Backward importance sampling for online estimation of models with intractable likelihood

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Abstract

This paper proposes a new Sequential Monte Carlo algorithm to perform maximum likelihood estimation in partially observed dynamical systems whose dynamics is unknown. Training such generative models and obtaining low variance estimators of the posterior distributions of the unobserved states given the observations is challenging as the transition densities of the states cannot be evaluated pointwise. In this paper, a backward importance sampling step is introduced to estimate such posterior distributions instead of the acceptance-rejection procedure used in the usual approach. In the context of multivariate stochastic differential equations, the proposed algorithm makes use of unbiased estimates of the unknown transition densities under much weaker assumptions than standard alternatives. The performance of this estimator is assessed in the case of a partially observed stochastic Lotka-Volterra model and more!

1 Introduction

Latent data models are all-pervasive in time series and sequential data analysis across a wide range of applied science and engineering domains such as movement ecology [Michelot et al., 2016], energy consumptions modelling [Candanedo et al., 2017], genomics [Yau et al., 2011, Gassiat et al., 2016, Wang et al., 2017], target tracking [Särkkä et al., 2007], enhancement and segmentation of speech and audio signals [Rabiner, 1989], see also [Särkkä, 2013, Douc et al., 2014, Zucchini et al., 2017] and the numerous references therein. Performing maximum likehood estimation (MLE) for instance with the Expectation Maximization (EM) algorithm [Dempster et al., 1977] or a stochastic gradient ascent ([Cappé et al., 2005] in the case of HMMs) is a challenging task. Both approaches involve conditional distributions of sequences of hidden states given the observation record (the *smoothing* distribution), which are not available explicitly.

Markov chain Monte Carlo (MCMC) and sequential Monte Carlo (SMC) methods (also known as particle filters or smoothers) are widespread solutions to propose consistent estimators of such distributions. A pivotal step of SMC approaches is the evaluation of the transition density of the hidden signal and of the density of the conditional distribution of an observation given the corresponding latent state (the marginal conditional likelihood). However, in many practical settings, no closed-form expressions of these distributions are available for instance in the case of partially observed diffusions [] or in the context of approximate

Bayesian computation smoothing []. A first step to bypass this shortcoming was proposed [] where the authors proposed an important contribution by showing that it is possible to implement importance sampling and filtering recursions, when the unavailable importance weights are replaced by random estimators. Standard data augmentation schemes were then used to extend this random-weight particle filter to provide new inference procedures for partially observed diffusion models [].

More recently, [Gloaguen et al., 2019] introduced a pseudo-marginal online smoother to approximate conditional expectations of additive functionals of the hidden states in a very general setting where the user can only evaluate (possibly biased) approximations of the transition density and/or of the marginal conditional likelihood. The online algorithm of [Gloaguen et al., 2019] may be used to approximate expectations of additive functionals under the smoothing distributions by processing the data stream online. This algorithm extends the particle-based rapid incremental smoother (PaRIS) of [Olsson et al., 2017]. This approach is an online version of the Forward Filtering Backward Simulation algorithm [Douc et al., 2011] specifically designed to approximate conditional expectations of additive functionals. Other smoothing algorithms such as two-filter based approaches [Briers et al., 2010, Fearnhead et al., 2010b, Nguyen et al., 2017] could be extended but they are intrisically not online procedures as they require the time horizon and all observations to be available to initialize a backward information filter. In [Gloaguen et al., 2019], the authors proposed several theoretical guarantees for this pseudo-marginal smoothing algorithm to assess the reach of its efficiency: strong consistency, asymptotic normality when the number of particles grows to infinity and control of the asymptotic variance. This extended the result of [Olsson et al., 2017], written only in the case of the bootstrap filter [Gordon et al., 1993], and the theoretical guarantees obtained for online sequential Monte Carlo smoothers given in [Del Moral et al., 2010, Douc et al., 2011, Dubarry and Le Corff, 2013, Gerber and Chopin, 2017].

However, a requirement to use this algorithm is that the estimate of the transition density and of the marginal likelihood is almost surely positive and upper bounded. This condition is required to perform a pivotal backward acceptance-rejection sampling procedure. In the context of diffusion processes, this assumption is very restrictive and narrows the possible models to the class of diffusions satisfying the Exact algorithm conditions of [Beskos et al., 2006a], for which General Poisson Estimators (GPEs) [Fearnhead et al., 2008] lead to eligible unbiased estimators. Add other settings where accept-reject is not a valid option.

In this paper, a new procedure is introduced to replace the backward acceptance-rejection step by an importance sampling estimate which leads to a smoothing algorithm that only requires an almost surely positive estimator of the transition density. In the context of partially observed diffusion processes, it is shown that such an estimator can be obtained for a wide range of models, using the parametrix estimators of [Andersson and Kohatsu-Higa, 2017] and [Fearnhead et al., 2017]. In this paper, we propose to use Wald's trick to obtain positive estimates of the transition densities as this is not guaranteed in the original parametrix estimators. The proposed method does not rely on any acceptance rejection procedure which reduces very significantly the computational time and its variance, as illustrated in extensive numerical experiments. Add bias.

2 Model and objectives

Let $(X_k)_{k\geq 0}$ be a Markov chain on $\mathbb{R}^d$ such that the distribution of X_0 has density χ with respect to the Lebesgue measure and for all $0 \leqslant k \leqslant n-1$, the conditional distribution of X_{k+1} given $(X_0, \ldots, X_k)$ has density $q_{k+1;\theta}(X_k, \cdot)$. It is assumed that this state is partially observed through an observation process $(Y_k)_{0\leqslant k\leqslant n}$ taking values in $\mathbb{R}^m$. For all $0 \leqslant k \leqslant n$, the distribution of Y_k given $(X_0, \ldots, X_n)$ depends on X_k only and has density $g_{k;\theta}$ with respect to the Lebesgue measure. In this setting, common learning

objectives are the *state estimation problem*, which aims at recovering the underlying signal X_k at time t_k given the observations $Y_{0:n}$, where $a_{u:v}$ is a short-hand notation for $(a_u, \ldots, a_v)$, and the *parameter inference problem* which aims at approximating

$$\widehat{\theta}_n = \mathrm{argmax}_{\theta \in \Theta} \, \mathsf{L}_n(\theta) \, ,$$

where $\mathsf{L}_n(\theta)$ is the likelihood of the observations. When θ is known, the state estimation problem is usually solved by approximating the posterior mean of X_k given the observations $Y_{0:n}$ when the model is driven by the parameter θ. In the context of parameter estimation, note that

$$\mathsf{L}_n(\theta) = \int \chi(x_0) g_{0;\theta}(x_0, Y_0) \prod_{k=0}^{n-1} \ell_{k;\theta}(x_k, x_{k+1}) \mathrm{d}x_{0:n},$$

where, for all $0 \leqslant k \leqslant n$ and all $\theta \in \Theta$,

$$\ell_{k;\theta}(x_k, x_{k+1}) = q_{k+1;\theta}(x_k, x_{k+1}) g_{k+1;\theta}(x_{k+1}, Y_{k+1}) \, .$$

Expectation Maximization based algorithms are appealing solutions to obtain an estimator of $\hat{\theta}_n$. The pivotal concept of the EM algorithm is that the intermediate quantity defined by

$$\theta \mapsto Q(\theta, \theta') = \mathbb{E}_{\theta'} \left[\sum_{k=0}^{n-1} \log \ell_{k;\theta}(X_k, X_{k+1}) \middle| Y_{0:n} \right] \tag{1}$$

may be used as a surrogate for $\mathsf{L}_n(\theta)$ in the maximization procedure, where $\mathbb{E}_{\theta'}$ is the expectation under the joint distribution of the latent states and the observations when the model is parameterized by θ. Therefore, the EM algorithm iteratively builds a sequence $(\theta_p)_{p \geqslant 0}$ of parameter estimates following the two steps: (i) compute $\theta \mapsto Q(\theta, \theta_p)$ and (ii) choose θ_{p+1} as a maximizer of $\theta \mapsto Q(\theta, \theta_p)$. Gradient ascent algorithms are compelling alternatives to the EM algorithm. In the context of HMMs, the gradient of the log-likelihood can also be expressed as an expectation of an additive functional of the hidden states given $Y_{0:n}$ ([Cappé et al., 2005], Chapter 10, or [Gloaguen et al., 2019] in the context of SDEs). A key feature here is that all the relevant estimators rely on computing, for some parameters θ and θ':

$$\mathbb{E}_{\theta'} \left[h_{0:n,\theta}(X_{0:n}) | Y_{0:n} \right] ,$$

where $h_{0:n,\theta}$ is an *additive functional*, *i.e.* satisfying:

$$h_{0:n,\theta} : x_{0:n} \mapsto \sum_{k=0}^{n-1} \tilde{h}_{k;\theta}(x_k, x_{k+1}),$$

where $\tilde{h}_{k;\theta}$ is a functional depending on the estimator. For any $\theta \in \Theta$, $0 \leqslant k_1 \leqslant k_2 \leqslant n$ and any bounded and measurable function h on $(\mathbb{R}^d)^{k_2 - k_1 + 1}$, define the *joint smoothing distributions* as:

$$\phi_{k_1:k_2|n;\theta}[h] := \mathbb{E}_\theta \left[h(X_{k_1:k_2}) | Y_{0:n} \right] \, . \tag{2}$$

For all $0 \leqslant k \leqslant n$, $\phi_{k;\theta} = \phi_{k:k|k;\theta}$ are the *filtering distributions*.

In the following, θ is dropped from the notations for better clarity when there is no possible confusion. As noted for instance in [Cappé et al., 2005], although the objective is to obtain approximation of smoothing distributions, the filtering distribution is crucial as, for additive functionals,

$$\phi_{0:n|n}[h_{0:n}] = \phi_n \left[\mathbf{T}_n[h_{0:n}] \right] ,$$

where

$$\mathbf{T}_n[h_{0:n}](X_n) = \mathbb{E}\left[h_n(X_{0:n})|X_n, Y_{0:n}\right]. \tag{3}$$

As a key consequence of the additive property, for all $1 \leqslant k \leqslant n$

$$\mathbf{T}_k[h_{0:k}](X_k) = \mathbb{E}\left[\mathbf{T}_{k-1}[h_{0:(k-1)}](X_{k-1}) + \tilde{h}_{k-1}(X_{k-1}, X_k)\middle| X_k, Y_{0:k-1}\right]. \tag{4}$$

However, the exact computation of all these key expectations is not possible in general state spaces.

The next section describes a Sequential Monte Carlo algorithm [Doucet et al., 2013] to approximate ϕ_n by weighted samples $\{(\omega_n^\ell, \xi_n^\ell)\}_{\ell=1}^N$ and the algorithm of [Gloaguen et al., 2018] to compute recursively, for each $1 \leqslant \ell \leqslant N$ an approximation τ_n^ℓ of $\mathbf{T}_n[h_{0:n}](\xi_n^\ell)$ so that the estimator of $\phi_{0:n|n}[h_{0:n}]$ is defined as

$$\phi_{0:n|n}^N[h_{0:n}] := \sum_{\ell=1}^N \frac{\omega_n^\ell}{\sum_{j=1}^N \omega_n^j} \tau_n^\ell \,. \tag{5}$$

3 Online sequential Monte Carlo smoothing

In many situations Add examples (taken from the paper with Jimmy), SMC methods cannot be used straightforwardly as the transition densities q_k, $0 \leqslant k \leqslant n-1$ and the marginal likelihood of the observations g_k, $0 \leqslant k \leqslant n-1$, are unknown. Pseudo-marginalisation was originally proposed in [**?**] in the framework of MCMC methods, and further analyzed in [**?**]. Following [Fearnhead et al., 2008, Olsson et al., 2011, Gloaguen et al., 2018], while the target density is intractable we assume that there exists some additional state space$(\mathsf{U}, \mathcal{B}(\mathsf{U}))$ such that the following assumption holds.

H1 For all $\theta \in \Theta$ and $k \geqslant 0$, there exists a Markov kernel on $(\mathbb{R}^d \times \mathbb{R}^d, \mathcal{B}(\mathsf{U}))$ with density $\mathbf{R}_{k;\theta}$ with respect to a reference measure μ on a general state space $(\mathsf{U}, \mathcal{B}(\mathsf{U}))$, and a positive mapping $\ell_{k;\theta}$ on $\mathbb{R}^d \times \mathbb{R}^d \times \mathsf{U}$ such that, for all $(x, x') \in \mathbb{R}^d \times \mathbb{R}^d$,

$$\int \mathbf{R}_{k;\theta}(x, x'; z)\ell_{k;\theta}\langle z\rangle(x, x')\mu(\mathrm{d}z) = \ell_{k;\theta}(x, x') \,.$$

Thus, a pointwise estimate of $\ell_{k;\theta}(x, x')$ can be obtained by generating ζ from $\mathbf{R}_{k;\theta}(x, x'; \mathrm{d}z)$ and computing the statistic $\ell_{k;\theta}\langle z\rangle(x, x')$. Interestingly, even though pseudo marginalisation is based on the plug-in principle, it preserves typically the consistency of an algorithm, see for instance in the case of pseudo-marginal SMC smoothers [Gloaguen et al., 2019].

3.1 Filtering

Let $(\xi_0^\ell)_{\ell=1}^N$ be independent and identically distributed according to an instrumental proposal density ρ_0 on $\mathbb{R}^d$ and define the importance weights $\omega_0^\ell := \chi(\xi_0^\ell)/\rho_0(\xi_0^\ell)$, where χ is the density of the distribution of X_0, see Section 2. For any bounded and measurable function f defined on $\mathbb{R}^d$,

$$\phi_0^N[f] := \Omega_0^{-1} \sum_{\ell=1}^N \omega_0^\ell f(\xi_0^\ell) \,, \quad \text{where} \quad \Omega_0 := \sum_{\ell=1}^N \omega_0^\ell \,.$$

is a consistent estimator of $\phi_0[f]$. Then, for all $k \geqslant 1$, once the observation Y_k is available, the weighted particle sample $\{(\omega_{k-1}^\ell, \xi_{k-1}^\ell)\}_{\ell=1}^N$ is transformed into a new weighted particle sample approximating ϕ_k. This update step is carried through in two steps, *selection* and *mutation*, using sequential importance sampling and resampling steps. New indices and particles $\{(I_k^\ell, \xi_k^\ell, \zeta_k^\ell)\}_{\ell=1}^N$ are simulated independently from the instrumental distribution with density on $\{1, \ldots, N\} \times \mathbb{R}^d \times \mathsf{U}$:

$$\upsilon_k(\ell, x, z) \propto \omega_{k-1}^\ell p_{k-1}(\xi_{k-1}^\ell, x) \mathbf{R}_k(\xi_{k-1}^\ell, x; z) \ ,$$

where p_{k-1} is a Markovian transition density. In practice, this step is performed as follows:

1. Sample I_k^ℓ in $\{1, \ldots, N\}$ with probabilities proportional to $\{\omega_{k-1}^j\}_{1 \leqslant j \leqslant N}$.

2. Sample ξ_k^ℓ with distribution $p_{k-1}(\xi_{k-1}^{I_k^\ell}, \cdot)$ and sample ζ_k^ℓ with distribution $\mathbf{R}_k(\xi_{k-1}^{I_k^\ell}, \xi_k^\ell; \cdot)$.

The choice of the proposal distribution p_{k-1} is a pivotal tuning step to obtain efficient estimations of the filtering distributions. In the context of this paper, a natural choice for p_k could be to use an approximation of the bootstrap filter, i.e. an approximation of q_{k-1} based for instance on a Euler discretization scheme. In the numerical section of this paper, we propose to use an approximation of the optimal filter which accounts for the newly obtained observation to propose new particles, see (10). For any $\ell \in \{1, \ldots, N\}$, ξ_k^ℓ is associated with the importance weight defined by:

$$\omega_k^\ell := \frac{\ell_{k-1}\langle \zeta_k^\ell \rangle(\xi_{k-1}^{I_k^\ell}, \xi_k^\ell)}{p_{k-1}(\xi_{k-1}^{I_k^\ell}, \xi_k^\ell)} \tag{6}$$

to produce the following approximation of $\phi_k[f]$:

$$\phi_k^N[f] := \Omega_k^{-1} \sum_{\ell=1}^N \omega_k^\ell f(\xi_k^\ell) \ , \quad \text{where} \quad \Omega_k := \sum_{\ell=1}^N \omega_k^\ell \ .$$

3.2 Smoothing

In the context of additive functionals, the forward-only smoothing algorithm introduced in [Del Moral et al., 2010] proposes a particle approximation of (3) that can be computed *online* using the recursion (4). This algorithm has a computational complexity which grows *quadratically* with the number of particles N. This computational cost can be reduced when the transition density of the hidden states is upper bounded following [Olsson et al., 2017] by applying the accept-reject sampling approach proposed in [Douc et al., 2011] and illustrated in [Dubarry and Le Corff, 2011]. Following [Gloaguen et al., 2019], the backward statistics $\mathbf{T}_{k+1}[h_{0:k+1}](\xi_{k+1}^i)$, where $\mathbf{T}_{k+1}$ is defined in (3), are estimated, for all $1 \leqslant i \leqslant N$, as follows,

$$\tau_{k+1}^i = \frac{1}{\widetilde{N}} \sum_{j=1}^{\widetilde{N}} \left(\tau_k^{J_{k+1}^{(i,j)}} + \tilde{h}_k \left(\xi_k^{J_{k+1}^{(i,j)}}, \xi_{k+1}^i \right) \right) \ ,$$

where $\widetilde{N} \geqslant 1$ is a sample size which is typically small compared to N and where $(J_{k+1}^{(i,j)}, \zeta_{k+1}^{(i,j)})$, $1 \leqslant j \leqslant \widetilde{N}$, are i.i.d. in $\{1, \ldots, N\} \times \mathsf{U}$ with distribution

$$\overline{v}_k^i(\ell, z) \propto \omega_k^\ell \ell_k \langle z \rangle(\xi_k^\ell, \xi_{k+1}^i) \mathbf{R}_k(\xi_k^\ell, \xi_{k+1}^i; z) \ .$$

In [Gloaguen et al., 2018], it is assumed that, for all $0 \leqslant k \leqslant n$ and $0 \leqslant i \leqslant N$, there exists an upper bound $\bar{\varepsilon}_k^i$ such that

$$\sup_{\ell,\zeta} \ell_k\langle\zeta\rangle(\xi_k^\ell, \xi_{k+1}^i) \leqslant \bar{\varepsilon}_k^i \ . \tag{7}$$

Then, for all $(i, z) \in \{1, \ldots, N\} \times \mathsf{U}$,

$$\omega_k^\ell \ell_k\langle z\rangle(\xi_k^\ell, \xi_{k+1}^i)\mathbf{R}_k(\xi_k^\ell, \xi_{k+1}^i; z) \leqslant \bar{\varepsilon}_k \omega_k^\ell \mathbf{R}_k(\xi_k^\ell, \xi_{k+1}^i; z) \ .$$

Therefore, the following accept-reject mechanism algorithm may be used to sample from $\overline{v}_k^i$.

1. A candidate (J^*, ζ^*) is sampled in $\{1, \ldots, N\} \times \mathsf{U}$ as follows:
   (a) J^* is sampled with probabilities proportional to $(\omega_k^\ell)_{\ell=1}^N$;
   (b) ζ^* is sampled independently with distribution $\mathbf{R}_k(\xi_k^{J^*}, \xi_{k+1}^i; \zeta^*)$.
2. (J^*, ζ^*) is then accepted with probability $\ell_k\langle\zeta^*\rangle(\xi_k^{J^*}, \xi_{k+1}^i)/\bar{\varepsilon}_k^i$ and, upon acceptance, $J_{k+1}^{(i,j)} = J^*$.

This algorithm is the only SMC smoother proposed in the literature with theoretical guarantees when no closed-form expressions of the transition densities and the conditional likelihood of the observations are available, assuming that the user can only evaluate approximations of these densities. This pseudo-marginal particle smoothing algorithm requires that the backward sampling step generates samples exactly according to $\overline{v}_k^i$. This leads in practice to strong assumptions to implement the accept-reject step: positiveness of the pseudo-marginal likelihood and the existence of the uper bound (7). In the next section, we propose an alternative to this step to obtain a computationally efficient pseudo-marginal smoother in a much wider range of applications in which such assumptions do not hold.

4 Pseudo-marginal backward importance sampling

4.1 Positive transition densities estimates

Parler d'estimateur positifs au sens large, pas necessairement parametrix et pour les EDS. In this section, we propose to use Wald's identity for martingales to obtain a new estimator which is guaranteed to be positive based on any estimator of the transition density. This identity was applied in [Fearnhead et al., 2010a] to Poisson based estimators. Our estimator is defined up to an unknown constant of proportionality, which is removed when the importance weights are normalized in equation (8). This approach, rather than setting negative weights to 0, which would lead to a biased estimate, uses extra simulation to obtain positiveness. This is done while ensuring that the weights remain unbiased up to a common constant of proportionality. Assume that the distribution $\mathbf{R}_k$ of the additional random variables ζ_k and the estimator ℓ_k are obtained with the parametrix estimator.

Particle filtering. For all $k \geqslant 0$, the Wald-based random weight particle filtering proceeds as follows.

1. For all $1 \leqslant i \leqslant N$, sample a new particle as described in Section 3.1.
   (a) Sample I_k^i in $\{1, \ldots, N\}$ with probabilities proportional to $\{\omega_{k-1}^j\}_{1 \leqslant j \leqslant N}$.
   (b) Sample ξ_k^i with distribution $p_{k-1}(\xi_{k-1}^{I_k^i}, \cdot)$.
2. For all $1 \leqslant i \leqslant N$, set $\omega_k^i = 0$.

3. While there exists $i_* \in \{1, \dots, N\}$ such that $\omega_k^{i_*} \leqslant 0$, for all $1 \leqslant i \leqslant N$, sample ζ_k^i with distribution $\mathbf{R}_k(\xi_{k-1}^{I_k^i}, \xi_k^i; \cdot)$ (i.e. compute a parametrix estimator of the transition density) and set

$$\omega_k^i = \omega_k^i + \frac{\ell_{k-1}\langle \zeta_k^i \rangle(\xi_{k-1}^{I_k^i}, \xi_k^i)}{p_{k-1}(\xi_{k-1}^{I_k^i}, \xi_k^i)} \, .$$

Backward simulation. For all $1 \leqslant i \leqslant N$, the backward importance sampling step proceeds then as follows.

1. For all $1 \leqslant j \leqslant \widetilde{N}$, sample $J_{k+1}^{(i,j)}$ in $\{1, \dots, N\}$ with probabilities proportional to $(\omega_k^i)_{i=1}^N$.
2. For all $1 \leqslant j \leqslant \widetilde{N}$, set $\varpi_k^{(i,j)} = 0$.
3. While there exist $j_* \in \{1, \dots, \widetilde{N}\}$ such that $\varpi_k^{(i,j)} \leqslant 0$, for all $1 \leqslant j \leqslant \widetilde{N}$, sample $\zeta_k^{(i,j)}$ with distribution $\mathbf{R}_k(\xi_k^{J_{k+1}^{(i,j)}}, \xi_{k+1}^i; \cdot)$ and set

$$\varpi_k^{(i,j)} = \varpi_k^{(i,j)} + \ell_k\langle \zeta_k^{(i,j)} \rangle(\xi_k^{J_{k+1}^{(i,j)}}, \xi_{k+1}^i) \, .$$

4.2 AR-free online smoothing

As the positive parametrix-based estimate does not satisfy the upper bound condition of (7), the statistics are updated recursively with an importance sampling step: for all $1 \leqslant i \leqslant N$,

$$\tau_{k+1}^i = \sum_{j=1}^{\widetilde{N}} \frac{\varpi_k^{(i,j)}}{\mathcal{W}_k^i} \left(\tau_k^{J_{k+1}^{(i,j)}} + \tilde{h}_k \left(\xi_k^{J_{k+1}^{(i,j)}}, \xi_{k+1}^i \right) \right) \, , \tag{8}$$

where $\varpi_k^{(i,j)}$, $1 \leqslant j \leqslant \widetilde{N}$ are computed using the parametrix estimate combined with Wald's identity and $\mathcal{W}_k^i = \sum_{j=1}^{\widetilde{N}} \varpi_k^{(i,j)}$. Then, the estimator of the conditional expectation of the additive functional is set as

$$\phi_{0:n|n}^{N,\mathrm{IS}}[h_{0:n}] := \sum_{i=1}^N \frac{\omega_n^i}{\Omega_n} \tau_n^i \, .$$

This estimator does not rely on an accept reject mechanism and is therefore less computationally intensive and can be used under reasonable assumptions for many SDEs. In addition, as shown in Section **??**, this does not affect the statistical efficiency of the algorithm.

5 Application to smoothing expectations and score estimation

5.1 Sine model

This section investigates the performance of the proposed algorithm to compute expectations under the smoothing distributions in a context where alternatives are available for comparison. Consider the Sine model where $(X_t)_{t \geqslant 0}$ is assumed to be a weak solution to

$$\mathrm{d}X_t = \sin(X_t - \theta)\mathrm{d}t + \mathrm{d}W_t \, , \quad X_0 = x_0 \, .$$

This simple model has no explicit transition density, however, a General Poisson estimator which satisfies (7) can be computed by simulating Brownian bridges, (see [Beskos et al., 2006b]). Therefore, the backward importance sampling technique proposed in this paper can be compared to the usual acceptance-rejection algorithm described in Section 3.2. For this simple comparison, observations are received at evenly spaced times $t_0 = 0, \dots, t_{10} = 5$ from the model

$$Y_k = X_{t_k} + \varepsilon_k,\ 0 \leqslant k \leqslant n = 10\ , \tag{9}$$

where $(\varepsilon_k)_{0\leqslant k\leqslant 10}$ are i.i.d. Gaussian random variables with mean 0 and variance 1. In this experiment $\theta = \pi/4$. The proposal distribution p_k for the particle filtering approximation is chosen as the following approximation of the optimal filter:

$$p_k(x_k, x_{k+1}) \propto q_{k+1}^{\mathsf{Eul}}(x_k, x_{k+1}) g_{k+1}(x_{k+1}, Y_{k+1})\ , \tag{10}$$

where q_{k+1}^{Eul} is the probability density function of Gaussian distibution with mean $\Delta \sin(x_k - \theta)$ and variance Δ where $\Delta = 1/2$, i.e. the Euler approximation of the Sine SDE, and g_k is the probability density function of the law of Y_k given X_{t_k} i.e. of a Gaussian random variable with mean X_{t_k} and variance 1. As the observation model is linear and Gaussian, the proposal distribution is therefore Gaussian with explicit mean and variance.

In this first experiment, particles are used to solve the state estimation problem for the first observation i.e. to compute an estimate of $\mathbb{E}[X_0|Y_{0:n}]$. Figure 1 displays the computational complexity and the estimation of the posterior mean with the acceptance-rejection algorithm and the proposed backward sampling technique as a function of $\widetilde{N}$. In this setting, $N = 100$, and each unbiased estimate of $\hat{q}$ is computed using 30 Monte Carlo replicates.

For $\widetilde{N} = 2$ (which is the recommended value for the PaRIS algorithm, see [Olsson et al., 2017]), our estimate shows a bias, which is no suprise, as it is based on a biased normalized importance sampling step. However, this bias quickly vanishes for $\widetilde{N} \geqslant 10$. Interestingly, our method comes with a drastic (a factor 10) reduction of computational time. The vanishing of the bias might induce more backward sampling, but this remains much faster than the acceptance rejection method with $\widetilde{N} = 2$.

Then, the same estimation was perfomed (on the same data set) for N varying from 50 to 2000. In this context, $\widetilde{N}$ was set to 2 for the AR method. To have an empirical intuition of how $\widetilde{N}$ must vary with N, the importance sampling algorithm is applied with $\widetilde{N} = N^{0.5}, N^{0.6}$ and $N/10$ (as this last value was sufficient in the first experiment to avoid any bias). The results are shown in Figure 2. A small bias might appear for $N = 2000$ and $\widetilde{N} = 45$ ($\approx 2000^{0.5}$), but no bias is visible for $N^{0.6}$ and $N/10$. As expected, the gain in time, compared to the state of the art algorithm, remains important (even if it decreases as $\widetilde{N}$ increases). It is worth noting that the variance of the computational time is greatly reduced compared to the AR technique.

5.2 Stochastic Lotka-Volterra model

This section sets the focus on a stochastic model describing in continuous time the population dynamics in a predator-prey system, as fully discussed in [Hening and Nguyen, 2018]. The bivariate process $(X_t)_{t\geqslant 0}$ of predators and preys abundances is assumed to follow the stochastic Lotka-Volterra model:

$$\mathrm{d}X_t = \alpha_\theta(X_t)\mathrm{d}t + \begin{pmatrix} X_1(t) & 0 \\ 0 & X_2(t) \end{pmatrix} \Gamma \mathrm{d}\mathbf{W}_t\ , \tag{11}$$

where $\mathbf{W}_t$ is a vector of independent standard Wiener processes, Γ a 2×2 matrix, and for $x = (x_1, x_2)^T$:

$$\alpha_\theta(x) = \begin{pmatrix} x_1(a_{10} - a_{11}x_1 - a_{12}x_2) \\ x_2(-a_{20} + a_{21}x_1 - a_{22}x_2) \end{pmatrix}\ .$$

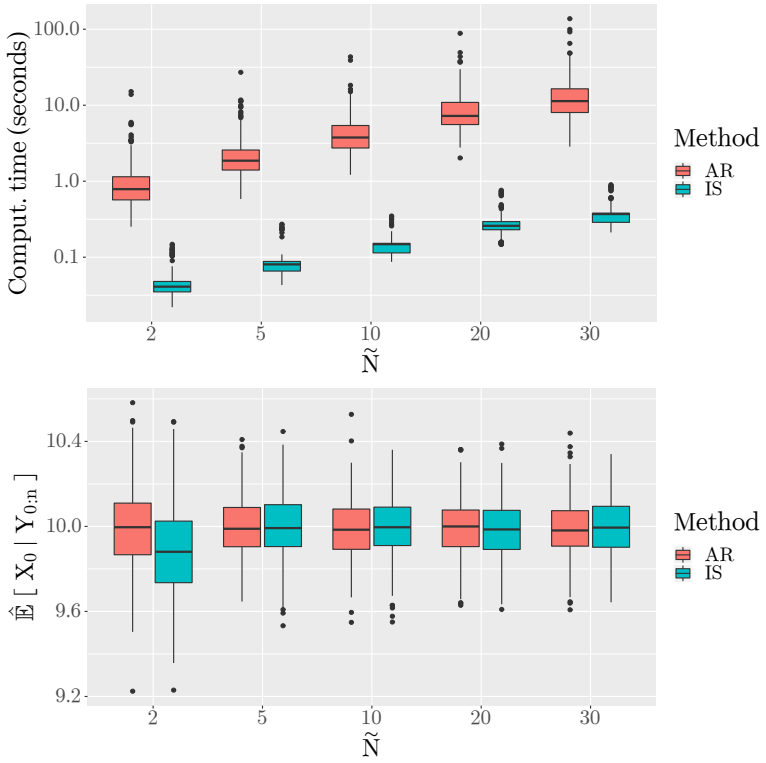

Figure 1: Computational complexity and estimation of a posterior mean as a function of the number of backward samples. Results are shown for the state of the art acceptance-rejection algorithm and the proposed backward importance sampling technique.

In this context, the unknow parameter to be estimated is $\theta = (a_{10}, a_{11}, a_{12}, a_{20}, a_{21}, a_{22}, \Gamma)$. The observation model follows a widespread framework in ecology where the abundance of preys and predators are observed through some abundance index at discrete times $t_0, \ldots, t_n$:

$$Y_{t_k} = \begin{pmatrix} \mathrm{c}_1 X_1(t_k) \mathrm{e}^{\epsilon_{t_k}^{(1)}} \\ \mathrm{c}_2 X_2(t_k) \mathrm{e}^{\epsilon_{t_k}^{(2)}} \end{pmatrix} , \tag{12}$$

where $\mathrm{c} = (\mathrm{c}_1, \mathrm{c}_2)^T$ is known (the observed fraction of the population) and $\{\epsilon_{t_k} = (\epsilon_{t_k}^{(1)}, \epsilon_{t_k}^{(2)})\}_{1 \leqslant k \leqslant n}$ are i.i.d. random variables distributed as a $\mathcal{N}_2(-\mathrm{diag}\, \Sigma/2, \Sigma)$ where Σ is an unknown 2×2 covariance matrix. It is straightforward to show that for a generic θ, in the SDE defined by (11), the drift function cannot be written (even after the Lamperti transform) as the gradient of a potential. Therefore, the General Poisson estimator cannot be used as an unbiased estimator of the transition density, and the method proposed in this paper is the only solution to obtain a consistent estimate of the target expectations. The proposal distribution for the particle filter is again a trade off between model dynamics and the observation model (full details are given in the appendix). The simulated set of particles is used to obtain estimates of the true abundances given the observations, both on synthetic and real data.

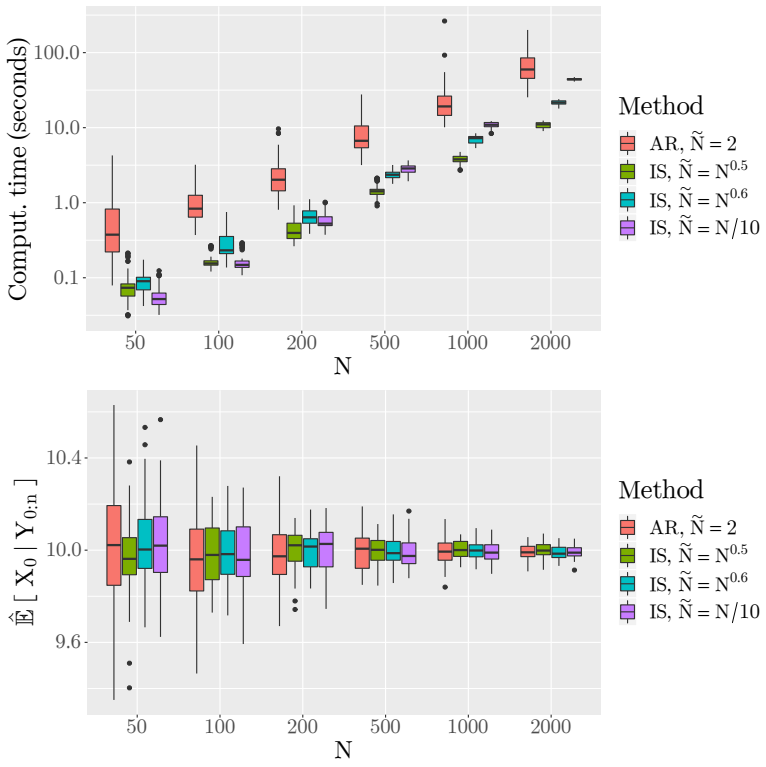

Figure 2: Computational complexity and estimation of a posterior mean as a function of the number of particles. Results are shown for the state of the art acceptance-rejection algorithm and the proposed backward importance sampling technique. The number of backward samples is set to 2 for the AR, and $N/10$ for the IS.

Synthetic data

In a first approach, simulated data are obtained from the model given by (11) and (12) for a known set of parameters. Chosen values of θ, Σ, c_1 and c_2 for the experiment are given in the appendix. The model is used to simulate abundances indexes $Y_0, \dots Y_{300}$ at times $t_0 = 0, \dots, t_{300} = 3$. The associated time series (after a division by c) is shown in Figure 3 (left panel). In this experiment, the goal is to obtain an estimate of the actual predator-prey abundances given all the observed abundances indexes $Y_{0:n}$. Our estimate is given by the set of conditional expectations $\{\mathbb{E}[X_k|Y_{0:n}]\}_{k=0,\dots,n}$, approximated using our backward importance sampling PaRIS smoother, which is run using the true parameters. Figure 3 shows the estimated abundance trajectory over time. The proposed algorithm manages to estimate efficiently the actual abundance from noisy data and a model with an intractable transition density.

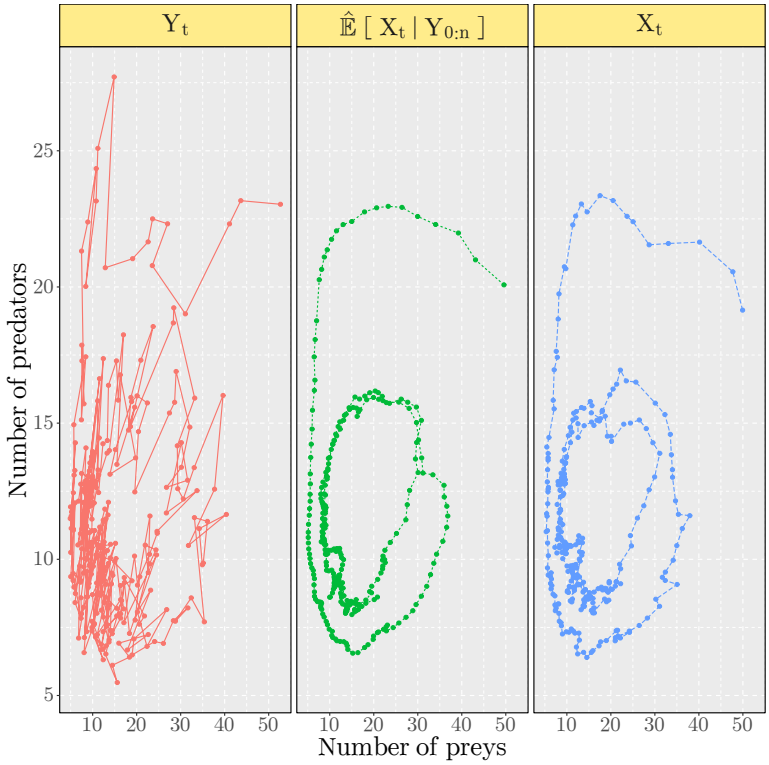

Figure 3: Estimated predator-prey abundances (center) in a stochastic Lotka Volterra model using our backward sampling estimate on simulated abundance indexes (left). Right panel shows the ground truth.

Hares and lynx data

In this section, the model defined by equations (11) and (12) is applied to the Hudson Bay company data, giving the number of hares and lynx trapped in Canada during the first 20 years of the 20th century (available in [Odum and Barrett, 1971]). As parameters are unknown in this case, maximum likelihood inference is performed using an EM [Dempster et al., 1977] algorithm to obtain an estimate $\hat{\theta}$. As explained in the introduction, it is then required to estimate iteratively, from an initial guess θ_0, the conditional expectation given in equation (1). This E step is performed using the particle smoother introduced in this paper. At each iteration, the estimator θ_k is updated by finding a parameter θ_{k+1} for which $\hat{Q}(\theta_{k+1}, \theta_k) > \hat{Q}(\theta_k, \theta_k)$, with a gradient free evolution strategy [Hansen, 2006]. The last estimate $\hat{\theta}$ obtained with this EM algorithm is used to estimate the actual abundances in the model (similarly to the synthetic data case). Figure 8 shows estimates of $\mathbb{E}_{\hat{\theta}}\left[X_k | Y_{0:n}\right]$ obtained with 30 independent runs of our algorithm. The particle smoother is implemented using $N = 200$ particles and $\tilde{N} = 20$. The replicates show that the variance of our estimator (for a given set of observations) is much smaller than the one of the *poor man smoother*. This algorithm approximates the smoothing distributions at time n by the weighted samples where the particle trajectories $\xi_{0:n}^{\ell}$, $1 \leqslant \ell \leqslant N$, are obtained using the ancestral line of each last sample. The variance of the estimates based on this ancestor tree is doomed to failure due to the degeneracy caused by the successive resampling steps.

5.3 Recurrent neural networks

6 Tangent filters and online recursive maximum likelihood

Let Θ be a parameter space. This section considers a family of transition kernels $(\mathbf{Q}_{k;\theta})_{\theta\in\Theta;0\leqslant k\leqslant n-1}$ on $\mathbb{R}^d \times \mathcal{B}(\mathbb{R}^d)$ and $(\mathbf{G}_{k;\theta})_{\theta\in\Theta;1\leqslant k\leqslant n}$ on $\mathbb{R}^d \times \mathcal{B}(\mathsf{Y})$ associated with densities $q_{k;\theta}$ and $g_{k;\theta}$ with respect to μ and ν. The joint smoothing distributions are then defined, for any $\theta \in \Theta$, $0 \leqslant k_1 \leqslant k_2 \leqslant n$ and any function $h \in \mathsf{F}((\mathbb{R}^d)^{k_2-k_1+1})$, by:

$$\phi_{k_1:k_2;\theta|n}[h] := \mathsf{L}_{n;\theta}^{-1}(Y_{1:n}) \int \chi(\mathrm{d}x_0) \prod_{k=0}^{n-1} \mathbf{Q}_{k;\theta}(x_k, \mathrm{d}x_{k+1}) g_{k+1;\theta}(x_{k+1}, Y_{k+1}) h(x_{k_1:k_2}) \;,$$

where

$$\mathsf{L}_{n;\theta}(Y_{1:n}) = \int \chi(\mathrm{d}x_0) \prod_{k=0}^{n-1} \mathbf{Q}_{k;\theta}(x_k, \mathrm{d}x_{k+1}) g_{k+1;\theta}(x_{k+1}, Y_{k+1})$$

As noted for instance in [**?**, Section 2] and [**?**], for all $\theta \in \Theta$ and all $f_{0:n} \in \mathsf{F}((\mathbb{R}^d)^{n+1})$,

$$\nabla_\theta \phi_{0:n;\theta|n-1}[f_{0:n}] = \phi_{0:n;\theta|n-1}[h_n f_{0:n}] - \phi_{0:n;\theta|n-1}[f_{0:n}] \times \phi_{0:n;\theta|n-1}[h_n] \;,$$

where

$$h_n(x_{0:n}) = \sum_{k=0}^{n-1} \tilde{h}_{k;\theta}(x_k, x_{k+1}) \;,$$

with, for all $0 \leqslant k \leqslant n-1$,

$$\tilde{h}_{k;\theta}(x_k, x_{k+1}) = \nabla_\theta \log g_{k+1;\theta}(x_{k+1}, Y_{k+1}) + \nabla_\theta \log q_{k;\theta}(x_k, x_{k+1}) \;.$$

Considering an objective function $f_n \in \mathsf{F}(\mathbb{R}^d)$ which depends on the last state x_n only, the tangent filter η_n is defined as the following signed measure:

$$\eta_{n;\theta}[f_n] := \nabla_\theta \pi_{n;\theta}[f_n] = \phi_{0:n;\theta|n-1}[h_{n;\theta} f_n] - \pi_{n;\theta}[f_n] \times \phi_{0:n;\theta|n-1}[h_n] \ ,$$

where $\pi_n = \phi_{n:n|n-1}$ is the predictive measure. The particle based estimator of $\pi_n[f]$ is given by:

$$\pi_n^N[f] = \frac{1}{N} \sum_{\ell=1}^N f(\xi_n^\ell) \ .$$

Using the tower property, (**??**) and the backward decomposition (**??**):

$$\eta_{n;\theta}[f_n] = \pi_{n;\theta}[(\mathbf{T}_n h_n - \pi_{n;\theta}[\mathbf{T}_n h_n]) f_n] \ . \tag{13}$$

Therefore, the tangent filter (13) can be approximated on-the-fly using the statistics $(\tilde{\tau}_n^i)_{i=1}^N$ and the weighted particles $\{(\xi_n^i, \omega_n^i)\}_{i=1}^N$:

$$\eta_{n;\theta}^{N,\mathrm{FFBS}}[f_n] = \frac{1}{N} \sum_{i=1}^N \tilde{\tau}_n^i f_n(\xi_i^n) - \left(\frac{1}{N} \sum_{i=1}^N \tilde{\tau}_n^i \right) \left(\frac{1}{N} \sum_{i=1}^N f_n(\xi_i^n) \right) \ . \tag{14}$$

In cases where ℓ_k, $0 \leqslant k \leqslant n-1$, is unknown and replaced by an unbiased estimate, the associated pseudo marginal particle-based approximation of the tangent filter is given by:

$$\widehat{\eta}_{n;\theta}^N[f_n] = \frac{1}{N} \sum_{i=1}^N \widehat{\tau}_n^i f_n(\xi_i^n) - \left(\frac{1}{N} \sum_{i=1}^N \widehat{\tau}_n^i \right) \left(\frac{1}{N} \sum_{i=1}^N f_n(\xi_i^n) \right) \ . \tag{15}$$

Given a set of observations $Y_{1:n}$, maximum likelihood estimation amounts at obtaining a parameter $\hat{\theta}_n \in \Theta$ such that $\hat{\theta}_n = \arg\max_{\theta \in \Theta} \ell_{\theta;n}(Y_{1:n})$, where $\ell_{\theta;n}(Y_{1:n}) = \log \mathsf{L}_{\theta;n}(Y_{1:n})$ is the logarithm of the likelihood given in (**??**). There are many different approaches to compute an estimator of $\hat{\theta}_n$, see for instance [**?**, Chapter 10]. Following [**?**], under strong mixing assumptions, for all $\theta \in \theta$, the extended process $\{(X_n, Y_n, \pi_n, \eta_n)\}_{n \geqslant 0}$ is an ergodic Markov chain and for all $\theta \in \theta$, the normalized score $\nabla_\theta \ell_\theta(Y_{1:n})/n$ of the observations may be shown to converge where:

$$\frac{1}{n} \nabla_\theta \ell_\theta(Y_{1:n}) = \frac{1}{n} \sum_{k=1}^n \nabla_\theta \ell_\theta(Y_k \mid Y_{1:k-1}) = \frac{1}{n} \sum_{k=0}^n \frac{\pi_{k;\theta}[\nabla_\theta g_{k;\theta}] + \eta_{k;\theta}[g_{k;\theta}]}{\pi_{k;\theta}[g_{k;\theta}]} \ .$$

Assuming that the observations $Y_{1:n}$ are generated by a model driven by a true parameter $\theta_\star$ for all $\theta \in \theta$ this normalized score converges almost surely to a limiting quantity $\lambda(\theta, \theta_\star)$ such that, under identifiability constraints, $\lambda(\theta_\star, \theta_\star) = 0$. A gradient ascent algorithm cannot be designed as the limiting function $\theta \mapsto \lambda(\theta, \theta_\star)$ is not available explicitly. Solving the equation $\lambda(\theta_\star, \theta_\star) = 0$ may be cast into the framework of *stochastic approximation* to produce parameter estimates using the *Robbins-Monro algorithm*

$$\theta_{n+1} = \theta_n + \gamma_{n+1} \zeta_{n+1} \ , \quad n \geqslant 0 \ , \tag{16}$$

where ζ_{n+1} is a noisy observation of $\lambda(\theta_n, \theta_\star)$. Obtaining such an observation is not possible in practice and following [**?**] this noisy observation is approximated by

$$\zeta_{n+1} := \frac{\zeta_{n+1}^1 + \zeta_{n+1}^2}{\zeta_{n+1}^3} \ , \tag{17}$$

where

$$\zeta_{n+1}^1 := \pi_{n+1;\theta_n}\left[(\nabla_\theta g_{n+1;\theta})_{|\theta=\theta_n}\right] , \quad \zeta_{n+1}^2 := \eta_{n+1;\theta_n}[g_{n+1;\theta_n}] \quad \text{and} \quad \zeta_{n+1}^3 := \pi_{n+1;\theta_n}[g_{n+1;\theta_n}] . \tag{18}$$

In (18), the measures $\pi_{n+1;\theta_n}$ and $\eta_{n+1;\theta_n}$ depend on *all* the past parameter values. In the case of a finite state space X the algorithm was studied in [**?**], which also provides assumptions under which the sequence $\{\theta_n\}_{n\geqslant 0}$ converges towards the parameter $\theta_\star$ (see also [**?**] for refinements). In more general cases, these measures may be estimated online using the pseudo marginal smoother presented in this paper.

6.1 Application to partially observed SDE

6.1.1 Unbiased estimators of the transition densities

The algorithm described above strongly relies on assumption H1. In the context of SDEs, when $g_{k+1;\theta}$ is available explicitly, this boils down to finding an unbiased estimate $\widehat{q}_{k+1;\theta}\langle\zeta\rangle(x,y)$ of $q_{k+1;\theta}(x,y)$ and defining

$$\ell_{k;\theta}\langle\zeta\rangle(x,y) = \widehat{q}_{k+1;\theta}\langle\zeta\rangle(x,y) g_{k+1;\theta}(x_{k+1}, Y_{k+1}) .$$

6.1.2 General Poisson Estimators

In [Olsson et al., 2011], [Gloaguen et al., 2018] and [Gloaguen et al., 2019], General Poisson Estimators (GPEs) are used to obtain an unbiased estimate of the transition density. However, designing such estimators requires three strong assumptions [Beskos et al., 2006a].

1. The diffusion defined by (20) can be transformed into a unit diffusion through the Lamperti transform, with drift function $\tilde{\alpha}_\theta(x)$.
2. The drift of this unit diffusion can be expressed as the gradient of a potential function, i.e., there exists a twice differentiable function $A_\theta : \mathbb{R}^d \to \mathbb{R}$ such $\tilde{\alpha}_\theta = \nabla_x A_\theta$.
3. The function $x \mapsto (\|\tilde{\alpha}_\theta(x)\|^2 + \Delta A_\theta(x))/2$ (where Δ denotes the Laplacian) is lower bounded.

Assumption (1) is used to define a proposal distribution absolutely continuous with respect to the target which is easy to sample from. Assumption (2) is necessary to obtain a tractable Radon-Nikodym derivative between the proposal and the target distributions using the Girsanov transformation. While these assumptions can be proved under mild assumptions for scalar diffusions, much stronger conditions are required in the multidimensional case [Aït-Shalia, 2008].

6.1.3 Parametrix estimators

More recently, [Andersson and Kohatsu-Higa, 2017] and [Fearnhead et al., 2017] proposed an algorithm which can be used under weaker assumptions. This parametrix algorithm draws weighted skeletons using an importance sampling mechanism for diffusion processes. In this case, the sampled paths are not distributed as the target process but the weighted samples produce unbiased estimates of expectations of functionals of this process. To obtain an unbiased estimator $\widehat{q}_{k+1}\langle\zeta\rangle(x,y)$, the parametrix algorithm draws weighted skeletons at random times $s_0 = 0 < s_1 < \cdots < s_j$, denoted by $\left\{(x_{s_j}, \mathsf{w}_{s_j})\right\}_{j\geqslant 0}$, where $x_0 = x$ and $\mathsf{w}_0 = 1$. The update times $(s_j)_{j\geqslant 0}$ are instances of an inhomogeneous Poisson process of intensity

$\lambda(t)$. Let $(x_{s_j}, \mathsf{w}_{s_j})$ be the last weighted sample and s_{j+1} be the next update time of the trajectory. While $s_{j+1} < \Delta t_k$, the new state is sampled using a simple Euler scheme, namely:

$$x_{s_{j+1}} := x_{s_j} + \Delta s_j \alpha_\theta(x_{s_j}) + (\Delta s_j)^{1/2} \sigma_\theta(x_{s_j}) \varepsilon_{j+1} \ ,$$

where $\Delta s_j := s_{j+1} - s_j$, $\Delta t_k = t_{k+1} - t_k$ and $\varepsilon_{j+1} \sim \mathcal{N}_d(0, I_d)$. The proposal density associated with this procedure is denoted by $m_{j;\theta}\left(x_{s_j}, \cdot, \Delta\tau_j\right)$. Let $\mathcal{K}^\theta$ (resp. $\mathcal{K}^{j,\theta}_{\mathrm{prop}}$) denote the Kolmogorov forward operator of the diffusion (resp. the Kolmogorov forward operator of the proposal distribution $m_{j;\theta}\left(x_{s_j}, \cdot, \Delta s_j\right)$). The forward operators write, for any function $h : \mathbb{R}^d \to \mathbb{R}$,

$$\mathcal{K}^\theta h\left(y\right) := -\sum_{i=1}^{d} \frac{\partial}{\partial y_i} \left\{\alpha_{\theta,i}(y) h\left(y\right)\right\} + \sum_{i,\ell=1}^{d} \frac{1}{2} \frac{\partial^2}{\partial y_i \partial y_\ell} \left\{\gamma_{\theta,i,\ell}(y) h\left(y\right)\right\} \ ,$$

where $\gamma_\theta = \sigma_\theta \sigma_\theta^T$. Then, following [Fearnhead et al., 2017], the weight is updated by

$$\mathsf{w}_{s_{j+1}} := \mathsf{w}_{s_j} \rho_j^\lambda \left(x_{s_j}, x_{s_{j+1}}, \Delta s_j\right) \ ,$$

where

$$\rho_j^\lambda\left(x, y, u\right) := 1 + \frac{\left(\mathcal{K} - \mathcal{K}^{j,\theta}_{\mathrm{prop}}\right) m_{j;\theta}\left(x, z, u\right)_{|z=y}}{\lambda(u) m_{j;\theta}\left(x, y, u\right)} \ . \tag{19}$$

It is worth noting that (19) can be computed using only first derivatives of α_θ and second derivatives of σ_θ. If N_k is the number of Poisson events between 0 and Δt_k, the parametrix unbiased estimate is then given by

$$\widehat{q}_{k+1}\langle\zeta_k\rangle(x, y) = \mathsf{w}_{s_{N_k}} m_{k;\theta}\left(x_{s_{N_k}}, y, t_{k+1} - s_{N_k}\right) \ ,$$

where ζ_k stands for all the randomness required to produce the parametrix estimator (Poisson process and Gaussian random variables).

The stability of this estimator is studied in [Fearnhead et al., 2017] which provides L_p controls for the weight $\mathsf{w}_{s_{N_k}}$. The parametrix algorithm mentioned above is a highly flexible procedure to obtain such an unbiased estimate for a much broader class of diffusions than Poisson based estimations which require strong assumptions. However, as the update (19) involves the difference of two Kolmogorov operators, the parametrix estimator of the transition density may be negative, and has no reason to satisfy (7). Thus, the SMC algorithms described above cannot be implemented. Let $(X_t)_{t\geq 0}$ be defined as a weak solution to the following Stochastic Differential Equation (SDE) in $\mathbb{R}^d$:

$$X_0 = x_0 \quad \text{and} \quad \mathrm{d}X_t = \alpha_\theta(X_t)\mathrm{d}t + \mathrm{d}W_t \ , \tag{20}$$

where $(W_t)_{t\geqslant 0}$ is a standard Brownian motion, $\alpha_\theta : \mathbb{R}^d \to \mathbb{R}^d$ is the drift function . The inference procedure presented in this paper is applied in the case where the solution to (20) is supposed to be partially observed at times $t_0 = 0, \ldots, t_n$, for a given $n \geqslant 1$, through an observation process $(Y_k)_{0\leqslant k\leqslant n}$ taking values in $\mathbb{R}^m$. For all $0 \leqslant k \leqslant n$, the distribution of Y_k given $(X_t)_{t\geqslant 0}$ depends on $X_k = X_{t_k}$ only and has density $g_{k;\theta}$ with respect to ν. The distribution of X_0 has density χ with respect to μ and for all $0 \leqslant k \leqslant n-1$, the conditional distribution of X_{k+1} given $(X_t)_{0\leqslant t\leqslant k}$ has density $q_{k+1;\theta}(X_k, \cdot)$ with respect to μ. This unknown density can be expressed as an expectation of a Brownian Bridge functional [**?**].

Let $\omega = (\omega_s)_{0\leq s\leq t}$ be the realization of a Brownian Bridge starting at x at time 0 and ending in y at time Δ. The distribution of ω is denoted by $\mathbb{W}_x^{\Delta,y}$. Moreover, suppose that for all $\theta \in \Theta$, α_θ is of a

gradient form $\alpha_\theta = \nabla_x A_\theta$ where $A_\theta : \mathbb{R}^d \to \mathbb{R}$ is a twice continuously differentiable function. Denoting, $\psi_\theta : \; x \mapsto \psi_\theta(x) = (\|\alpha_\theta(x)\|^2 + \Delta A_\theta(x))/2$, by Girsanov theorem, for all $x, y \in \mathbb{R}^d \times \mathbb{R}^d$

$$q_{k+1;\theta}(x,y) = \phi_{\Delta_k}(x-y)\exp\left(A_\theta(y) - A_\theta(x)\right)\mathbb{E}_{\mathbb{W}_x^{\Delta_k,y}}\left[\exp\left(-\int_0^{\Delta_k}\psi_\theta(\omega_s)\mathrm{d}s\right)\right] , \qquad (21)$$

where $\Delta_k = t_{k+1} - t_k$, for all $a > 0$, ϕ_a is the probability density function of a centered Gaussian random variable with variance a.

The transition density then cannot be computed as it involves an integration over the whole path between x and y. To perform the algorithm proposed in this paper, we therefore have to design a positive an unbiased estimator of $q_{k+1;\theta}(x,y)$. Moreover, maximum likelihood estimation of θ requires an unbiased estimator of $\nabla_\theta \log q_{k+1;\theta}(x,y)$. Such two estimators can be obtained using the General Poisson Estimator (GPE, [**?**]).

Unbiased GPE estimator for $q_{k+1;\theta}(x,y;\zeta)$. Assume that there exist random variables $\underline{m}_\theta$ and $\overline{m}_\theta$ such that for all $0 \leqslant s \leqslant \Delta_k$, $\underline{m}_\theta \leqslant \psi_\theta(\omega_s) \leqslant \overline{m}_\theta$. Let κ be a random variable taking values in $\mathbb{N}$ with distribution μ, $\omega = (\omega_s)_{0\leq s\leq\Delta_k}$ be the realization of a Brownian Bridge, and $(U_j)_{1\leqslant j\leqslant\kappa}$ be independent uniform random variables on $(0,\Delta_k)$ and $\zeta = (\kappa, \omega, U_1, \ldots, U_\kappa)$. As shown in [**?**], equation (21) leads to a positive unbiased estimator given by

$$\widehat{q}_{k+1;\theta}(x,y;\zeta) = \phi_{\Delta_k}(x-y)\exp\left(A_\theta(y) - A_\theta(x) - \underline{m}_\theta\Delta_k\right)\prod_{j=1}^{\kappa}\frac{\overline{m}_\theta - \psi_\theta(\omega_{U_j})}{\overline{m}_\theta - \underline{m}_\theta} .$$

Unbiased GPE estimator of $\nabla_\theta \log q_{k+1;\theta}(x,y)$. Let's denote $\varphi_\theta : \; x \mapsto \psi_\theta(x) - \underline{m}_\theta$. By (21),

$$\nabla_\theta \log q_{k+1;\theta}(x,y) = \nabla_\theta A_\theta(y) - \nabla_\theta A_\theta(x) - \nabla_\theta\underline{m}_\theta\Delta_k - \frac{\mathbb{E}_{\mathbb{W}_x^{\Delta_k,y}}\left[\left(\int_0^{\Delta_k}\nabla_\theta\varphi_\theta(\omega_s)\mathrm{d}s\right)\exp\left(-\int_0^{\Delta_k}\varphi_\theta(\omega_s)\mathrm{d}s\right)\right]}{\mathbb{E}_{\mathbb{W}_x^{\Delta_k,y}}\left[\exp\left(-\int_0^{\Delta_k}\varphi_\theta(\omega_s)\mathrm{d}s\right)\right]} .$$

On the other hand, the diffusion bridge $\mathbb{S}_{\theta,x}^{\Delta_k,y}$ associated with the SDE (20) is absolutely continuous with respect to $\mathbb{W}_x^{\Delta_k,y}$ with Radon-Nikodym derivative given by

$$\begin{aligned}\frac{\mathrm{d}\mathbb{S}_{\theta,x}^{\Delta_k,y}}{\mathrm{d}\mathbb{W}_x^{\Delta_k,y}}(\omega) &= \left[q_{k+1;\theta}(x,y)\right]^{-1}\phi_{\Delta_k}(x-y)\exp\left(A_\theta(y) - A_\theta(x) - \underline{m}_\theta\Delta_k - \int_0^{\Delta_k}\varphi_\theta(\omega_s)\mathrm{d}s\right) ,\\ &= \mathbb{E}_{\mathbb{W}_x^{\Delta_k,y}}\left[\exp\left(-\int_0^{\Delta_k}\varphi_\theta(\omega_s)\mathrm{d}s\right)\right]^{-1}\exp\left(-\int_0^{\Delta_k}\varphi_\theta(\omega_s)\mathrm{d}s\right) .\end{aligned}$$

This yields

$$\nabla_\theta \log q_{k+1;\theta}(x,y) = \left(\nabla_\theta A_\theta(y) - \nabla_\theta A_\theta(x) - \nabla_\theta\underline{m}_\theta\Delta_k\right) - \mathbb{E}_{\mathbb{S}_{\theta,x}^{\Delta_k,y}}\left[\int_0^{\Delta_k}\nabla_\theta\varphi_\theta(\omega_s)\mathrm{d}s\right]$$

and an unbiased estimator of $\nabla_\theta \log q_{k+1;\theta}(x,y)$ is given by

$$\mathsf{I}_{k+1;\theta}(x,y,\mathsf{s}_U^{\theta,x,y,\Delta_k}) = \left(\nabla_\theta A_\theta(y) - \nabla_\theta A_\theta(x) - \nabla_\theta\underline{m}_\theta\Delta_k\right) - \Delta_k\nabla_\theta\varphi_\theta(\mathsf{s}_U^{\theta,x,y,\Delta_k}) ,$$

where U is uniform on $(0,1)$ and independent of $\mathsf{s}^{\theta,x,y,\Delta_k} \sim \mathbb{S}_{\theta,x}^{\Delta_k,y}$. In the context of GPE, $\mathsf{s}^{\theta,x,y,\Delta_k}$ can be simulated exactly using exact algorithms for diffusion processes proposed in [Beskos et al., 2006a].

Experiments. Online recursive maximum likelihood using pseudo marginal SMC is illustrated when (20) has the specific form:

$$X_0 = x_0 \quad \text{and} \quad \mathrm{d}X_t = \sin(X_t - \theta)\mathrm{d}t + \mathrm{d}W_t \ , \tag{22}$$

where θ is an unknown parameter ranging between 0 and 2π. For this numerical experiments, we suppose that a realization of (22) is only observed at times $t_k = k$ for $0 \leqslant k \leqslant n$ with $n = 5000$ through a noisy observation process $(Y_k)_{0 \leqslant k \leqslant n}$ such for all $0 \leqslant k \leqslant n$,

$$Y_k = X_{t_k} + \varepsilon_k \ ,$$

where $(\varepsilon_k)_{0 \leqslant k \leqslant n}$ are i.i.d. standard Gaussian random variables, independent of $(W_t)_{t \geqslant 0}$. In this case $\alpha_\theta : x \mapsto \sin(x - \theta)$ and

$$\inf_{x \in \mathbb{R}} (\alpha_\theta^2(x) + \Delta A_\theta(x))/2 \geqslant -1/2$$

and for all $x \in \mathbb{R}$,

$$0 \leqslant \varphi_\theta(x) = (\alpha_\theta^2(x) + \Delta A_\theta(x))/2 + 1/2 \leqslant 9/8$$

and a GPE estimator of both the transition density and the gradient of its logarithm associated with the SINE model is straightforward to compute.

A simulated data set is displayed in Figure 4, where $\theta_* = \pi/4$. The solution to (22) is sampled at times $(t_k)_{0 \leqslant k \leqslant n}$ using the Exact algorithm of [Beskos et al., 2006a]. For all $0 \leqslant k \leqslant n-1$, $\widehat{q}_{k,\theta}$ and the GPE unbiased estimator of $\nabla_\theta q_{k,\theta}(x, y)$ are estimated using $M = 30$ independent Monte Carlo replications of the general Poisson estimator. The estimations of θ_* are given for 50 independent runs started at random locations θ_0 with $N = 100$ particles and $\widetilde{N} = 2$ backward samples. Following [**?**], the proposal distribution of the particle filter is obtained using an approximation of the fully adapted particle filter where $q_{k,\theta}$ is replaced by the its Euler scheme approximation.

Sensitivity to the starting point $\hat{\theta}_0$. The inference procedure was performed on the same data set from 50 different starting points uniformly chosen in $(0, 2\pi)$. The gradient step size γ_k of equation (16) was chosen constant (and equal to 0.5) for the first 300 time steps, and then decreasing with a rate proportional to $k^{-0.6}$. Results are given Figure 5. There is no sensitivity to the starting point of the algorithm, and after a couple of hundred observations, the estimates all concentrate around the true value. As the gradient step size decreases, the estimates stay around the true value following autocorrelated patterns that are common to all trajectories.

Asymptotic normality. The inference procedure was performed on 50 different data sets simulated with the same θ_*. The 50 estimates were obtained starting from the same starting point (fixed to θ_*, as Figure 5 shows no sensitivity to the starting point). Figure 6 shows the results for the raw and the averaged estimates. The averaged estimates $(\widetilde{\theta}_k)_{k \geqslant 0}$ consist in averaging the values produced by the estimation procedure after a burning phase of n_0 time steps (here $n_0 = 300$ time steps). This procedure allows to obtain an estimator whose convergence rate does not depend on the step sizes chosen by the user, see [**?**, **?**]. For all $0 \leqslant k \leqslant n_0$, $\widetilde{\theta}_k = \widehat{\theta}_k$ and for all $k > n_0$,

$$\widetilde{\theta}_k = \frac{1}{k - n_0} \sum_{j=n_0+1}^{k} \widehat{\theta}_j \ .$$

As expected, the estimated distribution of the final estimates tends to be Gaussian, centered around the true value.

Step size influence. To illustrate the influence of the gradient step sizes, different settings are considered. In each scenario, the sequence $(\gamma_k)_{k \geqslant 0}$ is given by

$$\gamma_k = \gamma_0 \mathbb{1}_{\{k \leq n_0\}} + \frac{\gamma_0}{(k - n_0)^\kappa} \mathbb{1}_{\{k > n_0\}} \ ,$$

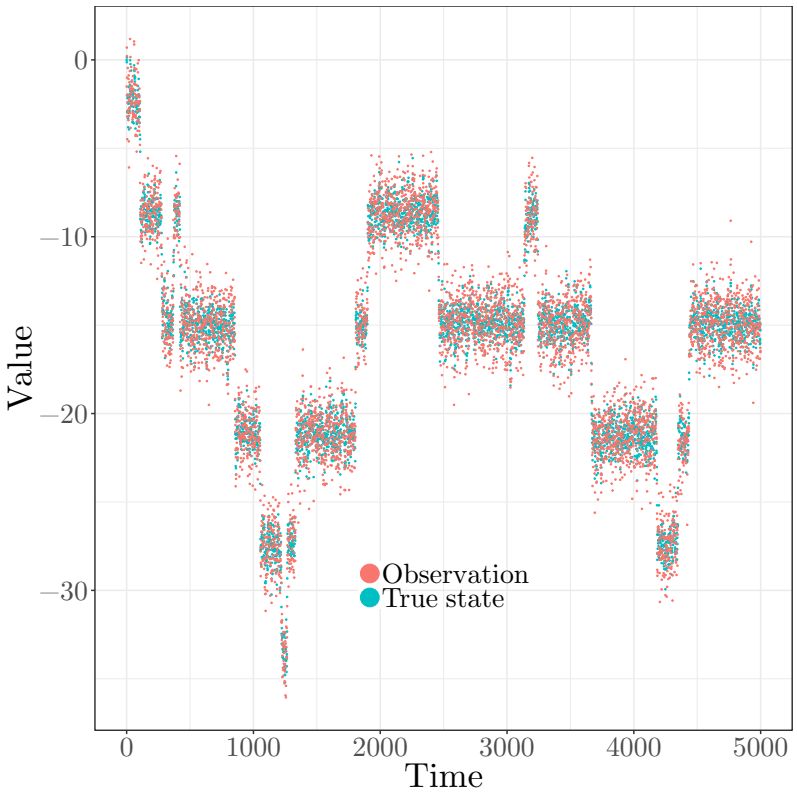

Figure 4: Data set simulated according to the SINE process, observed with noise at discrete time steps.

where $\gamma_0 = 0.5$. In this experiment $\kappa \in \{0.5, 0.6, 0.7, 0.8, 0.9, 1\}$. The results are shown in Figure 7. As expected, the raw estimator shows different rates of convergence depending on κ, whereas the averaged estimator has the same behavior in all cases.

7 Discussion

This paper proposes a solution to overcome the two main challenges when it comes to perform online smoothing for generic SDEs i.e. obtaining a positive and almost surely bounded estimate of the transition density to run the backward acceptance rejection mechanism.

Note that the proposed backward importance sampling may be used to approximate expectations under the smoothing distributions for general state space hidden Markov models and is not restricted to POD processes. As illustrated in Section **??** this approach may lead to significant gains in computational time for similar performance as the acceptance rejection approach.

The proposed estimator, unlike the existing methods such as GPE-based algorithms, applies to a large range of multivariate diffusion processes (see [Andersson and Kohatsu-Higa, 2017] and [Fearnhead et al., 2017]).

Theoretical guarantees, such as consistency and asymptotic normality of (5), remain to be proved. This should be an extension of [Gloaguen et al., 2019], however this would imply few technicalities which are

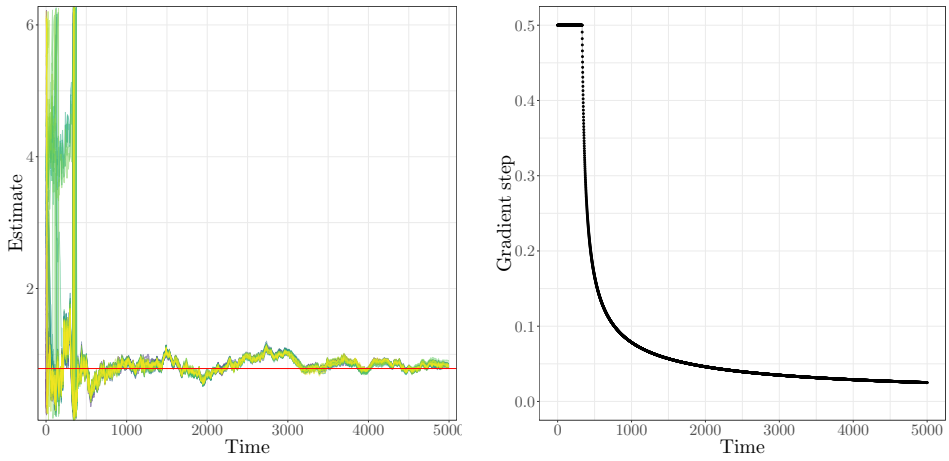

Figure 5: (*Left*) online estimation of θ for the data set presented in Figure 4. The algorithm is performed from 50 starting points. (*Right*) The gradient step sizes (defined in equation (16)).

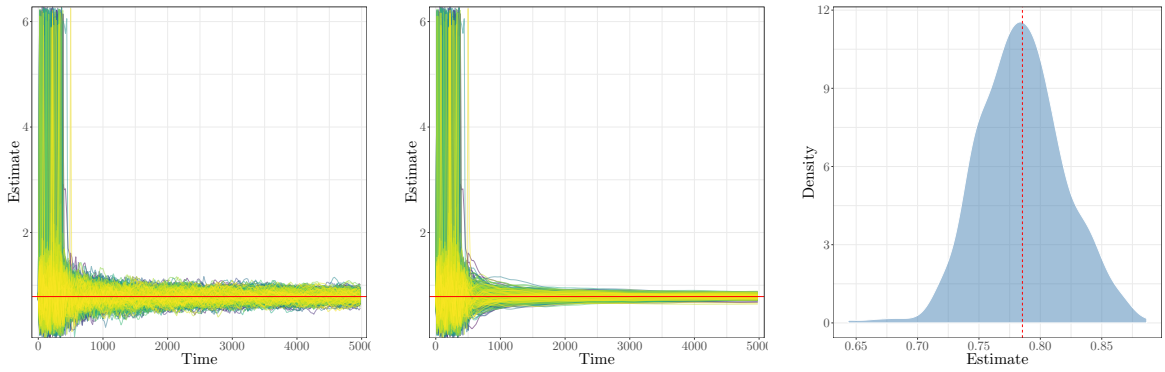

Figure 6: (*Left*) online estimation of θ for 50 different simulated data sets as presented in Figure 4. The algorithm is performed from 1 starting point with the gradient step size shown in Figure 5. (*Center*) Averaged estimator, where $\hat{\theta}$ is averaged after a burning phase of 300 time steps. (*Right*) Empirical distribution of $\hat{\theta}$. The red line is the value of θ^*.

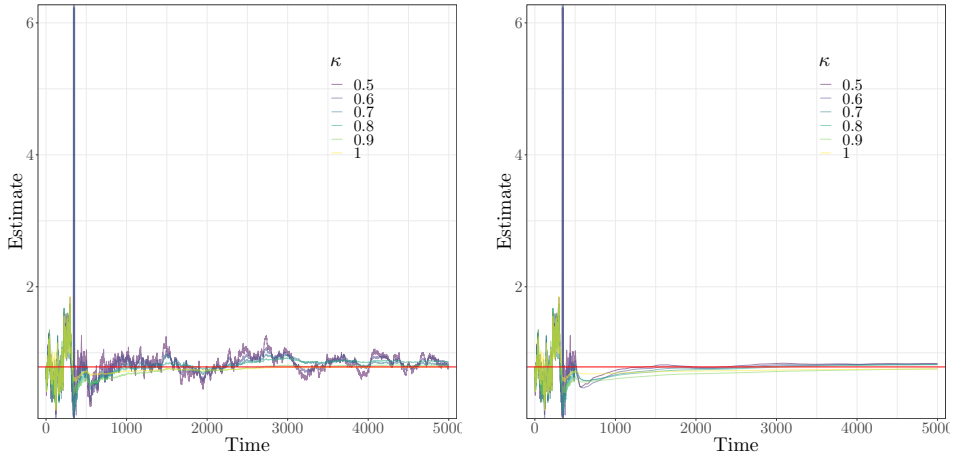

Figure 7: (*Left*) online estimation of θ for the data set presented in Figure 4, with different decreasing rates values κ. (*Right*) Averaged estimator, where $\hat{\theta}$ is averaged after a burning phase of 300 time steps.

out of the scope of this paper.

The bias of the PaRIS algorithm may be shown to be or order $\mathcal{O}((1+1/\widetilde{N})/N)$ and vanishes as N goes to infitnity for any choice of $\widetilde{N} \geqslant 2$. The exact sampling being replaced by an importance sampling step, the conjecture is that the bias of the proposed algorithm involves a $\mathcal{O}(1/\widetilde{N})$ term which does not vanish as N goes to infinity. However, the empirical study illustrates that $\widetilde{N}$ may be chosen to increase with N sufficiently slowly to remove the additional bias term while simultaneously ensuring better computational performance.

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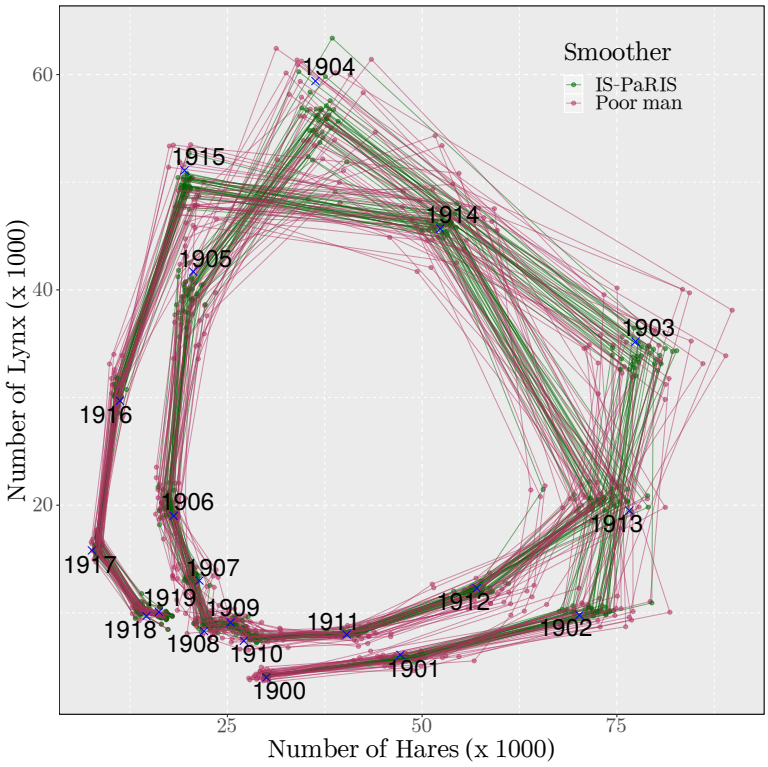

Figure 8: Estimated Hares-Lynx abundances using the Hudson bay company data set. Both our IS-PaRIS smoother and the poor man smoother are performed to approximate the MLE and solve the tracking problem. Blue crosses show the observations.

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