On embedded hidden Markov models and particle Markov chain Monte Carlo methods

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Abstract

The embedded hidden Markov models (EHMM) sampling method is a Markov chain Monte Carlo (MCMC) technique for state inference in non-linear non-Gaussian state-space models which was proposed in Neal (2003); Neal et al. (2004) and extended in Shestopaloff and Neal (2016). An extension to Bayesian parameter inference was presented in Shestopaloff and Neal (2013). An alternative class of MCMC schemes addressing similar inference problems is provided by particle Markov chain Monte Carlo (PMCMC) methods (Andrieu et al., 2009, 2010). All these methods rely on the introduction of artificial extended target distributions for multiple state sequences which, by construction, are such that one randomly indexed sequence is distributed according to the posterior of interest. By adapting the Metropolis–Hastings algorithms developed in the framework of PMCMC methods to the EHMM framework, we obtain novel particle filter (PF)-type algorithms for state inference and novel MCMC schemes for parameter and state inference. In addition, we show that most of these algorithms can be viewed as particular cases of a general PF and PMCMC framework. We compare the empirical performance of the various algorithms on low- to high-dimensional state-space models. We demonstrate that a properly tuned conditional PF with ‘local’ MCMC moves proposed in Shestopaloff and Neal (2016) can outperform the standard conditional PF significantly when applied to high-dimensional state-space models while the novel PF-type algorithm could prove to be an interesting alternative to standard PFs for likelihood estimation in some lower-dimensional scenarios.

1 Introduction

Throughout this work, for concreteness, we will describe both particle Markov chain Monte Carlo (PMCMC) and embedded hidden Markov models (EHMM) methods in the context of performing inference in non-linear state-space models. However, we stress that those methods can be used to perform inference in other contexts.

Non-linear non-Gaussian state-space models constitute a popular class of time series models which can be described in the time-homogeneous case as follows — throughout this paper we consider the time-homogeneous case, noting that the generalisation to time-inhomogeneous models is straightforward but notationally cumbersome. Let \( \{x_t\}_{t \geq 1} \) be an \( X \)-valued latent Markov process satisfying

\[
x_1 \sim \mu_\theta(\cdot) \quad \text{and} \quad x_t | (x_{t-1} = x) \sim f_\theta(\cdot | x), \quad \text{for } t \geq 2.
\]

(1)

and let \( \{y_t\}_{t \geq 1} \) be a sequence of \( Y \)-valued observations which are conditionally independent given \( \{x_t\}_{t \geq 1} \) and which satisfy

\[
y_t | (x_1, \ldots, x_t = x, x_{t+1}, \ldots) \sim g_\theta(\cdot | x), \quad \text{for } t \geq 1.
\]

(2)

Here \( \theta \in \Theta \) denotes the vector of parameters of the model.

Let \( z_{i,j} \) denotes the components \( (z_i, z_{i+1}, \ldots, z_j) \) of a generic sequence \( \{z_i\}_{i \geq 1} \). Assume that we have access to a realization of the observations \( Y_{1:T} = y_{1:T} \). If \( \theta \) is known, inference about the latent states \( x_{1:T} \) relies upon

\[
p_\theta(x_{1:T} | y_{1:T}) = \frac{p_\theta(x_{1:T}, y_{1:T})}{p_\theta(y_{1:T})},
\]

where

\[
p_\theta(x_{1:T}, y_{1:T}) = \mu_\theta(x_1) \prod_{t=2}^{T} f_\theta(x_t | x_{t-1}) \prod_{t=1}^{T} g_\theta(y_t | x_t).
\]
When θ is unknown, to conduct Bayesian inference a prior density \( p(θ) \) is assigned to the parameters and inference proceeds via the joint posterior density

\[
p(x_{1:T},θ|y_{1:T}) = p(θ|y_{1:T})p_0(x_{1:T}|y_{1:T}),
\]

where the marginal posterior distribution of the parameter satisfies

\[
p(θ|y_{1:T}) \propto p(θ)p_0(y_{1:T}),
\]

the likelihood \( p_0(y_{1:T}) \) being given by

\[
p_0(y_{1:T}) = \int p_0(x_{1:T},y_{1:T})dx_{1:T}.
\]

Many algorithms have been proposed over the past twenty-five years to perform inference for this class of models; see Kantas et al. (2015) for a recent survey. We focus here on the EHMM algorithm introduced in Neal (2003); Neal et al. (2004) and on PMCMC introduced in Andrieu et al. (2009, 2010). Both classes of methods are fairly generic and do not require the state-space model under consideration to possess additional structural properties beyond (1) and (2). The EHMM method has been recently extended in Shestopaloff and Neal (2013, 2016) while extensions of PMCMC have also been proposed in, among other works, Whiteley (2010) and Lindsten et al. (2014). In particular, Whiteley (2010) combined the conditional particle filter (PF) algorithm of Andrieu et al. (2009, 2010) with a backward sampling step. We will denote the resulting algorithm as the conditional PF with backward sampling (BS).

Both EHMM and PMCMC methods rely upon sampling a population of \( N \) particles for the state \( x_{1:T} \) and introducing an extended target distribution over the resulting \( NT \) potential sequences \( x_{1:T} \) such that one of the sequences selected uniformly at random is at equilibrium by construction. It was observed in Lindsten and Schön (2013, p. 116) that conditional PF with BS is reminiscent of the EHMM method proposed in Neal (2003); Neal et al. (2004) and some connections were made between some simple EHMM methods and PMCMC methods in Linker (2013, pp. 82–87) who also showed that both methods can be viewed as special cases of a much more general construction. However, to the best of our knowledge, the connections between the two classes of methods have never been investigated thoroughly. Indeed, such an analysis was deemed of interest in Shestopaloff and Neal (2014), where we note that EHMM methods are sometimes alternatively referred to as ensemble MCMC methods:

“It would be interesting to compare the performance of the ensemble MCMC method with the PMCMC-based methods of Andrieu et al. (2010) and also to see whether techniques used to improve particle MCMC methods can be used to improve ensemble methods and vice versa.”

In this work, we characterize this relationship and show that it is possible to exploit the similarities between these methods to derive new inference algorithms. The relationship between the various classes of algorithms discussed in this work is shown in Figure 1. The remainder of the paper is organized as follows.

Section 2 reviews some PMCMC schemes, including the particle marginal Metropolis–Hastings (PMMH) algorithm and particle Gibbs (PG) samplers. We recall how the validity of these algorithms can be established by showing that they are standard MCMC algorithms sampling from an extended target distribution. In particular, the PMMH algorithm can be thought of as a standard Metropolis–Hastings (MH) algorithm sampling from this extended target using a PF proposal for the states. Likewise, the theoretical validity of the conditional PF with BS can be established by showing that it corresponds to a “partially collapsed” – see Van Dyk and Park (2008) – Gibbs sampler (Whiteley 2010).

Section 3 is devoted to the ‘original’ EHMM from Neal (2003); Neal et al. (2004). At the core of this methodology is an extended target distribution which shares common features with the PMCMC target. We show that the EHMM method can be reinterpreted as a collapsed Gibbs sampling procedure for this target. This provides an alternative proof of validity of this algorithm. More interestingly, it is possible to come up with an original MH scheme to sample from this extended target distribution reminiscent of PMMH. However, whereas the PMMH algorithm relies on PF estimates of the likelihood \( p_0(y_{1:T}) \), this MH version of EHMM relies on an estimate of \( p_0(y_{1:T}) \) computed using a finite-state hidden Markov model (HMM), the cardinality of the state-space being \( N \). The computational cost of both of these original EHMM methods is \( O(N^2T) \) in contrast to the \( O(NT) \)-cost of PMCMC methods.

The high computational cost of the original EHMM method has partially motivated the development of a novel class of alternative EHMM methods which bring the computational complexity down to \( O(NT) \). As described in Section 4, this is done by introducing a set of auxiliary variables playing the same role as the ancestor indices generated in the resampling step of a standard PF. This leads to the extended target distribution introduced in Shestopaloff and Neal (2016). We show that this target coincides in a special case with the extended target of PMCMC when one uses the fully-adapted auxiliary particle filter (FA-APF) Pitt and Shephard (1999) and the resulting EHMM coincides with the conditional FA-APF with BS in this scenario.
We show once more that the validity of this novel EHMM method can be established by using a collapsed Gibbs sampler.

In Section 5, we derive several novel, practical extensions to the alternative EHMM method. First, we show that the alternative EHMM framework can also be used to derive an MH algorithm which, once again, mimics idealised Gibbs version of original EHMM. We show once more that the validity of this novel EHMM method can be established by using a collapsed Gibbs sampler before finally considering the case of general auxiliary particle filters.

2 PMCMC methods

This section reviews PMCMC methods. For transparency, we first restrict ourselves in this section to the scenario in which the underlying PF used is the bootstrap PF, and then discuss the fully-adapted auxiliary particle filter before finally considering the case of general auxiliary particle filters.

2.1 Extended target distribution

Let $N$ be an integer such that $N \geq 2$, PMCMC methods rely on the following extended target density on $\Theta \times \mathcal{X}^{NT} \times \{1, \ldots, N\}^{N(T-1)+1}$

$$\tilde{p}(\theta, b_{1:T}, x_{1:T}, a_{1:T-1}) := \frac{1}{N^T} \times \pi(\theta, x_{1:T}) \times \phi_{\theta}(x_{1:T}, a_{1:T-1} \mid a_{1:T-1}, b_{1:T}),$$

(3)

where $\pi(\theta, x_{1:T}) := p(x_{1:T}, \theta \mid y_{1:T})$ represents the posterior distribution of interest. In addition, the particles $x_t := \{x_{1:T}\} \in \mathcal{X}^N$, ancestor indices $a_t := \{a_{1:T}\} \in \{1, \ldots, N\}^N$ and particle indices $b_{1:T} := \{b_1, \ldots, b_T\}$ are related as

$$x_t^{b_t} = x_t \setminus x_t^{b_t}, \quad x_{1:T}^{b_T} = \{x_{1:b_1}, \ldots, x_{T:b_T}\}, \quad a_{t-1}^{b_t} = a_{t-1} \setminus a_{t-1}^{b_t}, \quad a_{1:T-1}^{b_T} = \{a_1^{b_2}, \ldots, a_{T-1}^{b_T}\}.$$
In particular, given \( b_T \), the particle indices \( b_{1:T−1} \) are deterministically related to the ancestor indices by the recursive relationship

\[
b_t = a_{t+1}^b, \quad \text{for } t = T − 1, \ldots, 1.
\]

Finally, for any \( (x_{1:T}^b, b_{1:T}) \in \mathcal{X}^N \times \{1, \ldots, N\}^N \), \( \phi_\theta \) denotes a conditional distribution induced by an algorithm referred to as a conditional particle filter (CPF)

\[
\phi_\theta(x_{1:T}^i, \mathbf{a}_{1:T}^i | x_{1:T}^b, b_{1:T}) := \prod_{t=1}^{N} \mu_\theta(x_t^i) \prod_{t=2}^{N} w_{\theta,t-1}^{-1} f_\theta(x_t^i | x_{t-1}^i),
\]

where

\[
w_{\theta,t}^i := \frac{g_\theta(y_t^i | x_t^i)}{\sum_{j=1}^{N} g_\theta(y_t^j | x_t^j)}
\]

represents the normalised weight associated with the \( i \)th particle at time \( t \).

The key feature of this high-dimensional target is that by construction it ensures that \((\theta, x_{1:T}^b)\) is distributed according to the posterior of interest. PMCMC methods are MCMC algorithms which sample from this extended target, hence from the posterior of interest.

### 2.2 Particle marginal Metropolis–Hastings

The particle marginal Metropolis–Hastings (PMMH) algorithm is a Metropolis–Hastings (MH) algorithm targeting \( \pi(\theta, b_{1:T}, \mathbf{x}_{1:T}, \mathbf{a}_{1:T−1}) \) defined through \((3), (4)\) and \((5)\) using a proposal of the form

\[
q(\theta', \theta) \times \Psi_\theta(x_{1:T}, \mathbf{a}_{1:T−1}) \times \text{path selection}
\]

where \( b_{1:T} \) is again obtained via the reparametrisation \( b_t = a_{t+1}^b \) for \( t = T − 1, \ldots, 1 \) and \( \Psi_\theta(x_{1:T}, \mathbf{a}_{1:T−1}) \) is the law induced by a bootstrap

\[
\Psi_\theta(x_{1:T}, \mathbf{a}_{1:T−1}) := \prod_{i=1}^{N} \mu_\theta(x_t^i) \prod_{t=2}^{N} w_{\theta,t-1}^{-1} f_\theta(x_t^i | x_{t-1}^i).
\]

The resulting MH acceptance probability is of the form

\[
\begin{align*}
1 \wedge \frac{\hat{p}_\theta(y_{1:T}) p(\theta') q(\theta', \theta)}{\hat{p}_\theta(y_{1:T}) p(\theta) q(\theta, \theta')}.
\end{align*}
\]

where

\[
\hat{p}_\theta(y_{1:T}) := \frac{1}{N} \sum_{i=1}^{N} g_\theta(y_t^i | x_t^i)
\]

is well known to be an unbiased estimate of \( p_\theta(y_{1:T}) \); see Del Moral [2004]. We stress that the unbiased estimates appearing in the numerator and denominator of \((6)\) each depends upon the particles (and ancestor indices) generated in distinct \([PF]s\) but we suppress this dependence to keep the notation as simple as is possible.

The validity of the expression in \((6)\) follows directly by noting that:

\[
\tilde{\pi}(\theta, b_{1:T}, \mathbf{x}_{1:T}, \mathbf{a}_{1:T−1}) = \frac{1}{\Psi_\theta(x_{1:T}, \mathbf{a}_{1:T−1})} \pi(\theta, x_{1:T}^b) \times \text{path selection}
\]

\[
= \frac{p(\theta | y_{1:T}) \hat{p}_\theta(y_{1:T}) p(\theta)}{\hat{p}_\theta(y_{1:T}) p(\theta) p(\theta | y_{1:T})} \approx \hat{p}_\theta(y_{1:T}) p(\theta),
\]

where we have again used that \( b_t = a_{t+1}^b \), for \( t = T − 1, \ldots, 1 \) and that \( p(\theta | y_{1:T}) / \hat{p}_\theta(y_{1:T}) = p(\theta) / p(y_{1:T}) \); see also [Andrieu et al. 2010, Theorem 2].
2.3 Particle Gibbs samplers

To sample from \( \pi(\theta, x_{1:T}) \), one can use the particle Gibbs (PG) sampler. The PG sampler mimics the block Gibbs sampler iterating draws from \( \pi(\theta|x_{1:T}) \) and \( \pi(x_{1:T}|\theta) \). As sampling from \( \pi(x_{1:T}|\theta) \) is typically impossible, we can use a so-called conditional PF kernel with backward sampling (BS) to emulate sampling from it. Given a current value of \( x_{1:T} \), we perform the following steps (see [Andrieu et al. (2009), Andrieu et al. (2010) Section 4.5]):

1. Sample \( b_{1:T} \) uniformly at random and set \( x_{1:T}^{'b_{1:T}} \leftarrow x_{1:T} \).
2. Run the conditional [PF] i.e. sample from \( \phi_\theta(x_{1:T}^{'b_{1:T}}, a_{1:T-1}^{'b_{1:T}}|x_{1:T}^{'b_{1:T}}, b_{1:T}) \).
3. Sample \( b_T \) according to \( \Pr(b_T = m) = w_{m,t}^b \) and set \( b_t = a_{t+1}^{b_{t+1}} \) for \( t = T - 1, \ldots, 1 \).

It was noticed in [Whiteley (2010)] that it is possible to improve Step 3 for \( t = T - 1, \ldots, 1 \), instead of deterministically setting \( b_t = a_{t+1}^{b_{t+1}} \), one can use a backward sampling step which samples

\[
\Pr(b_t = m) \propto w_{m,t}^b f_\theta(x_{t+1}^{'b_{t+1}}|x_t^{'m})
\]

To establish the validity of this procedure (i.e. of the conditional [PF] with [BS]), it was shown that this procedure is a (partially) collapsed Gibbs sampler of invariant distribution \( \tilde{\pi}(b_{1:T}, x_{1:T}, a_{1:T-1}|\theta) \), sampling recursively from \( \tilde{\pi}(b_t|\theta, x_{1:T}, a_{1:T-1}, x_{t+1:T}^{'b_{t+1}:t}, b_{1:T}) \), for \( t = T, T - 1, \ldots, 1 \). Indeed, we have

\[
\tilde{\pi}(b_t|\theta, x_{1:T}, a_{1:T-1}, x_{t+1:T}^{b_{t+1}:t}, b_{1:T}) \\
\propto \sum_{b_{1:t-1}} \sum_{a_{t-1}} \int \cdots \int \frac{\pi(\theta, x_{1:T}^{'b_{1:T}})}{N^T} \prod_{i=1}^{N} \mu_\theta(x_i^{'t}) \prod_{n=2}^{T} \prod_{i \neq b_n} \mu_{\theta,n-1}^{'n-1} f_\theta(x_n^{'n-1}|x_{n-1}^{'n-1}) \, dx_{t+1:T}^{'b_{t+1:T}}
\]

\[
\propto \sum_{b_{1:t-1}} \sum_{n=1}^{N} \frac{\pi(\theta, x_{1:T}^{'b_{1:T}})}{\mu_\theta(x_1^{'t})} \prod_{n=2}^{T} \prod_{i \neq b_n} \mu_{\theta,n-1}^{'n-1} f_\theta(x_n^{'n-1}|x_{n-1}^{'n-1})
\]

\[
= \pi(\theta, x_{1:T}^{'b_{1:T}}) \frac{N \prod_{n=1}^{N} \mu_\theta(x_1^{'t}) \prod_{i \neq b_n} \mu_{\theta,n-1}^{'n-1}}{\mu_\theta(\theta_1^{'t}) \prod_{n=2}^{T} \prod_{i \neq b_n} \mu_{\theta,n-1}^{'n-1}} f_\theta(x_{1:T}^{'b_{1:T}}|x_{1:T}^{'b_{1:T}}), \\
\text{as } a_{n-1}^{b_n} = b_{n-1},
\]

\[
\propto \sum_{b_{1:t-1}} \sum_{n=1}^{N} f_\theta(x_{t+1}^{'b_{t+1}}|x_t^{'b_t}) w_{b_t,t}^b \]

where we have used that the numerator of the ratio appearing in (7) is independent of \( b_{t-1} \).

2.4 Extension to the fully-adapted auxiliary particle filter

It is straightforward to employ a more general class of PFs in a PMCMC context. One such PF is the fully-adapted auxiliary particle filter (FA-APF) ([Pitt and Shephard (1999]) whose incorporation within PMCMC was explored in [Pitt et al. (2012)]. It is described in this subsection.

When it is possible to sample from \( p_\theta(x_1|y_1) \propto \mu_\theta(x_1) g_\theta(y_1|x_1) \) and \( p_\theta(x_t|x_{t-1}, y_t) \propto f_\theta(x_t|x_{t-1}) g_\theta(y_t|x_t) \) and to compute \( p_\theta(y_1) = \int \mu_\theta(x_1) g_\theta(y_1|x_1) \, dx_1 \) and \( p_\theta(y_t|x_{t-1}) = \int f_\theta(x_t|x_{t-1}) g_\theta(y_t|x_t) \, dx_t \), it is possible to define the target distribution \( \tilde{\pi}(\theta, b_{1:T}, x_{1:T}, a_{1:T-1}^{b_{1:T}}) \) using an alternative conditional [PF] - the conditional FA-APF - in (3) (more precisely, in these circumstances one can implement the associated [PF])

\[
\phi_\theta(x_{1:T}^{'b_{1:T}}, a_{1:T-1}^{b_{1:T}}|x_{1:T}^{'b_{1:T}}, b_{1:T}) = \prod_{i \neq b_1}^{N} p_\theta(x_1^{'i}|y_1) \prod_{t=2}^{T} \prod_{i \neq b_t}^{N} w_{b_t,t-1}^{'i} \phi_\theta(x_t^{b_t-t}|x_{t-1}^{b_t-t}, y_t),
\]

where

\[
w_{b_t,t}^{'i} \defeq \frac{p_\theta(y_{t+1}|x_t^{b_t-t})}{\sum_{j=1}^{N} p_\theta(y_{t+1}|x_t^{b_t-t})}.
\]

In this case, we can target the extended distribution \( \tilde{\pi}(\theta, b_{1:T}, x_{1:T}, a_{1:T-1}^{b_{1:T}}) \) defined through (3), (8) and (9) using a MH algorithm with proposal

\[
q(\theta, \theta') \times \psi_\theta(x_{1:T}, a_{1:T-1}) \times \frac{1}{N},
\]

law of FA-APF, path selection.
i.e. we pick $b_T$ uniformly at random, then set $b_t = a_t^{b_{t+1}}$ for $t = T - 1, \ldots, 1$ and $\Psi_\theta(x_{1:T}, a_{1:T-1})$ is the distribution associated with the FA-APF instead of the bootstrap PF.

$$\Psi_\theta(x_{1:T}, a_{1:T-1}) = \prod_{i=1}^{N} p_\theta(x_i^1 | y_i) \prod_{t=2}^{T} \prod_{i=1}^{N} w_{\theta,t-1}^{1:a_t\!-\!1} p_\theta(x_t^i | x_{t-1}^{a_t\!-\!1}, y_t).$$

It is easy to check that the resulting MH acceptance probability is also of the form given in (6) but with

$$\widetilde{p}_\theta(y_{1:T}) = p_\theta(y_1) \prod_{t=2}^{T} \left[ \frac{1}{N} \sum_{i=1}^{N} p_\theta(y_t | x_{t-1}^i) \right],$$

(10)

The conditional FA-APF with BS proceeds by first running the conditional FA-APF defined in [8], then sampling $b_T$ uniformly at random and finally sampling $b_{T-1}, \ldots, b_1$ backwards using

$$\pi(b_t | \theta, x_{1:T}, a_{1:T-1}, x_{t+1:T}, b_{t+1:T}) \propto f_\theta(x_{b_{t+1}} | x_t^b),$$

(11)

where the expression in (11) is obtained using calculations similar to those in [7].

2.5 Extension to general auxiliary particle filters

The previous section demonstrated that the FA-APF leads straightforwardly to valid PMCMC algorithms and will allow natural connections to be made to certain EHHM methods. Here, we show that as was established in Pitt et al. [2012] Appendix 8.2), any general auxiliary particle filter (APF) can be employed in this context and will lead to natural extensions of these methods.

To facilitate later developments, an explicit representation of the associated extended target distribution and related quantities is useful. Viewing the APF as a sequential importance resampling algorithm for an appropriate sequence of target distributions as described in Johansen and Doucet [2008], it is immediate that the density associated with such an algorithm is simply:

$$\Psi_{\theta}^q(x_{1:T}, a_{1:T-1}) = \prod_{i=1}^{N} q_{\theta,i}(x_i^1) \prod_{t=2}^{T} w_{\theta,t-1}^{1:a_t\!-\!1} q_{\theta,i}(x_t^i | x_{t-1}^{a_t\!-\!1}),$$

where $q_\theta = (q_{\theta,t})_{t=1}^{T}$ and $q_{\theta,t}$ denotes the proposal distribution employed at time $t$ (with dependence of this distribution upon the observation sequence suppressed from the notation) and $w_{\theta,t} = v_{\theta,t} / \sum_{j=1}^{N} v_{\theta,t}$, with:

$$v_{\theta,t} = \begin{cases} 
\mu_\theta(x_t^1) \pi_\theta(y_1 | x_1^1) \widetilde{p}_\theta(y_2 | x_1^1), & \text{if } t = 1, \\
 f_{\theta}(x_t^1 | x_{t-1}^{a_t\!-\!1}) \pi_\theta(y_t | x_t^1) \widetilde{p}_\theta(y_{t+1} | x_t^1), & \text{if } 1 < t < T, \\
 q_{\theta,T}(x_T^1 | x_{T-1}^{a_T\!-\!1}) \pi_\theta(y_T | x_T^1), & \text{if } t = T, 
\end{cases}$$

(12)

and $\widetilde{p}_\theta(y_{t+1} | x_t^i)$ denoting the approximation of the predictive likelihood employed within the weighting of the APF. Note that $\widetilde{p}_\theta(y_{t+1} | x_t^i)$ can be any positive function of $x_t$ and the simpler sequential importance resampling PF is recovered by setting $\widetilde{p}_\theta(y_{t+1} | x_t^i) \equiv 1$, with the bootstrap PF emerging as a particular case thereof when $q_{\theta,t}(x_t | x_{t-1}^i) = f_\theta(x_t | x_{t-1}^i)$.

Associated with the APF is a conditional PF of the form:

$$\phi_\theta^q(x_{1:T}^{b_1:T}, a_{1:T-1}^{b_1:T} | x_{b_1:T}, b_{1:T}) = \prod_{i=1}^{N} q_{\theta,i}(x_i^1) \prod_{t=2}^{T} w_{\theta,t-1}^{1:a_t\!-\!1} q_{\theta,i}(x_t^i | x_{t-1}^{a_t\!-\!1}).$$

A PMCMC algorithm is arrived at by employing the extended target distribution,

$$\pi_{\theta}(\theta, b_{1:T}, x_{1:T}, a_{1:T-1}^{b_{1:T}}) = \frac{1}{N_T} \times \pi(\theta, x_{b_1:T}^{b_1:T}) \times \phi_\theta^q(x_{1:T}^{b_1:T}, a_{1:T-1}^{b_{1:T}} | x_{b_1:T}, b_{1:T}),$$

and proposal distribution,

$$q(\theta, \theta') \times \Psi_{\theta'}^q(x_{1:T}, a_{1:T-1}) \times w_{\theta', T}^{b_T},$$

law of conditional APF

law of APF

path selection

\text{law of APF}

\text{path selection}

6
One can straightforwardly verify that this leads to a MH acceptance probability of the form stated in (6) but using the natural unbiased estimator of the normalising constant associated with the APF

\[ \hat{p}_\theta(y_{1:T}) = \prod_{t=1}^{T} \left[ \frac{1}{N} \sum_{i=1}^{N} v_{\theta,t}^{i} \right]. \]

We conclude this section by noting that although the constructions developed above were presented for simplicity with multinomial resampling employed during every iteration of the algorithm, it is straightforward to incorporate more sophisticated, adaptive resampling schemes within this framework.

### 3 Original embedded hidden Markov models

#### 3.1 Extended target distribution

The embedded Markov models (EHMM) method of Neal (2003; Neal et al. 2004) is based on the introduction of a target distribution on \( \Theta \times X^{NT} \times \{1, \ldots, N\}^{T} \) of the form

\[ \tilde{\pi} (\theta, b_{1:T}, x_{1:T}) = \frac{1}{N^T} \times \pi (\theta, x_{1:T}^{b_{1:T}}) \times \prod_{t=1}^{T} \left\{ \prod_{i=b_{t-1}+1}^{b_{t}} \tilde{R}_{\theta,t}(x_{i}^{t} | x_{i-1}^{t-1}) \right\}, \]

(13)

where \( \tilde{R}_{\theta,t} \) is a \( \rho_{\theta,t} \)-invariant Markov transition kernel, i.e. \( \int \rho_{\theta,t}(x) \tilde{R}_{\theta,t}(x'|x) dx = \rho_{\theta,t}(x') \), and \( \tilde{R}_{\theta,t} \) is its reversal, i.e. \( \tilde{R}_{\theta,t}(x'|x) = \rho_{\theta,t}(x' \rho_{\theta,t}(x) / \rho_{\theta,t}(x)) \) (for \( \rho_{\theta,t} \)-almost every \( x \) and \( x' \)).

Similarly to the PMC extended target distribution, the key feature of \( \tilde{\pi} (\theta, b_{1:T}, x_{1:T}) \) is that, by construction, it ensures that the associated marginal distribution of \( (\theta, x_{1:T}^{b_{1:T}}) \) is the posterior of interest.

#### 3.2 Metropolis–Hastings algorithm

As detailed in the next section, the algorithm proposed in Neal (2003) can be reinterpreted as a Gibbs sampler targeting \( \tilde{\pi} (b_{1:T}, x_{1:T}|\theta) \). We present here an alternative, original MH algorithm to sample from \( \tilde{\pi} (\theta, b_{1:T}, x_{1:T}) \).

It relies on a proposal of the form

\[ q (\theta', \theta) \times \Psi_{\theta} (x_{1:T}) \times q_{\theta} (b_{1:T}|x_{1:T}), \]

(14)

where

\[ \Psi_{\theta} (x_{1:T}) := \frac{1}{N^T} \prod_{t=1}^{T} \left\{ \rho_{\theta,t}(x_{1}^{t}) \prod_{i=2}^{N} \tilde{R}_{\theta,t}(x_{i}^{t} | x_{i-1}^{t-1}) \right\} \]

is sometimes referred to as the ensemble base measure (Neal 2011) and

\[ q_{\theta} (b_{1:T}|x_{1:T}) := \frac{\tilde{p}_{\theta}(x_{1:T}^{b_{1:T}}, y_{1:T})}{\sum_{b_{1:T}} \tilde{p}_{\theta}(x_{1:T}^{b_{1:T}}, y_{1:T})} = \frac{1}{N^T} \tilde{p}_{\theta}(x_{1:T}^{b_{1:T}}, y_{1:T}). \]

In this expression, we have (where we note that this is no longer a probability density with respect to Lebesgue measure)

\[ \tilde{p}_{\theta}(x_{1:T}^{b_{1:T}}, y_{1:T}) := \frac{\mu_{\theta}(x_{1} | x_{1}) \prod_{t=2}^{T} f_{\theta}(x_{t} | x_{t-1}) g_{\theta}(y_{t} | x_{t})}{\rho_{\theta,t}(x_{1:T})}, \]

and

\[ \tilde{p}_{\theta}(y_{1:T}) := \frac{1}{N^T} \sum_{b_{1:T}} \tilde{p}_{\theta}(x_{1:T}^{b_{1:T}}, y_{1:T}). \]

To sample from \( \Psi_{\theta} (x_{1:T}) \), we sample \( x_{i}^{t} \sim \rho_{\theta,t}(x_{i}^{t}) \) and \( x_{i}^{-1} \sim \prod_{t=2}^{T} \tilde{R}_{\theta,t}(x_{i}^{t} | x_{i-1}^{t-1}) \) for \( t = 1, \ldots, T \). Hence, at time \( t \) all of the particles are marginally distributed according to \( \rho_{\theta,t} \). When \( \rho_{\theta,t}(x') = \rho_{\theta,t}(x) \), this corresponds to the algorithm proposed in Lin et al. (2005). Sampling from the high-dimensional discrete distribution \( q_{\theta}(b_{1:T}|x_{1:T}) \) can be performed in \( O(N^2T) \) operations with the finite state-space hidden Markov model (HMM) filter using the \( N \) states \( (x_{i}^{t}) \) at time \( t \), transition probabilities proportional to \( f_{\theta}(x_{i}^{t} | x_{i-1}^{t-1}) \) and conditional probabilities of the observations proportional to \( g_{\theta}(y_{t} | x_{i}^{t}) / \rho_{\theta,t}(x_{i}^{t}) \). We also obtain as a by-product \( \tilde{p}_{\theta}(y_{1:T}) \), which is an unbiased estimate of \( p_{\theta}(y_{1:T}) \).
The resulting MH algorithm targeting the extended distribution given in (13) with the proposal given in (14) admits an acceptance probability of the form

\[ 1 \wedge \frac{\tilde{p}(y_{1:T})p(\theta')}{\tilde{p}(y_{1:T})p(\theta)} = q(\theta', \theta) q(\theta, \theta'), \tag{15} \]

i.e., it looks very much like the PMMH algorithm, except that instead of having likelihood terms estimated by a particle filter, these likelihood terms are estimated using a finite state-space HMM filter.

To establish the correctness of the acceptance probability given in (15), we note that

\[ \tilde{p}(\theta, b_{1:T}, x_{1:T}) = N(T) \pi(\theta, x_{1:T}) \prod_{t=1}^{T} \left\{ \prod_{i=b_{t-1}}^{b_{t}} \tilde{R}_{\theta, n}(x_{i}^{t} | x_{i}^{t-1}) \cdot \prod_{i=b_{t}+1}^{N} R_{\theta, n}(x_{i}^{t} | x_{i+1}^{t-1}) \right\} \]

\[ \times \prod_{t=1}^{T} \left\{ \prod_{i=b_{t}}^{b_{t+1} - 1} \rho_{\theta, t}(x_{i}^{t}) \right\} \prod_{t=1}^{T} \left\{ \prod_{i=b_{t}+1}^{N} \rho_{\theta, t}(x_{i}^{t}) \right\}^{-1} \]

\[ = p(\theta | y_{1:T}) \tilde{p}_{b}(y_{1:T}) \tilde{p}(y_{1:T}) \]

where we have used that

\[ \tilde{p}_{b}(y_{1:T}) = p_{b}(x_{1:T}, y_{1:T}) p_{b}(y_{1:T}) \sum_{b_{1:T}}^{T} p_{b}(x_{1:T}, y_{1:T}) \]

In addition, we have used the following identity which we will also exploit in the next section: if \( R \) is a \( \rho \)-invariant Markov kernel and \( \bar{R} \) the associated reversal, then for any \( b, c \in \{1, \ldots, N\} \),

\[ \prod_{i=b-1}^{1} R(x_{i}^{t} | x_{i}^{t+1}) \cdot \rho(x_{i}^{t}) \cdot \prod_{i=c+1}^{N} R(x_{i}^{t} | x_{i-1}^{t}) = \prod_{i=c-1}^{1} R(x_{i}^{t} | x_{i+1}^{t}) \cdot \rho(x_{i}^{t}) \cdot \prod_{i=c+1}^{N} R(x_{i}^{t} | x_{i-1}^{t}). \tag{16} \]

### 3.3 Interpretation as a collapsed Gibbs sampler

Consider the following Gibbs sampler type algorithm to sample from \( \pi(x_{1:T} | \theta) \):

1. Sample \( b_{1:T} \) uniformly at random on \( \{1, \ldots, N\} \) and set \( x_{1:T} ^{b_{1:T}} \leftarrow x_{1:T} \);
2. Sample \( \tilde{\pi}(x_{1:T}^{b_{1:T}} | \theta, b_{1:T}, x_{1:T}) \);
3. Sample \( y_{1:T} \sim \tilde{\pi}(y_{1:T} | \theta, x_{1:T}) \) then \( b_{1:T} \sim \tilde{\pi}(b_{1:T} | \theta, x_{1:T}) \) and so on.

It is obvious that Steps 1 and 2 coincide with the first steps of the EHMM algorithm described in [Neal, 2003]. For Step 3 we note that

\[ \tilde{\pi}(b_{1:T} | \theta, x_{1:T}) \propto \prod_{b_{1:T}}^{T} \left\{ \prod_{n=1}^{b_{n}} \tilde{R}_{\theta, n}(x_{n}^{t} | x_{n+1}^{t-1}) \cdot \prod_{n=1}^{b_{n}} \bar{R}_{\theta, n}(x_{n}^{t+1} | x_{n}^{t}) \right\} \]

\[ = \prod_{n=1}^{T} \left\{ \prod_{i=b_{n}}^{b_{n+1} - 1} \rho_{\theta, n}(x_{i}^{t}) \right\} \]

where by (16), the numerator in the penultimate line is independent of \( b_{n} \). Since

\[ \frac{\pi(\theta, x_{1:T})}{\prod_{n=1}^{T} \rho_{\theta, n}(x_{n}^{t})} \propto \prod_{n=1}^{T} \rho_{\theta, n}(x_{n}^{t}) \]

\[ \propto \prod_{n=1}^{T} f_{\theta}(x_{n}^{t} | x_{n-1}^{t-1}) g_{\theta}(y_{n} | x_{n}^{t}) \]

\[ \propto \prod_{n=1}^{T} f_{\theta}(x_{n}^{t} | x_{n-1}^{t-1}) g_{\theta}(y_{n} | x_{n}^{t}) \]

modified posterior \( \tilde{p}_{b}(x_{1:T}^{b_{1:T}} | y_{1:T}) \)
we can compute the marginal \( \tilde{p}_\theta (x_{b1}^b | y_{1:t}) := \sum_{b_{t+1}^T} \tilde{p}_\theta (x_{b1+1}^b | y_{1:t}) \) using the same (finite state-space) HMM filter discussed in the previous section and so
\[
\tilde{\pi} (b_t | \theta , x_{1:t} , x_{t+1:T}^b , b_{t+1:T}) \propto \tilde{p}_\theta (x_t^b | y_{1:t}) f_\theta (x_{t+1}^b | x_t^b)
\]
coinciding with the expression obtained in [Neal (2003)]. This is an alternative proof of validity of the algorithm. The present derivation is more complex than that in [Neal (2003)] which relies on a simple detailed balance argument. One potential benefit of our approach is that it can be extended systematically to any extended target admitting a similar structure; see for example [Lindsten and Schön (2013, p. 116)] for extensions to the non-Markovian case. Finally, we note that this algorithm may be viewed as a special case of the framework proposed in [Tjelmeland (2004)] and simplifies to Barker’s kernel (Barker, 1965) if \( N = 2 \) and \( T = 1 \).

4 Alternative embedded hidden Markov models

In its original version, the EHMM method has a computational cost per iteration of order \( O(N^2T) \) compared to \( O(NT) \) for PMCMC methods and it samples particles independently across time which can be inefficient if the latent states are strongly correlated. The new version of EHMM methods, which was proposed in [Shestopaloff (2015)] compared to those in [Neal (2003)] which relies on a proposal of order \( N \times T \) for PMCMC methods.

The present derivation is more complex than that in [Neal (2003)] which relies on a simple detailed balance argument. One potential benefit of our approach is that it can be extended systematically to any extended target admitting a similar structure; see for example [Lindsten and Schön (2013, p. 116)] for extensions to the non-Markovian case. Finally, we note that this algorithm may be viewed as a special case of the framework proposed in [Tjelmeland (2004)] and simplifies to Barker’s kernel (Barker, 1965) if \( N = 2 \) and \( T = 1 \).

4.1 Extended target distribution

This version of the EHMM henceforth referred to as the alternative EHMM method, relies on the extended target distribution
\[
\tilde{\pi} (\theta , b_{1:T} , x_{1:T} , a_{1:T-1} \cdot | \cdot ) := \frac{1}{N^T} \times \pi (\theta , x_{1:T}^b) \times \phi_\theta (x_{1:T}^b , a_{1:T-1} \cdot | \cdot )
\]
where we will refer to the algorithm inducing the following distribution as the conditional MCMC FA-APF for reasons which are made clear below:
\[
\phi_\theta (x_{1:T}^b , a_{1:T-1} \cdot | \cdot ) := \frac{1}{N^T} \prod_{i=0}^N \left( \prod_{i=0}^N \tilde{R}_{\theta,t} (x_t^i , a_{t-1}^i \cdot | \cdot ) \right)
\]
with \( b_t = a_t^b \) as for PMCMC methods.

Here \( R_{\theta,t} \) is invariant with respect to \( \rho_{\theta,1} (x_1) = p_\theta (x_1 | y_1) \) whereas, for \( t = 2, \ldots , T \), \( R_{\theta,t}( \cdot , x_{t-1} \cdot | \cdot ) \) is invariant w.r.t.
\[
\rho_{\theta,t} (x_t , a_{t-1} \cdot | x_{t-1} \cdot ) = \frac{g_\theta (y_t | x_t^i) f_\theta (x_t | x_{t-1}^a)}{\sum_{i=0}^N g_\theta (y_t | x_t^i) f_\theta (x_t | x_{t-1}^a)},
\]
while, for \( t = 1, \ldots , T \), \( R_{\theta,t}( \cdot , x_{t-1} \cdot | x_{t-1} \cdot ) \) denotes the reversal of the kernel \( R_{\theta,t}( \cdot , x_{t-1} \cdot | x_{t-1} \cdot ) \) with respect to its invariant distribution.

Note that if \( R_{\theta,1} (x_{1}^i | x_1) = \rho_{\theta,1} (x_1^i) \) and \( R_{\theta,t} (x_t^i , a_{t-1}^i | x_t , a_{t-1}^i ; x_{t-1}) = \rho_{\theta,t} (x_t^i , a_{t-1}^i | x_{t-1}) \), the extended target \( \tilde{\pi} (\theta , b_{1:T} , x_{1:T} , a_{1:T-1} \cdot | \cdot ) \) coincides exactly with the extended target associated with the FA-APF described in Section 2.7. As explored in the following two sections, this allows us to understand this EHMM approach as the incorporation of a slightly more general class of PFs within a PMCMC framework and ultimately suggests further generalisations of these algorithms.

4.2 Metropolis–Hastings algorithm

We now consider the following MH algorithm to sample from \( \tilde{\pi} (\theta , b_{1:T} , x_{1:T} , a_{1:T-1} \cdot | \cdot ) \). It relies on a proposal of the form
\[
q(\theta , \theta') \times \Psi_{\theta'} (x_{1:T} , a_{1:T-1} \cdot | \cdot ) \times \frac{1}{N^T}.
\]
i.e. to sample \( b_t \) uniformly at random, then set \( b_t = a_t^{b_{t+1}} \) for \( t = T - 1, \ldots, 1 \). Moreover,

\[
\Psi_\theta(x_{1:T}, a_{1:T-1}) = \rho_{\theta,1}(x_1^1) \prod_{i=2}^{N} \rho_{\theta,i}(x_i^1 | x_{1}^{i-1}) \\
\times \prod_{t=2}^{T} \left\{ \rho_{\theta,t}(x_t^1, a_t^{-1} | x_{t-1}^1, a_{t-1}^{-1}; x_{t-1}) \right\}
\]

(17)

is the law of a novel PF type algorithm, which we refer to as the MCMC FA-APF; again the reason for this terminology should become clear below.

The MCMC FA-APF proceeds as follows.

1. At time 1, sample \( x_1^1 \sim \rho_{\theta,1}(x_1^1) \) and then \( x_1^{-1} \sim \prod_{i=2}^{N} \rho_{\theta,1}(x_i^1 | x_{1}^{i-1}) \).

2. At time \( t = 2, \ldots, T \), sample
   
   \[
   \begin{align*}
   &\text{a)} \ (x_t^1, a_t^{-1}) \sim \rho_{\theta,t}(x_t^1, a_t^{-1} | x_{t-1}^1, a_{t-1}; x_{t-1}) \\
   &\text{b)} \ (x_t^{-1}, a_t^{-1}) \sim \prod_{i=2}^{N} \rho_{\theta,t}(x_i^1, a_i^{-1} | x_{t-1}^1, a_{t-1}; x_{t-1}).
   \end{align*}
   \]

If \( \rho_{\theta,1}(x_1^1 | x_1^t) = \rho_{\theta,1}(x_1^t) \) and \( \rho_{\theta,t}(x_t^1, a_t^{-1} | x_t^t, a_t; x_t) = \rho_{\theta,t}(x_t^t, a_t^{-1} | x_t) \), this corresponds to the standard FA-APF.

The resulting [MH] algorithm targeting the extended distribution defined in (13) and using the proposal defined in (14) admits an acceptance probability of the form

\[
1 \wedge \frac{\tilde{p}(y_{1:T})p(\theta') q(\theta, \theta')}{\tilde{p}(y_{1:T})p(\theta)} q(\theta, \theta')
\]

(18)

i.e. it looks very much like the PMMH except that here \( \tilde{p}(y_{1:T}) \) is given by the expression in (10) with particles generated via (17). Note that this estimate is unbiased.

The validity of the acceptance probability in (18) can be established by calculating

\[
\frac{\tilde{p}(\theta, b_{1:T}, x_{1:T}, a_{1:T-1})}{\Psi_\theta(a_{1:T-1}, x_{1:T})} = \frac{N \pi(\theta, x_{1:T}^{b_{1:T}}) \prod_{i=b_1}^{1} \rho_{\theta,i}(x_1^1 | x_{1}^{i-1}) \cdot \prod_{i=b_t+1}^{N} \rho_{\theta,i}(x_1^1 | x_{1}^{i-1})}{\rho_{\theta,1}(x_1^1) \prod_{i=2}^{N} \rho_{\theta,i}(x_i^1 | x_{1}^{i-1})} \\
\times \prod_{t=2}^{T} \frac{\tilde{R}_{\theta,t}(x_t^1, a_t^1 | x_t^1, a_t^1, x_{1}^{i-1}) \cdot \prod_{i=b_t+1}^{N} \rho_{\theta,i}(x_t^1, a_t^1 | x_t^1, a_t^1; x_{t-1})}{\rho_{\theta,t}(x_t^1, a_t^{-1} | x_{t-1}^1, a_{t-1}; x_{t-1})} \\
= \frac{N^{-1} \pi(\theta, x_{1:T}^{b_{1:T}})}{\rho_{\theta,1}(x_1^1) \prod_{i=2}^{T} \rho_{\theta,i}(x_t^1, a_t^1 | x_{1}^{i-1})} \\
= \frac{N^{-1} \pi(\theta, x_{1:T}^{b_{1:T}})}{\rho_{\theta}(x_1^1, y_{1:T}) \prod_{i=2}^{T} f_{\theta}(x_t^1 | x_{1:t-1}^i ; \rho_{\theta}(y_{1:T})) \sum_{i=1}^{N} \rho_{\theta}(y_{1:T})} = \frac{p(\theta | y_{1:T}) \tilde{p}_{\theta}(y_{1:T})}{p_{\theta}(y_{1:T})}.
\]

We have again used identity (16) and additionally that \( b_t = a_t^{b_{t+1}} \), for \( t = T - 1, \ldots, 1 \).

### 4.3 Gibbs sampler

The EHMM method of [Shestopaloff and Neal (2016)] can be reinterpreted as a collapsed Gibbs sampler to sample from the extended target distribution \( \tilde{p}(\theta, b_{1:T}, x_{1:T}, a_{1:T-1}) \). Given a current value of \( x_{1:T} \), the algorithm proceeds as follows.

1. Sample \( b_{1:T} \) uniformly at random and set \( x_{1:T}^{b_{1:T}} \leftarrow x_{1:T} \).

2. Run the conditional MCMC FA-APF i.e. sample from \( \phi_\theta(x_{1:T}^{b_{1:T}}, a_{1:T-1}^{b_{1:T}} | x_{1:T}^{b_{1:T}}, b_{1:T}) \).

3. Sample \( bt \) according to \( \Pr(b_T = m) = 1/N \) and then, for \( t = T - 1, \ldots, 1 \), sample \( b_t \) according to a distribution proportional to \( f_\theta(x_t^{b_{t+1}} | x_{1:T}^{b_{t+1}}) \).

The validity of the algorithm is established using a detailed balance argument in [Shestopaloff and Neal (2016)]. Alternatively, we can show using simple calculations similar to the ones presented earlier that

\[
\tilde{p}(b_t | \theta, x_{1:T}, x_{t+1:T}^{b_{t+1}}, b_{1:T}) \propto f_\theta(x_t^{b_{t+1}} | x_{1:T}^{b_{t+1}}).
\]
In the standard conditional PF, the particles are conditionally independent given the previously sampled values. The conditional MCMC FA-APF allows for conditional dependence between all the particles (and ancestor indices) generated in one time step. Indeed, we can choose the kernels $p^q_{\theta,t}(\cdot \mid x_{t-2:t-1}, a_{t-2})$ such that they induce only small, local moves. This can improve the performance of PF samplers in high dimensions: as with standard MCMC schemes, less ambitious local moves are much more likely to be accepted. Of course, as with any local proposal one could not expect such a strategy to work well with strongly multi-modal target distributions without further refinements.

5 Novel practical extensions

Motivated by the connections identified above, we now develop extensions based upon the more general PMCMC algorithms described above, in particular considering constructions based around general APFs. In particular, we relax the requirement in the MCMC algorithm from Section 4.2 that it is possible to sample from the proposal distribution of the FA-APF (which is possible in only a small number of tractable models) and to compute its associated importance weight.

5.1 MCMC APF

Generalising the MCMC FA-APF in the same manner as the APF generalises the FA-APF leads us to propose a (general) auxiliary particle filter with MCMC moves (MCMC APF). Set

$$
\rho_{\theta,t}^{q_\theta}(x_t, a_{t-1} \mid x_{t-2:t-1}, a_{t-2}) = \begin{cases} 
q_\theta(x_1), & \text{if } t = 1, \\
\frac{v_{\theta,t-1}}{\sum_{i=1}^N v_{\theta,t-1}} q_\theta(x_t \mid a_{t-1}^{t-1}), & \text{if } t > 1,
\end{cases}
$$

where $v_{\theta,t-1}$ are as defined in (12), and is responsible for the dependence upon $a_{t-1}$ and $x_{t-2}$ in particular, and we allow $p^q_{\theta,t} \left( \cdot \mid x_{t-2:t-1}, a_{t-2} \right)$ and $p^q_{\theta,t} \left( \cdot \mid x_{t-2:t-1}, a_{t-2} \right)$ to respectively denote a $\rho^q_{\theta,t}(\cdot \mid x_{t-2:t-1}, a_{t-2})$-invariant Markov kernel and the associated reversal kernel. Although this expression superficially resembles the mixture proposal of the marginalised APF (Klass et al., 2005), by explicitly including the ancestry variables it avoids incurring the $O(N^2)$ cost and allows an approximation of smoothing distributions. We then define the law of the MCMC APF via:

$$
\Psi^{q}_\theta(x_{1:T}, a_{1:T-1}) := \rho^{q}_\theta(x_{1}^T) \prod_{i=2}^N p^{q}_{\theta,i-1}(x_{i}^T \mid a_{i-1}^{i-1}) 
\times \prod_{t=2}^T \left\{ \rho^{q}_{\theta,t}(x_{i}^t, a_{i-1}^t \mid x_{t-2:t-1}, a_{t-2}) \prod_{i=2}^N p^{q}_{\theta,i}(x_{i}^t, a_{i-1}^t \mid x_{t-2:t-1}, a_{t-2}) \right\}.
$$

The corresponding extended PMCMC target distribution is simply:

$$
\pi_q(\theta, b_{1:T}, x_{1:T}, a_{1:T}, b_{1:T}) = \frac{1}{N^T} \prod_{t=1}^T \pi(\theta, x_{t+1:T}) \phi^{q}_\theta(x_{1:T}, a_{1:T}, b_{1:T})
$$

where, as might be expected:

$$
\phi^{q}_\theta(x_{1:T}, a_{1:T}, b_{1:T}) = \prod_{t=1}^T \prod_{i=1}^{b_{t-1}} p^{q}_{\theta,i}(x_{i}^t \mid a_{i-1}^t), \prod_{i=1}^{b_{t-1}} p^{q}_{\theta,i}(x_{i}^t \mid a_{i-1}^t)
\times \prod_{t=2}^T \left\{ \prod_{i=1}^{b_{t-1}} p^{q}_{\theta,i}(x_{i}^t, a_{i-1}^t \mid x_{t-2:t-1}, a_{t-2}) \prod_{i=1}^{b_{t-1}} p^{q}_{\theta,i}(x_{i}^t, a_{i-1}^t \mid x_{t-2:t-1}, a_{t-2}) \right\}.
$$

Note that the MCMC FA-APF can be viewed as a special case of the MCMC APF in much the same way that the FA-APF from Section 2.4 can be viewed as a special case of the (general) APF from Section 2.3.

5.2 Metropolis–Hastings algorithms

We arrive at a PMMH-type algorithm based around the MCMC APF by considering proposal distributions of the form:

$$
q(\theta, \theta') \times q^{q_\theta}_\theta(x_{1:T}, a_{1:T-1}) \times a_{b_{t-1}}
$$

path selection
where, as in Section 2, \( w^t_{i,T} = v^t_{θ,T} / \sum_{j=1}^N v^t_{θ,T} \) and \( \tilde{ρ}_0(y_{1:T}) = \prod_{t=1}^T N^{-1} \sum_{i=1}^N v^t_{θ,t} \) is again an unbiased estimate of the marginal likelihood.

Note that the \( \text{PMMH}\) type variant of the \( \text{MCMC FA-APF} \) cannot often be used in realistic scenarios because it requires sampling from \( p_0(x_1|x_{t-1}, y_t) \) and evaluating \( x_{t-1} \mapsto p_0(y_t|x_{t-1}) \) in order to implement the \( \text{FA-APF} \) in (19). To circumvent this problem, we can define a special case of the \( \text{MCMC APF} \) algorithm which requires neither sampling from \( p_0(x_1|x_{t-1}, y_t) \) nor evaluating \( x_{t-1} \mapsto p_0(y_t|x_{t-1}) \). This algorithm, obtained by setting \( p_0(y|x) \equiv 1 \), will be called (bootstrap) particle filter with \( \text{MCMC moves} \) \( \text{(MCMC PF)} \) as it represents an analogue of the (bootstrap) \( \text{PF} \). At time 1, the \( \text{MCMC PF} \) uses the \( \text{MCMC kernels} \) \( R_θ,1 \) which are invariant w.r.t. \( ρ_{θ,t}(x_1) = \mu_θ(x_1) \). At time \( t, t > 1 \), the \( \text{MCMC PF} \) uses the kernels \( R_θ,t(\cdot | \cdot ; x_{t-1}) \) which are invariant w.r.t.

\[
ρ_{θ,t}(x_{t-1}, a_{t-1}|x_{t-1}) := \frac{g_θ(y_{t-1}|x^a_{t-1})}{\sum_{i=1}^N g_θ(y_{t-1}|x^i_{t-1})} f_0(x_t|x^a_{t-1}).
\] (19)

The \( \text{PMMH}\) type variant of the \( \text{MCMC PF} \) may be useful if the \( \text{PMMH}\) type variant of the \( \text{MCMC FA-APF} \) cannot be implemented.

### 5.3 Gibbs samplers

Given the extended target construction of the \( \text{MCMC APF} \) algorithm, it is straightforward to implement \( \text{PG} \) algorithms \([55]\) (or similarly with ancestor sampling \([\text{AS}]\)) see Section 6.3 which target it.

However, Gibbs samplers based around the (conditional) \( \text{MCMC PF} \) do not appear useful as they might be expected to perform less well than the Gibbs sampler based around the \( \text{MCMC FA-APF} \) and are no more easy to implement: in contrast to the \( \text{PMMH}\) type algorithms, the Gibbs sampler based around the (conditional) \( \text{MCMC FA-APF} \) does not generally require sampling from \( p_0(x_1|x_{t-1}, y_t) \) and it only requires evaluation of the unnormalised density \( p_0(y_t|x_t) f_0(x_t|x_{t-1}) \) in the transition density of the \( \text{FA-APF} \) in (19).

### 6 General particle Markov chain Monte Carlo methods

In this section, we describe a slight generalisation of \( \text{PMCMC} \) methods which admits both the standard \( \text{PMCMC} \) methods from Section 2 as well as the alternative \( \text{EHMM} \) methods from Section 4 as special cases. In addition, we derive both the backward sampling and ancestor sampling recursions for this algorithm. We note that this section is necessarily slightly more abstract than the previous sections. As the details developed below are not required for understanding the remainder of this work, this section may be skipped on a first reading.

#### 6.1 Extended target distribution

We define \( z_1 := x_1 \) and \( z_t := (x_t, a_{t-1}) \). For notational brevity, also define \( z^{-i}_t := z_1 \setminus x^i_1, z^{-i}_t := z_t \setminus (x^i_1, a^i_{t-1}) \) as well as \( z^{-b_{i-1}}_t = (z^{-b_{i-1}}, \ldots, z^{-b_{i-1}}_t) \). We note that further auxiliary variables could be included in \( z_t \) without changing anything in the construction developed below. The law of a general \( \text{PF} \) is given by

\[
ψ_θ(z_{1:T}) := ψ_{θ,1}(z_1) \prod_{t=2}^T ψ_{θ,t}(z_t|z_{1:t-1}).
\]

With this notation, general \( \text{PMCMC} \) methods target the following extended distribution:

\[
\tilde{π}(θ, z_{1:T}, b_{1:T}) := \frac{1}{N^T} × \tau(θ, x^{b_{1:T}}_{1:T}) × ϕ_θ(z^{-b_{1:T}}_{1:T} | x^{b_{1:T}}_{1:T}, b_{1:T}),
\]

where the law of the conditional general \( \text{PF} \) is given by

\[
ϕ_θ(z^{-b_{1:T}}_{1:T} | x^{b_{1:T}}_{1:T}, b_{1:T}) := ψ_{θ,1}(z^{-b_{1:T}}_1) \prod_{t=2}^T ψ_{θ,t}^{-b_{1:T}}(z^{-b_{1:T}}_{t-1} | z_{1:t-1}, x^{b_{1:T}}_t),
\]

with

\[
ψ_{θ,t}^{-b_{1:T}}(z^{-b_{1:T}}_{t-1} | x^{b_{1:T}}_t) := \frac{ψ_{θ,t}(z_t|z_{1:t-1})}{ψ^{-b_{1:T}}_{θ,t}(x_t, a^i_{t-1} | z_{1:t-1}, x^{b_{1:T}}_t)}.
\]

\[
\]
Here, $\psi_{\theta,t}^i(\cdot|z_{1:t-1})$ denotes the marginal distribution of the $i$th components of $x_t$ and $a_{t-1}$ under the distribution $\psi_{\theta,t}^i(\cdot|z_{1:t-1})$. Finally, for any $t \in \{1, \ldots, T\}$, we define the following unnormalised weight

$$v_{\theta,t}^{b_t} := \frac{1}{N^T} \psi_{\theta,1}^i(x_{b_t}^i) \prod_{n=2}^T \psi_{\theta,n}^i(x_{b_n}^i, a_{n-1}^i|z_{1:n-1}),$$

where $b_{1:t-1}$ on the r.h.s. are to be interpreted as functions of $b_t$ and the ancestry variables via the usual recursion $b_t = d_{b_t}$. Here, $\gamma_{\theta,t}(x_{1:t})$ is the unnormalised density targeted at the $t$th step of the general PF – for all the algorithms discussed in this work, we will state these densities explicitly in Appendix A in particular,

$$\gamma_{\theta,t}(x_{1:t}) = p_{\theta}(x_{1:T}, y_{1:T}).$$

We make the following minimal assumption to ensure the validity of the (general) PMCMC algorithms.

**Assumption 1 (absolute continuity).** For any $t \in \{1, \ldots, T\}$, any $i \in \{1, \ldots, N\}$ and any $z_{1:t-1}$, the support of $(x_t, b_t) \mapsto \psi_{\theta,t}^i(x_t, b_t-1|z_{1:t-1})$ includes the support of $(x_t, b_t) \mapsto \gamma_{\theta,t}(x_{1:t-1}, x_t)$.

We also make the following assumption which requires that all marginals of the conditional distributions $\psi_{\theta,t}^i(\cdot|z_{1:t-1})$ are identical.

**Assumption 2 (identical marginals).** For any $(i, j) \in \{1, \ldots, N\}^2$ and any $t \in \{1, \ldots, T\}$, $\psi_{\theta,t}^i = \psi_{\theta,t}^j$.

**Remark 1.** Assumption 2 can be easily dropped in favour of selecting a suitable (non-uniform) distribution for the particle indices $b_{1:T}$ in [20]. Indeed, more elaborate constructions could be used to justify resampling schemes which, unlike multinomial resampling, are not exchangeable in the sense of Andrieu et al. (2010) Assumption 2) (unless one permutes the particle indices uniformly at random at the end of each step as mentioned in Andrieu et al. (2010)). Similarly, such more general constructions would allow us to view the use of more sophisticated PFS such as the discrete particle filter of Fearnhead (1998), with PMCMC schemes as special cases of this framework as shown in Fink (2015) Section 2.3.4).

In Examples 1 and 2, we show how APFs with antithetic variables (Bizjajeva and Olsson, 2016) and (randomised) sequential quasi Monte Carlo (SQMC) methods (Gerber and Chopin 2015) can be considered as special cases of the framework described in this section even though these methods cannot easily be viewed as conventional PFS because the particles are not sampled conditionally independently at each step.

**Example 1 (APFs with antithetic variables).** The APFs with antithetic variables from Bizjajeva and Olsson (2016) aim to improve the performance of APFs by introducing negative correlation into the particle population. To that end, the $N$ particles are divided into $M$ groups of $K$ particles; the particles in each group then share the same ancestor index and given the ancestor particle, they are sampled in such a way that they are negatively correlated.

Assume that there exists $K, M \in \mathbb{N}$ such that $N = KM$ and for $z_t := (\tilde{x}_t^1, \ldots, \tilde{x}_t^K) \in \mathcal{X}^K$ let $\bar{q}_{\theta,t}(\tilde{x}_t|z_{1:t-1})$ denote some joint proposal kernel for $K$ particles such that if $(\tilde{x}_t^1, \ldots, \tilde{x}_t^K) \sim \bar{q}_{\theta,t}(\cdot|z_{1:t-1})$ then $1. \tilde{x}_t^1, \ldots, \tilde{x}_t^K$ are (pairwise) negatively correlated, $2.$ marginally, $\tilde{x}_t^k \sim q_{\theta,t}(\cdot|z_{1:t-1})$ for all $k \in \{1, \ldots, K\}$.

Given $z_{1:t-1}$, the APF with antithetic variables generates $z_t = (a_{t-1}, x_t)$ as follows (we use the convention that any action prescribed for some $m$ is to be performed for all $m \in \{1, \ldots, M\}$).

1. Set $a_{t-1}^{(m-1)K+1} = i$ w.p. proportional to $v_{\theta,t-1}^{i}$.
2. Sample $x_{t}^{(m-1)K+k} := a_{t-1}^{(m-1)K+1}$ for all $k \in \{2, \ldots, K\}$.
3. Permute the particle indices on $z_{1:t-1}^{1}, \ldots, z_{1:t-1}^{N}$ uniformly at random.

**Example 2 (sequential quasi Monte Carlo).** Let $\mathcal{X} = \mathbb{R}^d$. Randomised SQMC algorithms are general PFS which stratify sampling of the ancestor indices and particles $z_t = (a_{t-1}, x_t)$ by computing them as a deterministic transformation of a set of randomised quasi Monte Carlo points $u_t := (u_t^1, \ldots, u_t^N) \in [0, 1)^{(d+1)N}$. By construction, 1. the set $u_t$ is $(\mathbb{U}^d)^N$ has a low discrepancy, 2. for each $i \in \{1, \ldots, N\}$, $u_t^i$ is (marginally) uniformly distributed on the $(d+1)$-dimensional hypercube.

Write $u_t^i = (u_t^{i1}, u_t^{i2})$ with $u_t^{i1} \in [0,1)$ and $u_t^{i2} \in [0,1)^d$. Given $z_{1:t-1}$, the algorithm (Gerber and Chopin 2015 Algorithm 3) transforms $u_t \rightarrow z_t = (a_{t-1}, x_t)$ as follows (using the convention that any action mentioned for some $i$ is to be performed for all $i \in \{1, \ldots, N\}$).

1. Find a suitable permutation $\sigma_{t-1} : \{1, \ldots, N\} \rightarrow \{1, \ldots, N\}$ such that $x_{t-1}^{\sigma_{t-1}(1)} \leq \ldots \leq x_{t-1}^{\sigma_{t-1}(N)}$, if $d = 1; \text{if } d > 1$, the permutation $\sigma_{t-1}$ is obtained by mapping the particles to the hypercube $[0, 1)^d$ and projecting them onto $\{0, 1\}$ using the pseudo-inverse of the Hilbert space-filling curve. These projections are then ordered as for $d = 1$ (see Gerber and Chopin (2015) for details).
2. Set \( a^i := F^{-1}(\tilde{a}_i^t) \), where \( F^{-1} \) denotes the generalised inverse of the cumulative distribution function (CDF) \( F : \{1, \ldots, N\} \rightarrow [0, 1] \), defined by \( F(i) := \sum_{j=1}^{i} \sigma_{t-1}^{\psi}(j) / \sum_{j=1}^{N} \sigma_{t-1}^{\psi} \).

3. Set \( a_{t-1}^i := \sigma_{t-1}(a^i) \) and \( x_i^t := \Gamma_{\theta, t}(a_{t-1}^i, \tilde{\epsilon}_t^i) \). Here, if \( d = 1 \), the function \( \Gamma_{\theta, t}(\cdot, \cdot) \) is the (generalised) inverse of the CDF associated with \( q_{\theta, t}(\cdot|\cdot) \); if \( d > 1 \), this can be generalised via the Rosenblatt transform.

4. Permute the particle indices on \( z_1^t, \ldots, z_N^t \) uniformly at random.

While the joint kernel \( \psi_{\theta, t}(z_1|1_{t-1}) \) is potentially intractable in both examples, the random permutation of the particle indices (i.e. Step 4 in Example 1 and also Step 4 in Example 2) ensures that Assumption 2 is satisfied. Indeed, it can be easily verified that in both examples, for any \((i, j) \in \{1, \ldots, N\}^2\),

\[
\psi_{\theta, t}(x_i, a_{t-1}|z_{1:t-1}) = \rho_{\theta, t}(x_i, a_{t-1}|x_{t-2:t-1}, a_{t-2}) = \psi_{\theta, t}(x_i, a_{t-1}|z_{1:t-1}).
\]

As pointed out in Remark 1, Assumption 2 is not actually necessary and can be easily dropped in favour of a slightly more general construction of the extended target distribution which is implicitly employed by Bizjakova and Olsson (2016); Gerber and Chopin (2015) (who therefore do not require the random permutation of the particle indices).

### 6.2 General particle marginal Metropolis–Hastings

In this section, we use the general PMCMC framework to derive a general PMMH algorithm. All PMMH algorithms and MH versions of the alternative EHMM methods can then be seen as special cases of this general scheme as shown in Appendix A. As with the standard PMMH, we may use an MH algorithm to target the extended distribution \( \tilde{\pi}(\theta, z_{1:T}, b_{1:T}) \) using a proposal of the form

\[
q(\theta', \theta) \times \frac{\psi_{\theta}(z_{1:T})}{\text{law of general PF}} \times \frac{q_{\theta}(b_{1:T}|z_{1:T})}{\text{path selection}}.
\]

where we have defined the selection probability

\[
q_{\theta}(b_{1:T}|z_{1:T}) := \frac{\psi_{\theta}(b_{1:T})}{\sum_{i=1}^{N} \psi_{\theta}(b_{1:T})}.
\]

Define the usual unbiased estimate of the marginal likelihood

\[
\hat{p}_{\theta}(y_{1:T}) := \sum_{i=1}^{N} \tilde{v}_{\theta, t}^i.
\]

Then we obtain the following general PMMH algorithm (Algorithm 1) the validity of which can be established by checking that indeed,

\[
\frac{\tilde{\pi}(\theta, z_{1:T}, b_{1:T})}{\psi_{\theta}(z_{1:T}) q_{\theta}(b_{1:T}|z_{1:T})} = \frac{p(\theta|y_{1:T}) \hat{p}_{\theta}(y_{1:T})}{p(\theta|y_{1:T}) \hat{p}_{\theta}(y_{1:T})}
\]

**Algorithm 1 (general PMMH algorithm).** Given \((\theta, z_{1:T}, b_{1:T}) \sim \tilde{\pi}(\theta, z_{1:T}, b_{1:T})\) with associated likelihood estimate \(\hat{p}_{\theta}(y_{1:T})\).

1. Propose \(\theta' \sim q(\theta, \theta')\), \(z'_{1:T} \sim \psi_{\theta'}(z'_{1:T})\) and \(b'_{1:T} \sim q_{\theta'}(b'_{1:T}|z'_{1:T})\).
2. Compute likelihood estimate \(\hat{p}_{\theta'}(y_{1:T})\) based on \(z'_{1:T}\).
3. Set \((\theta, z_{1:T}, b_{1:T}) \leftarrow (\theta', z'_{1:T}, b'_{1:T})\) w.p. 1 \(\frac{\hat{p}_{\theta'}(y_{1:T}) q(\theta', \theta)}{\hat{p}_{\theta}(y_{1:T}) q(\theta, \theta')}\).

### 6.3 General particle Gibbs samplers

In this section, we use the general PMCMC framework to derive a general PG sampler. We also derive backward sampling (BS) (Whiteley [2010]) and ancestor sampling (AS) (Lindsten et al. [2014]) recursions and prove that they leave the target distribution of interest invariant. As before, all PG samplers and Gibbs
versions of the alternative EHHM method can then be seen as special cases of this general scheme as shown in Appendix A. Set
\[ \gamma_\theta(x_{t+1:T} | x_{1:t}) := \frac{\gamma_{\theta, T}(x_{1:T})}{\gamma_{\theta, t}(x_{1:t})}. \]
We are then ready to state both (general) PG samplers. For the remainder of this section, we let \( \tilde{x}_{1:t} \) denote the \( i \)th particle lineage at time \( t \), i.e. \( \tilde{x}_{1:t} = x_{1:t}^{i} \), where \( i_t = i \) and \( i_n = a_n^{b_{n+1}} \), for \( n = t - 1, \ldots, 1 \).

**Algorithm 2 (general PG sampler with BS).** Given \((\theta, x_{1:T}) \sim \pi\), obtain \((\theta', x'_{1:T}) \sim \pi\) as follows.
1. Sample \( \theta' \) via some \( \pi(\cdot | x_{1:T}) \)-invariant MCMC kernel.
2. For \( t = 1, \ldots, T \), perform the following steps.
   (a) If \( t = 1 \), sample \( b_1 \) uniformly on \( \{1, \ldots, N\} \), set \( x_1^{b_1} := x_1 \) and sample \( z_1^{-b_1} \sim \pi_{\theta', 1}^{-b_1}(z_1^{-b_1} | x_1^{b_1}) \).
   (b) If \( t > 1 \), sample \( b_t \) uniformly on \( \{1, \ldots, N\} \), set \( x_t^{b_t} := x_t \), \( a_{t-1}^{b_t} := b_{t-1} \) and sample \( z_t^{-b_t} \sim \pi_{\theta', t}^{-b_t}(z_t^{-b_t} | z_{1:t-1}, x_t^{b_t}) \).
3. Sample \( b_T \sim \pi_{\theta', T}(b_T | z_{1:T}) \) and for \( t = T - 1, \ldots, 1 \), set \( b_t = i \) w.p. proportional to \( \tilde{v}_{\theta', t}^{-b_t} \gamma_{\theta}(x_{t+1:T} | x_{1:t}^{i}) \).
4. Set \( x'_{1:T} := x_{1:T}^{b_T} \).

**Algorithm 3 (general PG sampler with AS).** Given \((\theta, x_{1:T}) \sim \pi\), obtain \((\theta', x'_{1:T}) \sim \pi\) as follows.
1. Sample \( \theta' \) via some \( \pi(\cdot | x_{1:T}) \)-invariant MCMC kernel.
2. For \( t = 1, \ldots, T \), perform the following steps.
   (a) If \( t = 1 \), sample \( b_1 \) uniformly on \( \{1, \ldots, N\} \), set \( x_1^{b_1} := x_1 \) and sample \( z_1^{-b_1} \sim \pi_{\theta, 1}^{-b_1}(z_1^{-b_1} | x_1^{b_1}) \).
   (b) If \( t > 1 \), sample \( b_t \) uniformly on \( \{1, \ldots, N\} \), set \( x_t^{b_t} := x_t \), \( a_{t-1}^{b_t} := i \) w.p. proportional to \( \tilde{v}_{\theta, t-1}^{-b_t} \gamma_{\theta}(x_{1:T}^{b_t} | x_{1:t-1}^{i}) \), obtain \((\theta, x_{1:T}^{b_t}) \) and sample \( z_t^{-b_t} \sim \pi_{\theta, t}^{-b_t}(z_t^{-b_t} | z_{1:t-1}^{i}, x_t^{b_t}) \).
3. Sample \( b_T \sim \pi_{\theta, T}(b_T | z_{1:T}) \) and for \( t = T - 1, \ldots, 1 \), set \( b_t = a_{t+1}^{b_{t+1}} \).
4. Set \( x'_{1:T} := x_{1:T}^{b_T} \).

As in previous sections, the BS recursion in Algorithm 2 may be justified via appropriate partially-collapsed Gibbs sampler arguments by noting that
\[ \tilde{\pi}(b_t | \theta, z_{1:t}, x_{1:T}^{b_{t+1}}) \propto \tilde{v}_{\theta, t}^{b_t} \gamma_{\theta}(x_{t+1:T}^{b_t} | x_{1:t}^{b_t}). \]
The AS steps in Algorithm 3 follow similarly since \( a_{t+1}^{b_{t+1}} = b_t \), by construction.

Alternatively – without invoking partially-collapsed Gibbs sampler arguments – the validity of BS can be established by even further extending the space to include the new particle indices generated via BS. As shown in Finke (2015, Chapter 3.4.3), this construction also proves a particular duality of BS and AS.

### 7 Empirical study

In this section, we empirically compare the performance of some of the algorithms described in this work on a \( d \)-dimensional linear-Gaussian state-space model.

#### 7.1 Model

The model considered throughout this section is given by
\[
\begin{align*}
\mu_{\theta}(x_1) & = \text{Normal}(x_1; m_0, C_0), \\
f_{\theta}(x_t | x_{t-1}) & = \text{Normal}(x_t; Ax_{t-1}, \sigma^2 I_d), \quad \text{for } t > 1, \\
g_{\theta}(y_t | x_t) & = \text{Normal}(y_t; x_t, \tau^2 I_d), \quad \text{for } t \geq 1,
\end{align*}
\]
where \( x_1, y_t \in \mathbb{R}^d \), \( \sigma, \tau > 0 \), \( I_d \) denotes the \((d, d)\)-dimensional identity matrix and \( A \) is the \((d, d)\)-dimensional symmetric banded matrix with upper and lower bandwidth 1, with entries \( a_0 \in \mathbb{R} \) on the main diagonal, and with entries \( a_1 \in \mathbb{R} \) on the remaining bands, i.e.

\[
A = \begin{bmatrix}
a_0 & a_1 & 0 & \ldots & 0 \\
a_1 & a_0 & a_1 & \ddots & \vdots \\
0 & a_1 & \ddots & \ddots & 0 \\
\vdots & \ddots & \ddots & \ddots & 0 \\
0 & \ldots & 0 & a_1 & a_0
\end{bmatrix}
\]

For simplicity, we assume that the initial mean \( m_0 := \mathbf{0}_d \in \mathbb{R}^d \) (where \( \mathbf{0}_d \) denotes a vector of zeros of length \( d \)) and the initial \((d, d)\)-dimensional covariance matrix \( C_0 = I_d \) are known. Thus, the task is to approximate the posterior distribution of the remaining parameters \( \theta := (a_0, a_1, \sigma, \tau) \). The true values of these parameters, i.e. the values used for simulating the data are \((0.5, 0.2, 1, 1)\). As prior distributions, we take uniform distributions on \((-1, 1)\) for \( a_0 \) and \( a_1 \) and inverse-gamma distributions on \( \sigma \) and \( \tau \) each with shape parameter 1 and scale parameter 0.5. All parameters are assumed to be independent a priori. In all algorithms, we propose new values \( \theta' \) for \( \theta \) via a simple Gaussian random-walk kernel, i.e. we use \( q(\theta; \theta') := \text{Normal}(\theta'; \theta, (100d_0dT)^{-1}I_{d_0}) \), where \( d_0 \) is the dimension of the parameter vector \( \theta \), i.e. \( d_0 = 4 \).

7.2 Algorithms

In this subsection, we detail the specific algorithms whose empirical performance we compare in our simulation study.

**Standard PMCMC** We implement the (bootstrap) PF and the FA-APF using multinomial resampling at every step. Though we note that more sophisticated resampling schemes, e.g. adaptive systematic resampling, could easily be employed. As described above, we can implement both MH algorithms (i.e. the PMMH) and Gibbs samplers based around these standard PFs. For the latter, we make use of AS in the conditional PFs.

**Original EHMM** We implement the algorithms with \( \rho_{\theta,t}(x) = \text{Normal}(x; \mu, \Sigma) \), where \( \mu \) and \( \Sigma \) represent the mean and covariance matrix associated with the stationary distribution of the latent Markov chain \((X_t)_{t \in \mathbb{N}}\).

We compare two different options for constructing the kernels \( R_{\theta,t} \) which leave this distribution invariant.

(I) The kernel \( R_{\theta,t} \) generates independent and identically distributed (IID) samples from its invariant distribution, i.e. \( R_{\theta,t}(x_t'|x_t) = \rho_{\theta,t}(x_t') \).

(II) The kernel \( R_{\theta,t} \) is a standard MH kernel which proposes a value \( x_t^* \) using the Gaussian random-walk proposal \( \text{Normal}(x_t^*; x_t, d^{-1}I_d) \).

**Alternative EHMM** We compare four different versions of the MCMC PF and MCMC FA-APF methods outlined above. Again, we implement both MH algorithms and Gibbs samplers (with AS) based around these methods. Below, we describe the specific versions which we are comparing. The kernels \( R_{\theta,t}(\cdot; x_{t-1}) \) employed in the MCMC PF and the kernels \( R_{\theta,t}(\cdot; x_{t-1}) \) employed in the MCMC FA-APF are all taken to be MH kernels which, given \((x_t, a_{t-1})\), propose a new value \((x_t^*, a_{t-1}^*)\) using a proposal of the following form

\[
\frac{a_{t-1}^*}{\sum_{i=1}^N v_{\theta,t-1}^i} s_{\theta,t}(x_t^*; x_t; x_{t-1}, a_{t-1}^*).
\]

We compare two different approaches for generating a new value for the particle, \( x_t^* \).

(I) The first proposal uses a simple Gaussian random-walk kernel, i.e.

\[
s_{\theta,t}(x_t^*; x_t; x_{t-1}, a_{t-1}^*) = \text{Normal}(x_t^*; x_t, d^{-1}I_d),
\]

where the scaling of the covariance matrix is motivated by existing results on optimal scaling for such random-walk proposal kernels \cite{gelman96, roberts97}.

(II) The second proposal uses the *autoregressive* proposal employed by Shestopaloff and Neal \citeyear{shresthal16}, i.e.

\[
s_{\theta,t}(x_t^*; x_t; x_{t-1}, a_{t-1}^*) = \text{Normal}(x_t^*; \mu + \sqrt{1 - \varepsilon^2}(x_t - \mu), \varepsilon^2 \Sigma),
\]

where \( \mu \) and \( \Sigma \) denote the mean and covariance matrix of \( f_{\theta}(x_t|x_{t-1}) = \text{Normal}(x_t; \mu, \Sigma) \), i.e. \( \Sigma = \sigma^2 I \) and \( \mu = Ax_{t-1} \). To scale the covariance matrix of this proposal with the dimension \( d \), we set \( \varepsilon := \sqrt{d^{-1}} \).
Idealised. We also implement the algorithms which the above-mentioned algorithms seek to mimic. The idealised Gibbs sampler, is a (Metropolis-within-)Gibbs algorithm which updates the latent states $x_{1:T}$ as one block by sampling them from their full conditional posterior distribution. The idealised marginal MH algorithm analytically evaluates the marginal likelihood $p_\theta(y_{1:T})$ via the Kalman filter.

### 7.3 Results for general PMMH algorithms

In this subsection, we empirically compare the performance of various PMMH type samplers. First, we fix $\theta$ in order to assess the variability of the estimates of the marginal likelihood, $\hat{p}_\theta(y_{1:T})$, which is a key ingredient in (general) PMMH algorithms. Then, we perform inference about $\theta$.

Recall that in order to implement the MH version of the MCMC FA-APF we need to sample at least one particle from $p_\theta(x_t| x_{t-1}, y_t)$ at each time $t$ and we need to be able to evaluate the function $x_{t-1} \mapsto p_\theta(y_t|x_{t-1})$. In other words, whenever we can implement this algorithm we can also implement a standard PMMH algorithm based around the FA-APF.

Figure 2 shows the relative estimates of the marginal likelihood obtained from the various algorithms described in this work for various model dimensions. Unsurprisingly, the PF resp. FA-APF provides lower variance estimates than its corresponding MCMC PF resp. MCMC FA-APF counterparts. However, more interestingly, the MCMC FA-APF can provide lower variance estimates than the standard PF and could prove useful in more realistic scenarios where it is computationally very expensive to run the FA-APF. As expected, the original EHMM method described in Section 3 breaks down very quickly as the dimension $d$ increases.

![Figure 2: Relative estimates of the marginal likelihood $p_\theta(y_{1:T})$. Based on 1000 independent runs of each algorithm (and writing $\hat{p}_\theta(y_{1:T}) = \tilde{p}_\theta(y_{1:T})$ in the case of the original EHMM method) with each run using a different data sequence of length $T = 10$ simulated from the model. The number of particles was $N = 1000$ for the $O(N)$ methods and $N = 100$ for the $O(N^2)$ methods.](image)

$a$: $d = 2$.  
$b$: $d = 5$.  
$c$: $d = 10$.  
$d$: $d = 25$.  

The right panel of Figure 3 shows kernel-density plots of the estimates of parameter $a_0$ obtained from various PMMH-type algorithms. Clearly, the PMMH-type algorithms based around the (bootstrap) PF or the MCMC PF were unable to obtain sensible parameter estimates within the number of iterations that we fixed. The left panel of Figure 3 shows the corresponding empirical autocorrelation. The results are consistent with the efficiency of the likelihood estimates illustrated in Figure 2. That is, at least in this setting, the standard MH version of the alternative EHMM method does not outperform standard PMMH algorithms. The estimates of the other parameters behaved similarly and the results for $(a_1, \sigma, \tau)$ are therefore omitted.
Figure 3: Autocorrelation (left panel) and kernel-density estimate (right panel) of the estimates of Parameter $a_0$ for model dimension $d = 25$ and with $T = 10$ observations. Obtained from $10^6$ iterations (of which the initial 10% were discarded as burn-in) of standard PMMH algorithms and MH versions of the alternative EHMM method using $N = 1000$ particles. The autocorrelations shown on the r.h.s. are averages over four independent runs of each algorithm. Note: the PMMH algorithms based on the (bootstrap) PF and based on the MCMC PF failed to yield meaningful approximations of the posterior distribution and the corresponding kernel-density estimates are therefore suppressed.

7.4 Results for general particle Gibbs samplers

In this subsection, we compare empirically the performance of various PG type samplers (all using AS). Gibbs samplers based on the original EHMM method failed to yield meaningful estimates for the model dimensions considered in this subsection and at a similar computational cost as the other algorithms. We therefore do not show results for the original EHMM method in the figures below.

Recall that in order to implement the conditional MCMC FA-APF, we do not need to sample from $p_\theta(x_t|x_{t-1}, y_t)$ nor evaluate the function $x_{t-1} \mapsto p_\theta(y_t|x_{t-1})$. In other words, we can implement the conditional MCMC FA-APF in many situations in which implementing a standard conditional FA-APF is impossible.

Figure 4 shows the autocorrelation of estimates of the first component of $x_1$ obtained from various PG samplers for model dimension $d = 100$. For the moment, we have kept $\theta$ fixed to the true values. It appears that in high dimensions, the conditional PFs with MCMC moves are able to outperform standard conditional PFs. Note that although, unsurprisingly, the best performance is obtained with the MCMC FA-APF, the simpler MCMC PF is able to substantially outperform the approach based upon a standard PF. This is supported by Figure 5 which shows that the conditional PFs with MCMC moves lead to a higher estimated effective sample size (ESS) in this setting. The acceptance rates associated with the MH kernels are shown in Figure 6.

Figure 4: Autocorrelation (left panel) and kernel-density estimate (right panel) of the estimates of the first component of $x_1$ for the state-space model in dimension $d = 100$ with $T = 10$ observations. Obtained from three independent runs of each of the various Gibbs samplers comprising $500000$ iterations (of which the initial 10% were discarded as burn-in) and using $N = 100$ particles. Here, $\theta$ was fixed to the true parameters throughout each run. The autocorrelations shown on the r.h.s. are averages over the three independent runs of each algorithm. Note: the conditional (bootstrap) PF almost never managed to update the states: the corresponding kernel-density estimates were therefore not meaningful and are hence suppressed.
Figure 5: Average ESS for the same setting and colour-coding as in Figure 4. The results are averaged over three independent runs of each algorithm. It is worth noting that the ESS does not take the autocorrelation of the state-estimates (over iterations of the (particle) PMCMC chain) into account and so may flatter MCMC PFs to an extent but does illustrate the lessening of weight degeneracy within the particle set which they achieve.

Figure 6: Average acceptance rates for the MH kernels $\bar{R}_{\theta,t}(\cdot|\cdot;x_{t-1})$ and $R_{\theta,t}(\cdot|\cdot;x_{t-1})$ for same setting and colour-coding as in Figure 4. Note that standard PFs can always be interpreted as using a MH kernel that proposes IID samples from its invariant distribution so that the acceptance rate is always 1 in this case. Again the acceptance rates are averaged over three independent runs of each algorithm.

We conclude this section by showing (in Figure 7) simulation results for the estimates of Parameter $a_0$ obtained from the various PG samplers. The MH kernel which updates $\theta$ was employed 100 times per iteration, i.e. 100 times between each conditional PF update of the latent states as the former is relatively computationally cheap compared to the latter.

Note that as indicated by the kernel-density estimates in the right panel of Figure 7 the Gibbs sampler based around the PF did not manage to sufficiently explore the support of the posterior distribution within the number of iterations that we fixed. This lack of convergence also caused the comparatively low empirical autocorrelation of the PG chains based around the (bootstrap) PF in the left panel of Figure 7 as the chain did not sufficiently traverse support of the target distribution – due to poor mixing of the state-updates as illustrated in Figure 4 – the empirical autocorrelation shown in Figure 7 is a poor estimate of the (theoretical) autocorrelation of the chain. More specifically, the former greatly underestimates the latter.

The estimates of the other parameters behaved similarly and the results for $(a_1, \sigma, \tau)$ are therefore omitted.
Figure 7: Autocorrelation (left panel) and kernel-density estimate (right panel) of the estimates of Parameter $a_0$ for $T = 10$ observations. Obtained one run of the various Gibbs samplers comprising $10^6$ iterations (of which the initial 10% were discarded as burn-in) and using $N = 100$ particles. The autocorrelations shown on the l.h.s. are averages over the two independent runs of each algorithm.

### 8 Discussion

In this work, we have discussed the connections between the particle Markov chain Monte Carlo (PMCMC) and embedded hidden Markov models (EHMM) methodologies and have obtained novel Bayesian inference algorithms for state and parameter estimation in state-space models. We have compared the empirical performance of the various PMCMC and EHMM algorithms on a simple high-dimensional state-space model. We have found that a properly tuned conditional particle filter (PF) which employs local Metropolis–Hastings moves proposed in Shestopaloff and Neal (2016) can dramatically outperform the standard conditional PFs in high dimensions. Additionally, by formally establishing that PMCMC and the (alternative) EHMM methods can be viewed as a special case of a general PMCMC framework, we have derived both backward sampling and ancestor sampling for this general framework. This provides a promising strategy for extending the range of applicability of particle Gibbs algorithms as well as providing a novel class of PFs which might be useful.

There are numerous other potential extensions of these ideas. For instance, many existing extensions of standard PMCMC methods could also be considered for the alternative EHMM methods, e.g. incorporating gradient-information into the parameter proposals $q(\theta, \theta')$ or exploiting correlated pseudo-marginal ideas (Deligiannidis et al., 2015). Clearly, further generalisation of the target distribution and associated algorithms introduced here are possible. Many other processes for simulating from an extended target admitting a single random trajectory with the correct marginal distribution are possible, e.g. along the lines of Lindsten et al. (2016).

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A Special cases of the general PMCMC algorithm

In this appendix, we show that all PMCMC and alternative EHMM methods described this work can be recovered as special cases of the general PMCMC framework from Section 6. For completeness, we explicitly derive all algorithms as special cases of the general framework even though PMCMC methods based around the (bootstrap) PF and FA-APF were already shown to be special cases of PMCMC methods based around the general APF and even though, alternative EHMM methods based around the MCMC PF and MCMC APF were already shown to be special cases of alternative EHMM methods based around the MCMC APF.

(Bootstrap) PF In this case, \( \psi_0,1(z_t) = \prod_{i=1}^{N} \mu_0(x_t^i) = \prod_{i=1}^{N} \rho_0,1(x_t^i) \), and, for \( t > 1 \),

\[
\psi_0,t(z_t|z_{1:t-1}) = \prod_{i=1}^{N} \frac{q_0(y_{t-1}^i|x_{t-1}^i)}{\sum_{j=1}^{N} q_0(y_{t-1}^i|x_{t-1}^i)} f_0(x_t^i|\alpha_{t-1}^i) = \prod_{i=1}^{N} \rho_0,t(x_t^i, a_{t-1}^i|x_{t-1}^i),
\]

while \( \gamma_0,t(x_t, t) := \rho_0(x_{1:t}, y_{1:t}), \) for any \( t \leq T \). This implies that \( \tilde{v}_0,t = \frac{1}{N} \sum_{i=1}^{N} \rho_0(y_t^i|x_t^i) \prod_{j=t-1}^{T-1} \frac{1}{N} \sum_{i=1}^{N} q_0(y_{t-1}^i|x_{t-1}^i) \), so that we obtain \( q_0(i|z_{1:T}) = g_0(y_T|x_T^i) / \sum_{i=1}^{N} g_0(y_T|x_T^i) \) and \( \tilde{p}_0(y_{1:T}) = \prod_{t=1}^{T} \frac{1}{N} \sum_{i=1}^{N} \rho_0(y_t^i|x_t^i) \), as stated in Section 2.

FA-APF In this case, \( \psi_0,1(z_t) = \prod_{i=1}^{N} \rho_0(x_t^i|y_t) = \prod_{i=1}^{N} \rho_{0,1}(x_t^i) \), and, for \( t > 1 \),

\[
\psi_0,t(z_t|z_{1:t-1}) = \prod_{i=1}^{N} \frac{q_0(y_{t-1}^i|x_{t-1}^i)}{\sum_{j=1}^{N} q_0(y_{t-1}^i|x_{t-1}^i)} \rho_0(x_t^i|a_{t-1}^i, y_t) = \prod_{i=1}^{N} \rho_{0,t}(x_t^i, a_{t-1}^i|x_{t-1}^i),
\]

while \( \gamma_0,t(x_t, t) := \rho_0(x_{1:t}, y_{1:t}) \rho_0(y_{1:t-1}|x_{t-1}) \), for \( t < T \), and \( \gamma_0,0(x_{1:T}) := \rho_0(x_{1:T}, y_{1:T}) \). This implies that \( \tilde{v}_0,t = \frac{1}{N} \sum_{i=1}^{N} \rho_0(y_t^i|x_t^i) \prod_{j=t-1}^{T-1} \frac{1}{N} \sum_{i=1}^{N} \rho_0(y_{t-1}^i|x_{t-1}^i) \), so that we obtain the selection probability \( q_0(i|z_{1:T}) = 1/N \) and the marginal-likelihood estimate \( \tilde{p}_0(y_{1:T}) = \prod_{t=1}^{T} \rho_0(y_t) / \sum_{i=1}^{N} \rho_0(y_t|x_t^i) \), as stated in Section 2.

General APF In this case, \( \psi_0,1(z_t) = \prod_{i=1}^{N} q_{0,1}(x_t^i) = \prod_{i=1}^{N} \rho_{0,1}(x_t^i) \), and, for \( t > 1 \),

\[
\psi_0,t(z_t|z_{1:t-1}) = \prod_{i=1}^{N} \frac{q_{0,1}(x_t^i|y_t)}{\sum_{j=1}^{N} q_{0,1}(x_t^i|y_t)} \rho_{0,t}(x_t^i, a_{t-1}^i, y_t, \theta, x_{2:t-1}, a_{t-2}) = \prod_{i=1}^{N} \rho_{0,t}(x_t^i, a_{t-1}^i|x_{t-1}^i),
\]

while \( \gamma_0,t(x_t, t) := \rho_0(x_{1:t}, y_{1:t}) \rho_0(y_{t-1}|x_{t-1}) \), for \( t < T \), and \( \gamma_0,0(x_{1:T}) := \rho_0(x_{1:T}, y_{1:T}) \). This implies that \( \tilde{v}_0,t = \frac{1}{N} \prod_{i=1}^{N} \frac{1}{N} \sum_{j=1}^{N} \rho_{0,t}(x_t^i, a_{t-1}^i, \theta, y_t, x_{2:t-1}, a_{t-2}) \), so that we obtain the selection probability \( q_0(i|z_{1:T}) = v_{t,\theta} / \sum_{j=1}^{N} v_{t,\theta} \) and the marginal-likelihood estimate \( \tilde{p}_0(y_{1:T}) = \prod_{t=1}^{T} \frac{1}{N} \sum_{i=1}^{N} \rho_{0,t}(y_t|x_t^i, \theta) \), as stated in Section 2.

MCMC PF In this case, \( \psi_0,1(z_t) = \rho_{0,1}(x_{t}^i) \prod_{i=2}^{N} R_{0,1}(x_{t}^i|x_{t-1}^i) \), and, for \( t > 1 \),

\[
\psi_0,t(z_t|z_{1:t-1}) = \rho_{0,t}(x_t^i, a_{t-1}^i|x_{t-1}^i) \prod_{i=2}^{N} R_{0,t}(x_t^i, a_{t-1}^i|x_{t-1}^i),
\]

while \( \gamma_0,t(x_t, t) \) and \( \tilde{p}_0(y_{1:T}) \) are the same as for PMCMC methods using the bootstrap PF.

MCMC FA-APF In this case, \( \psi_0,1(z_t) = \rho_{0,1}(x_{t}^i) \prod_{i=2}^{N} R_{0,1}(x_{t}^i|x_{t-1}^i) \), and, for \( t > 1 \),

\[
\psi_0,t(z_t|z_{1:t-1}) = \rho_{0,t}(x_t^i, a_{t-1}^i|x_{t-1}^i) \prod_{i=2}^{N} R_{0,t}(x_t^i, a_{t-1}^i|x_{t-1}^i),
\]

while \( \gamma_0,t(x_t, t) \) and \( \tilde{p}_0(y_{1:T}) \) are the same as for PMCMC methods using the FA-APF.
In this case, \( \psi_{\theta,1}(z_1) = \rho_{\theta,1}^{q_{\theta}}(x_1^1) \prod_{i=2}^{N} R_{\theta,1}^{q_{\theta}}(x_i^i|x_1^{i-1}) \), and, for \( t > 1 \),

\[
\psi_{\theta,t}(z_t|z_{1:t-1}) = \rho_{\theta,1}^{q_{\theta}}(x_t^1, a_{t-1}^1|x_{t-2:t-1}, a_{t-2}) \prod_{i=2}^{N} R_{\theta,1}^{q_{\theta}}(x_t^i, a_{t-1}^i|x_t^{i-1}, a_{t-1}^{i-1}, x_{t-2:t-1}, a_{t-2}),
\]

while \( \gamma_{\theta,t}(x_{1:t}) \), \( q_{\theta}(y_T|z_1:T) \) and \( \hat{p}_{\theta}(y_{1:T}) \) are the same as for PMCMC methods using the general APF.