)$ using SMC - Estimation of $p(\omega_1|Y)$ (top) and $p(\omega_2|Y)$ (bottom).

5 Discussion

In this article, we have presented a class of methods to sample from distributions known up to a normalizing constant. These methods are based on SMC algorithms. This framework is very general and flexible. Several points not discussed here are detailed in (Del Moral and Doucet, 2003).

- In the homogeneous case, assume that we do not initialize the algorithm in the stationary regime, i.e. we do not correct for the discrepancy between $v_0$ and $\pi$. This has to be paralleled with MCMC algorithms which are not initialized in the stationary regime. Under regularity assumptions, it can be shown that the distribution flow still converges towards the target distribution $\pi$. Moreover, it converges at a rate only dependent on the mixing properties of $L$. This is in contrast with the MH algorithm whose rate of convergence is dependent on $\pi$ and $M$. 
• The algorithm we have presented can be used to simulate a Markov chain with a fixed terminal point. Indeed, one obtains at time $n$ samples from (1). By setting $L_0(x_1, dx_0) = \delta_x(dx_0)$ and reversing the time index, one obtains an approximate realization of a Markov process of initial distribution $\pi_n$ at time 0, transition $\{L_n\}$ and terminal point $x$ at time $n + 1$. This has applications in genetics and physics.

There are also several important open methodological and theoretical problems to study.

• Similarly to MCMC methods, one needs to carefully design the various components of the algorithm to get good performance. In particular, it would be of interest to come up with an automated choice for $L_n$ given $M_n$. For the homogeneous case, one could look at minimizing the variance of (3). It involves a tradeoff between the mixing properties of $L$ and the variance of the importance weights (2). This point is currently under study.

• It would be interesting to weaken the assumptions of the results in (Del Moral and Miclo, 2000; Del Moral and Doucet, 2003) which mostly only hold for compact spaces.

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