An extended space approach for particle Markov chain Monte Carlo methods

Christopher K. Carter    Eduardo F. Mendes    Robert Kohn

July 31, 2014

Abstract

In this paper we consider fully Bayesian inference in general state space models. Existing particle Markov chain Monte Carlo (MCMC) algorithms use an augmented model that takes into account all the variable sampled in a sequential Monte Carlo algorithm. This paper describes an approach that also uses sequential Monte Carlo to construct an approximation to the state space, but generates extra states using MCMC runs at each time point. We construct an augmented model for our extended space with the marginal distribution of the sampled states matching the posterior distribution of the state vector. We show how our method may be combined with particle independent Metropolis-Hastings or particle Gibbs steps to obtain a smoothing algorithm. All the Metropolis acceptance probabilities are identical to those obtained in existing approaches, so there is no extra cost in term of Metropolis-Hastings rejections when using our approach. The number of MCMC iterates at each time point is chosen by the user and our augmented model collapses back to the model in Olsson and Ryden (2011) when the number of MCMC iterations reduces. We show empirically that our approach works well on applied examples and can outperform existing methods.

1 Introduction

Our article deals with statistical inference for non-Gaussian state space models. Its main goal is to provide flexible methods that give efficient estimates for a wide class of state space models. This work extends the methods proposed by Andrieu et al. (2010), Bunch and Godsill (2013), Lindsten and Schön (2012), Lindsten et al. (2014) and Olsson and Ryden (2011).

MCMC methods for Bayesian inference for Gaussian state space models or conditionally Gaussian state space models are well developed with algorithms to generate from the joint distribution of all the state vectors and to generate from marginal distributions with the state vectors integrated out—see, for example, Carter and Kohn (1994), Frühwirth-Schnatter (1994), Gerlach et al. (2000) and Frühwirth-Schnatter (2006). Bayesian inference for general non-Gaussian state space models has proved to be a much harder problem. MCMC approaches include single-site updating of the state vectors in Carlin et al. (1992) and block-updating of the state vectors in Shephard and Pitt (1997). These approaches apply to general models, but they can be inefficient for some cases and can require numerical approximations over high dimensional spaces. MCMC methods based on the particle filter have proved to be an attractive alternative. A class of MCMC methods involving unbiased
estimation of the likelihood was introduced by Beaumont (2003) and its theoretical properties are discussed in Andrieu and Roberts (2009).

Andrieu et al. (2010) extend these methods by constructing a joint distribution for the output of the particle filter that has a marginal distribution equal to the posterior distribution of the states in a state space model. This marginal distribution involves the states determined by tracing back the ancestors of a selected particle and is called the ancestral tracing approach by Andrieu et al. (2010). They show that previous approaches involving unbiased estimation of the likelihood correspond to Metropolis-Hastings sampling schemes under their joint distribution. The methods in Andrieu et al. (2010) can also be viewed as a fully Bayesian approach to the smoothing algorithm of Kitagawa (1996). The Andrieu et al. (2010) approach also allows other possible MCMC sampling schemes and they construct a particle Gibbs sampler which targets the same joint distribution. Lindsten et al. (2014) construct another particle Gibbs sampler for this model and give empirical evidence that their sampler improves the mixing properties of the resulting Markov chains. Dubarry and Douc (2011) give a smoothing method based on single-site MCMC updating of the generated trajectories from the ancestral tracing approach in Andrieu et al. (2010).

Olsson and Ryden (2011) extend the methods in Andrieu et al. (2010) by constructing a joint distribution on the output of the particle filter together with a series of indices corresponding to the selected states. The sampling of indices is based on the forward filtering backward simulation approach in Godsill et al. (2004) and is called the backward simulation approach in the literature. Their joint distribution also has a marginal distribution equal to the posterior distribution of the states in a state space model and their Metropolis-Hastings sampling schemes have the same acceptance probabilities as the Andrieu et al. (2010) approach. Lindsten and Schönborg (2012) constructs a particle Gibbs algorithm for the Olsson and Ryden (2011) model and gives empirical results showing improved efficiency over previous approaches. Chopin and Singh (2013) gives theoretical results showing the particle Gibbs with backward simulation in Lindsten and Schönborg (2012) has a smaller integrated autocorrelation time compared to the Andrieu et al. (2010) particle Gibbs sampler.

Bunch and Godsill (2013) give a smoothing algorithm which runs the particle filter and then uses a backwards simulation approach that involves running an MCMC at each time point. They show that the advantage of their method is that new values of the state vectors are generated during the backward simulation step, whereas many other approaches are restricted to the output of the particle filter. Fearnhead et al. (2010) give a smoothing algorithm based on combining particles from a forward filter and a backward information filter, which also generates new values of the state vectors.

Our work extends the methods in Olsson and Ryden (2011), Lindsten and Schönborg (2012) and Bunch and Godsill (2013) by using an augmented model that includes the results of the particle filter, a series of indices which correspond to starting values of an MCMC run at each time point, and the output of the MCMC runs. We construct a joint distribution for our augmented space which has a marginal distribution equal to the posterior distribution of the states in a state space model and we show that our Metropolis-Hastings sampling schemes have the same acceptance probabilities as the approaches in Andrieu et al. (2010) and Olsson and Ryden (2011). The advantage of our approach is that the MCMC runs at each time point generate new values of the state vectors, so we are not restricted to the output of the particle filter. Our method can be used to obtain generated states from the smoothing distrution or for Bayesian inference involving parameters. Our method is fully Bayesian, so the output of our MCMC convergences to the posterior distribution given suitable
regularity conditions which we discuss. We derive a particle Gibbs sampler for our augmented model.

The paper is organised as follows. Section 2 describes our state space model and sequential Monte Carlo algorithm. This section also constructs the joint distribution we use for Bayesian inference, describes the properties of this distribution, and gives our particle Gibbs algorithm. Section 3 describes our MCMC sampling schemes to carry out smoothing and Bayesian inference and discusses their convergence properties. Section 4 reports the empirical results. Proofs are given in an Appendix.

2 Generating the states

This section gives the technical results that are required for the Markov chain Monte Carlo methods described in Section 3. We describe the State Space Model, the Sequential Monte Carlo algorithm to generate the particles, and the extra Markov chain Monte Carlo steps in our method to generate the states. We then derive the properties of the distributions resulting from our algorithms. We also give a conditional sequential Monte Carlo algorithm that is used for particle Gibbs steps in Section 3. We use the standard convention where capital letters denote random variables and lower case letters denote their values.

2.1 State Space Model

Consider the state space model with states denoted by \( \{X_t : t = 1, \ldots, T\} \subset \mathcal{X}_T \) and observations denoted by \( \{Y_t : t = 1, \ldots, T\} \). We will assume the transition and observation distributions have positive densities denoted by

\[
X_1 \sim f_1(\cdot | \theta) \quad \text{and} \quad X_t | (X_{t-1} = x) \sim f_t(\cdot | x, \theta) \quad t = 2, \ldots, T \tag{2.1}
\]

\[
Y_t | (X_t = x) \sim g_t(\cdot | x, \theta) \quad t = 1, \ldots, T. \tag{2.2}
\]

All the densities are with respect to Lebesgue measure for continuous variables and counting measure for discrete valued variables unless otherwise indicated. The vector \( \theta \in \Theta \) represents parameters which are discussed in Section 3 and in the examples in Section 4. We use the following notation for sequences, \( z_{i:j} = (z_i, \ldots, z_j) \) and we denote the joint density of \( \{y_{1:T}, x_{1:T}\} \) given \( \theta \) by

\[
p(y_{1:T}, x_{1:T}|\theta) := g_1(y_1|x_1, \theta) f_1(x_1|\theta) \prod_{t=2}^{T} g_t(y_t|x_t, \theta) f_t(x_t|x_{t-1}, \theta). \tag{2.4}
\]

2.2 Sequential Monte Carlo algorithm

The Sequential Monte Carlo algorithm we use for the state space model defined by (2.1)–(2.4) at time \( t \) constructs a sample of particles denoted by \( \{X_{1:t}^i, \ldots, X_{N_t}^i\} \) with associated normalized
weights $\mathbf{W}_t = \left\{ W^1_t, \ldots, W^{N_t}_t \right\}$ that approximates the distribution $p(dx_{1:t}|y_{1:t}, \theta)$ by

$$
\tilde{p}(dx_{1:t}|y_{1:t}, \theta) := \sum_{i=1}^{N_t} W^i_t \delta_{X^i_{1:t}}(dx_{1:t}).
$$

(2.5)

In the pseudocode of the sequential Monte Carlo Algorithm 1 described below we denote the unnormalized weights at time $t$ by $\mathbf{w}_t = \left\{ w^1_t, \ldots, w^{N_t}_t \right\}$ and use the notation $\mathcal{F}(\cdot|\mathbf{p})$ for the discrete probability distribution on $\{1, \ldots, m\}$ of parameter $\mathbf{p} = (p_1, \ldots, p_m)$, with $p_i \geq 0$ and $p_1 + \ldots + p_m = 1$, for some $m \in \mathbb{N}$. Algorithm 1 uses the importance densities $M_1(x_1|y_1, \theta)$ and $M_t(x_t|y_t, x_{t-1}, \theta)$, for $t = 2, \ldots, T$. We make Assumption 1 about these importance densities for the results in later sections.

**Assumption 1** $M_1(x_1|y_1, \theta)$ and $M_t(x_t|y_t, x_{t-1}, \theta)$, for $t = 2, \ldots, T$ are finite strictly positive densities.

Algorithm 1 is based on Andrieu et al. (2010) and we include it for completeness and notational consistency. We use the convention that whenever the index $i$ is used for a particular value of $t$ we mean ‘for all $i \in \{1, \ldots, N_t\}$’.

**Algorithm 1 (Sequential Monte Carlo)**

**Step 1** For $t = 1$,

**Step 1.1** sample $X^i_1 \sim M_1(\cdot|y_1, \theta)$,

**Step 1.2** compute and normalize the weights

$$
w^i_1 = \frac{p(y_1|X^i_1, \theta) p(X^i_1|\theta)}{M_1(X^i_1|y_1, \theta)}.
$$

(2.6)

$$
W^i_1 = \frac{w^i_1}{\sum_{j=1}^{N_1} w^j_1}.
$$

**Step 2** For $t = 2, \ldots, T$,

**Step 2.1** sample $A^i_{t-1} \sim \mathcal{F}(\cdot|\mathbf{W}_{t-1})$,

**Step 2.2** sample $X^i_t \sim M_t(\cdot|y_t, X^{A^i_{t-1}}_{t-1}, \theta)$,

**Step 2.3** compute and normalize the weights

$$
w^i_t = \frac{p(y_t|X^i_t, \theta) p(X^i_t|X^{A^i_{t-1}}_{t-1}, \theta)}{M_t(X^i_t|y_t, X^{A^i_{t-1}}_{t-1}, \theta)}.
$$

(2.7)

$$
W^i_t = \frac{w^i_t}{\sum_{j=1}^{N_t} w^j_t}.
$$
The variable $A_{t-1}^i$ in the above algorithm represents the index of the parent at time $t-1$ of particle $X_{1:t}^i$. Our methods do not require the full trajectory of the states in a particle and are more concerned with the individual values $X_t^i$ for $t = 1, \ldots, T$ and $A_t^i$ for $t = 1, \ldots, T-1$. We denote the collection of states at time $t$ by $\mathbf{X}_t = \{X_t^i : i = 1, \ldots, N_t\}$ for $t = 1, \ldots, T$ and the corresponding collection of parent indices by $\mathbf{A}_t = \{A_t^i, \ldots, A_t^{N_t}\}$ for $t = 1, \ldots, T-1$. We will also use the notation for sequences $\mathbf{X}_{i:j} = (\mathbf{X}_i, \ldots, \mathbf{X}_j)$ and $\mathbf{A}_{i:j} = (\mathbf{A}_i, \ldots, \mathbf{A}_j)$.

2.3 MCMC steps to generate states

Algorithm [2] described below takes the output of the Sequential Monte Carlo steps described in Algorithm [1] and runs a backward simulation algorithm to generate extra state values. The state at time $t$ is generated using the approach in [Andrieu et al. (2010)] and the states at times $T - 1, \ldots, 1$ are generated using an approach related to that of Bunch and Godsill (2013), which, at time $t$, involves a Markov chain Monte Carlo run of length $C_t$. We denote the generated values at time $t$ by $\mathbf{X}_t = \{X_t^i : i = 1, \ldots, C_t\}$ for $t = 1, \ldots, T-1$ and use the sequence notation $\mathbf{X}_{i:j} = (\mathbf{X}_i, \ldots, \mathbf{X}_j)$.

These Markov chain Monte Carlo runs involve the following components. For $t = 1$, the target density for the Metropolis-Hasting steps is

$$p \left( x_t | y_{1:t}, x_{t+1} \right) \propto g_t \left( y_t | x_t, \theta \right) f_t \left( x_{t+1} | x_t, \theta \right),$$

so no approximation using the output from Algorithm [1] is required. For $t = 2, \ldots, T-2$, the target densities for the Metropolis-Hasting steps are

$$\tilde{p} \left( x_t | \mathbf{X}_{1:t-1}, \tilde{x}_{t+1}, \tilde{a}_{1:t-2}, \theta \right) \propto g_t \left( y_t | x_t, \theta \right) f_{t+1} \left( \tilde{x}_{t+1} | x_t, \theta \right) \sum_{i=1}^{N_{t-1}} w_{t-1}^i f_t \left( x_t | x_{t-1}^i, \theta \right), \tag{2.8}$$

which approximates

$$p \left( x_t | y_{1:t}, x_{t+1} = \tilde{x}_{t+1}, \theta \right) \propto g_t \left( y_t | x_t, \theta \right) f_{t+1} \left( \tilde{x}_{t+1} | x_t, \theta \right) \times \int p \left( x_t | y_{1:t-1}, x_{t-1}, \theta \right) p \left( x_{t-1} | y_{1:t-1}, \theta \right) dx_{t-1}$$

based on the output from Algorithm [1]. Similarly, for $t = T-1$ the target density for the Metropolis-Hasting steps is

$$\tilde{p} \left( x_{T-1} | \mathbf{X}_{1:T-2}, \tilde{x}_T^b, \tilde{a}_{1:T-3}, \theta \right) \propto g_{T-1} \left( y_{T-1} | x_{T-1}, \theta \right) f_T \left( x_T^b | x_{T-1}, \theta \right) \sum_{i=1}^{N_{T-2}} w_{T-2}^i f_{T-1} \left( x_{T-1} | x_{T-2}^i, \theta \right), \tag{2.9}$$

which approximates

$$p \left( x_{T-1} | y_{1:T-1}, X_T = x_T^b, \theta \right) \propto g_{T-1} \left( y_{T-1} | x_{T-1}, \theta \right) f_T \left( x_T^b | x_{T-1}, \theta \right) \times \int p \left( x_{T-1} | y_{1:T-2}, x_{T-2}, \theta \right) p \left( x_{T-2} | y_{1:T-2}, \theta \right) dx_{T-2}.$$

The following lemma follows immediately from the assumption that $g_t \left( y_t | x_t, \theta \right)$ and $f_t \left( x_t | x_{t-1}, \theta \right)$ are strictly positive densities for $t = 1, \ldots, T$. 


Lemma 1 The densities \( \tilde{p} \left( x_t | \mathbf{x}_{1:t-1}, \mathbf{x}^{C_{t+1}}_{t+1}, \mathbf{a}_{1:t-2}, \theta \right) \) for \( t = 2, \ldots, T-1 \) and \( \tilde{p} \left( x_{T-1} | \mathbf{x}_{1:T-2}, x^{B_T}_{T}, \mathbf{a}_{1:T-3}, \theta \right) \) are strictly positive.

We denote the MCMC transition kernels by

\[
K_t \left( x_t, dx_t | \mathbf{x}_{1:t-1}, \mathbf{x}^{-b_t}_{t}, \mathbf{x}^{C_{t+1}}_{t+1}, \mathbf{a}_{1:t-2}, \mathbf{a}^{-b_t}_{t-1}, \theta \right),
\]

for \( t = 1, \ldots, T - 2 \) and

\[
K_{T-1} \left( x_{T-1}, dx_{T-1} | \mathbf{x}_{1:T-2}, \mathbf{x}^{-b_{T-1}}_{T-1}, x^{B_T}_{T}, \mathbf{a}_{1:T-3}, \mathbf{a}^{-b_{T-1}}_{T-2}, \theta \right).
\]

The choice of Metropolis-Hastings proposal is determined by the user, but the conditioning indicated in (2.10) and (2.11) is sufficient for the results given in Sections 2.4 and 2.5. We require the standard reversibility condition of detailed balance as described in Assumption 2. Sections 3.3 and 4.1 give more detail on the transition kernels.

Assumption 2 (Detailed balance) For all \( \theta \in \Theta \)

(a)

\[
p( dx_1 | y_1, \mathbf{x}^{C_2}_{2}, \theta ) K_1 \left( x_1, dx_1 | \mathbf{x}^{-b_1}_{1}, \mathbf{x}^{C_2}_{2}, \theta \right) = p( dx'_1 | y_1, \mathbf{x}^{C_2}_{2}, \theta ) K_1 \left( x'_1, dx_1 | \mathbf{x}^{-b_1}_{1}, \mathbf{x}^{C_2}_{2}, \theta \right),
\]

(b)

\[
\tilde{p} \left( dx_t | \mathbf{x}_{1:t-1}, \mathbf{x}^{C_{t+1}}_{t+1}, \mathbf{a}_{1:t-2}, \theta \right) K_t \left( x_t, dx_t | \mathbf{x}_{1:t-1}, \mathbf{x}^{-b_t}_{t}, \mathbf{x}^{C_{t+1}}_{t+1}, \mathbf{a}_{1:t-2}, \mathbf{a}^{-b_t}_{t-1}, \theta \right)
= \tilde{p} \left( dx'_t | \mathbf{x}_{1:t-1}, \mathbf{x}^{C_{t+1}}_{t+1}, \mathbf{a}_{1:t-2}, \theta \right) K_t \left( x'_t, dx_t | \mathbf{x}_{1:t-1}, \mathbf{x}^{-b_t}_{t}, \mathbf{x}^{C_{t+1}}_{t+1}, \mathbf{a}_{1:t-2}, \mathbf{a}^{-b_t}_{t-1}, \theta \right),
\]

for \( t = 2, \ldots, T - 2 \) and

(c)

\[
\tilde{p} \left( dx_{T-1} | \mathbf{x}_{1:T-2}, x^{B_T}_{T}, \mathbf{a}_{1:T-3}, \theta \right) K_t \left( x_{T-1}, dx_{T-1} | \mathbf{x}_{1:T-2}, \mathbf{x}^{-b_{T-1}}_{T-1}, x^{B_T}_{T}, \mathbf{a}_{1:T-3}, \mathbf{a}^{-b_{T-1}}_{T-2}, \theta \right)
= \tilde{p} \left( dx'_{T-1} | \mathbf{x}_{1:T-2}, x^{B_T}_{T}, \mathbf{a}_{1:T-3}, \theta \right) K_t \left( x'_{T-1}, dx_{T-1} | \mathbf{x}_{1:T-2}, \mathbf{x}^{-b_{T-1}}_{T-1}, x^{B_T}_{T}, \mathbf{a}_{1:T-3}, \mathbf{a}^{-b_{T-1}}_{T-2}, \theta \right).
\]

Algorithm 2 generates the states using Markov chain Monte Carlo runs.

Algorithm 2 (Markov chain Monte Carlo)

**Step 1** Run the sequential Monte Carlo algorithm (Algorithm 1) to obtain \( \hat{\mathbf{x}}_{1:T} \) and \( \hat{\mathbf{a}}_{1:T-1} \).

**Step 2** For \( t = T \), sample \( B_T \sim \mathcal{F} ( \cdot | \mathbf{W}_T ) \).

**Step 3** For \( t = T - 1 \), sample \( \hat{X}^{C_{T-1}}_{T-1} \) as follows
**Step 3.1** compute and normalize the weights

\[
\tilde{w}_T^{i} = w_{T-1}^i f_T \left( X_T^{B_T} \mid X_{T-1}^i , \theta \right) \tag{2.12}
\]

\[
\tilde{W}_{T-1}^i = \frac{\tilde{w}_{T-1}^i}{\sum_{j=1}^{N_{T-1}} \tilde{w}_{T-1}^j},
\]

**Step 3.2** sample \( B_{T-1} \sim \mathcal{F} \left( \mid \tilde{W}_{T-1} \right) \),

**Step 3.3** set

\[ \tilde{X}_{T-1}^{old} = X_{T-1}^{B_{T-1}} \],

**Step 3.4** For \( j = 1, \ldots, C_{T-1} \)

**Step 3.4.1** sample

\[ \tilde{X}_{T-1}^j \sim K_{T-1} \left( \tilde{X}_{T-1}^{old}, \mathbf{X}_{1:t-2}, X_{T-1}^{B_{T-1}}, X_T^{B_T}, \mathbf{X}_1^{t-3}, \mathbf{A}_{t-2}^{B_{T-1}}, \theta \right) \],

**Step 3.4.2** set

\[ \tilde{X}_{T-1}^{old} = \tilde{X}_{T-1}^j \].

**Step 4** For \( t = T - 2, \ldots, 1 \)

**Step 4.1** compute and normalize the weights

\[
\tilde{w}_t^{i} = w_t^i f_{t+1} \left( X_{t+1}^{C_{t+1}} \mid X_t^i , \theta \right) \tag{2.13}
\]

\[
\tilde{W}_t^i = \frac{\tilde{w}_t^i}{\sum_{j=1}^{N_t} \tilde{w}_t^j},
\]

**Step 4.2** sample \( B_t \sim \mathcal{F} \left( \mid \tilde{W}_t \right) \),

**Step 4.3** set

\[ \tilde{X}_t^{old} = X_t^{B_t} \],

**Step 4.4** For \( j = 1, \ldots, C_t \)

**Step 4.4.1** sample

\[ \tilde{X}_t^j \sim K_t \left( \tilde{X}_t^{old}, \mathbf{X}_{1:t-1}, X_t^{B_t}, X_{t+1}^{C_{t+1}}, \mathbf{X}_{1:t-2}, \mathbf{A}_{t-2}^{B_{t-1}}, \theta \right) \],

**Step 4.4.2** set

\[ \tilde{X}_t^{old} = \tilde{X}_t^j \].
2.4 Distributions on the extended space

This section first gives the joint probability distribution of the variables generated by Algorithms 1 and 2 before constructing our target distribution and deriving its properties. To simplify the notation, we group the variables together as $U_{1:T} = \left( X_{1:T}, \bar{X}_{1:T-1}, B_{1:T}, \bar{X}_{1:T-1} \right)$. We denote the sample space of $U_{1:T}$ by

$$U_{1:T} = \prod_{t=1}^{T} \mathcal{X}^{N_t} \times \prod_{t=1}^{T-1} \{1, \ldots, N_t\}^{N_{i+1}} \times \prod_{t=1}^{T} \{1, \ldots, N_t\} \times \prod_{t=1}^{T-1} \mathcal{X}^{C_t},$$

and the joint distribution of $U_{1:T}$ generated by Algorithms 1 and 2 by $\Psi\left(du_{1:T}\right) = \Psi\left(dX_{1:T}, \bar{X}_{1:T-1}, b_{1:T}, d\bar{X}_{1:T-1}\right)$. Let

$$r(\bar{x}_t|w_t) := \prod_{i=1}^{N_t} \mathcal{F}(a_i^t|w_t).$$

It is straightforward to show that the distribution $\Psi\left(dX_{1:T}, \bar{X}_{1:T-1}\right)$ of the variables $X_{1:T}, \bar{X}_{1:T-1}$ generated by Algorithm 1 is

$$\Psi\left(dX_{1:T}, \bar{X}_{1:T-1}\right) = \left\{ \prod_{i=1}^{N_t} M_1\left(x_1^i|y_1, \theta\right) \right\} \prod_{t=2}^{T} \left\{ r(\bar{x}_{t-1}|w_{t-1}) \prod_{i=1}^{N_t} M_t\left(x_t^i|y_t, x_{t-1}^i, \theta\right) \right\} dX_{1:T};$$

see Andrieu et al. (2010) for details.

The conditional distribution $\Psi\left(B_{1:T}, d\bar{X}_{1:T-1}|X_{1:T}, \bar{X}_{1:T-1}\right)$ generated by Algorithm 2 is

$$\Psi\left(b_{1:T}, d\bar{X}_{1:T-1}|X_{1:T}, \bar{X}_{1:T-1}, \theta\right) = W^{b_T} T^{b_{T-1}} K_{T-1}\left(x_T^{b_T}, d\bar{x}_{T-1}^{b_{T-1}}|X_{1:T-2}, x_T^{b_T}, \bar{X}_{1:T-3}, \bar{a}_{T-2}^{b_{T-1}}, \theta\right)$$

$$\prod_{j=2}^{C_T-1} K_{T-1}\left(x_T^{j-1}, d\bar{x}_{T-1}^{j-1}|X_{1:T-2}, x_T^{j}, \bar{X}_{1:T-1}, \bar{a}_{T-2}^{b_{T-1}}, \theta\right)$$

$$\prod_{t=1}^{T-2} \left\{ W^{b_t} T^{b_t} K_t\left(x_t^{b_t}, d\bar{x}_t^{b_t}|X_{1:t-1}, x_t^{b_t}, \bar{X}_{1:t-1}, \bar{a}_{t-1}^{b_t}, \theta\right) \right\},$$

and hence the joint distribution of $\Psi\left(du_{1:T}\right)$ is the product of (2.14) and (2.15).

We now construct a joint distribution on the variable $U$ that will be the target distribution of a Markov chain Monte Carlo sampling scheme to generate a sample from the posterior distribution of the states in a state space model. To simplify the notation, define

$$\pi\left(x_{1:T}|\theta\right) := p\left(x_{1:T}|y_{1:T}, \theta\right)$$

(2.16)
as the posterior density of the states in the state space model defined by (2.1)–(2.4). The distribution we construct is

\[
\Pi \left( d\mathbf{u}_{1:T} \mid \theta \right) := \pi \left( \tilde{x}^{C_1}_1, \ldots, \tilde{x}^{C_{T-1}}_T, x^b_T \mid \theta \right) \, d\tilde{x}^{C_1}_1 \ldots d\tilde{x}^{C_{T-1}}_T \, dx^b_T \left( \frac{1}{N_T} \right)
\]

\[
\frac{\Psi (d\mathbf{x}_{1:T}, \mathbf{a}_{1:T-1} \mid \theta)}{M_1 \left( dx^b_1 \mid y_1, \theta \right) \prod_{t=2}^{T} \left\{ W_{t-1}^{a_{t-1}} \frac{d\mathbf{u}_t^{a_{t-1}}}{d\mathbf{x}_{t-1}^{a_{t-1}}} \mid \theta \right\}} \prod_{t=2}^{T} \sum_{i=1}^{N_{t-1}} w_{t-1}^i f_t \left( \frac{d\mathbf{u}_t^i}{d\mathbf{x}_{t-1}^i} \mid \theta \right)
\]

\[
\left( \frac{1}{N_{T-1}} \right) \prod_{j=2}^{C_{T-1}} K_{T-1} \left( \tilde{x}_T^j, d\tilde{x}_T^{j-1} \mid \mathbf{x}_{1:T-2}, \mathbf{x}_{T-1}^{b_{T-1}}, x^b_T, \mathbf{a}_{1:T-3}, \mathbf{a}_{T-2}^{b_{T-2}}, \theta \right)
\]

\[
K_{T-1} \left( \tilde{x}_{T-1}^j, d\tilde{x}_{T-1}^{j-1} \mid \mathbf{x}_{1:T-2}, \mathbf{x}_{T-1}^{b_{T-1}}, x^b_T, \mathbf{a}_{1:T-3}, \mathbf{a}_{T-2}^{b_{T-2}}, \theta \right)
\]

\[
\prod_{t=1}^{T-2} \left\{ \left( \frac{1}{N_t} \right) \frac{C_t}{\prod_{j=2}^{C_t} K_t \left( \tilde{x}_t^j, d\tilde{x}_t^{j-1} \mid \mathbf{x}_{1:t-1}, \mathbf{x}_{t-1}^{b_{t-1}}, \mathbf{x}_{t+1}^{C_t+1}, \mathbf{a}_{1:t-2}, \mathbf{a}_{t-1}^{b_{t-1}}, \theta \right)} \frac{d\mathbf{u}_t}{d\mathbf{x}_t} \right\}, \tag{2.17}
\]

which is well defined by Assumption \[\text{[1]}\]

The following lemma describes the properties of the distribution defined in (2.17). Its proof is given in the Appendix.

**Lemma 2** (i) The joint distribution \( \Pi (d\mathbf{u}_{1:T} \mid \theta) \) has marginal distribution

\[
\Pi \left( d\tilde{x}^{C_1}_1, \ldots, d\tilde{x}^{C_{T-1}}_T, dx^b_T, b_T \mid \theta \right) = \pi \left( \tilde{x}^{C_1}_1, \ldots, \tilde{x}^{C_{T-1}}_T, x^b_T \mid \theta \right) \, d\tilde{x}^{C_1}_1 \ldots d\tilde{x}^{C_{T-1}}_T \, dx^b_T \left( \frac{1}{N_T} \right).
\]

(ii) For all \( \theta \in \Theta \), the measures \( \Pi (\cdot \mid \theta) \) and \( \Psi (\cdot \mid \theta) \) are equivalent.

(iii) There exists a version of the density

\[
h \left( \mathbf{u}_{1:T} \mid \theta \right) = \frac{\Pi (d\mathbf{u}_{1:T} \mid \theta)}{\Psi (d\mathbf{u}_{1:T} \mid \theta)}
\]

with

\[
h \left( \mathbf{u}_{1:T} \mid \theta \right) = \frac{\prod_{t=1}^{T} \left\{ \left( \sum_{i=1}^{N_t} w_t^i \right) \frac{1}{N_t} \right\} \, d\mathbf{u}_t}{p (y_{1:T} \mid \theta)} \tag{2.18}
\]

**Lemma 3** shows how to generate a sample from the distribution

\[
\Pi \left( b_{1:T}, \tilde{\mathbf{x}}_{1:T-1} \mid \mathbf{x}_{1:T}, \mathbf{a}_{1:T-1}, \theta \right). \tag{2.19}
\]

Its proof is given in the appendix.
Lemma 3
\[ \Pi (b_{1:T}, \bar{x}_{1:T-1}, \bar{a}_{1:T-1}, \theta) = \Psi (b_{1:T}, \bar{x}_{1:T-1}, \bar{a}_{1:T-1}, \theta), \]
and hence Algorithm 2 generates a sample from the distribution given in (2.19).

2.5 Conditional sequential Monte Carlo

This section gives a conditional sequential Monte Carlo algorithm that is used to construct a particle
Gibbs step later in the paper. We first describe the algorithm and derive its properties. Section 3
shows how to use it in Markov chain Monte Carlo sampling schemes.

Algorithm 3 generates from the conditional distribution
\[ \Pi \left( d_{1:T-1}, d_{x_{-b_{T}}}^{T}, \bar{a}_{1:T-1}, b_{1:T-1}, d_{x_{-b_{T}}}^{T}, \bar{a}_{1:T-1}, x_{1:T-1}, \bar{x}_{1:T-1}, \bar{a}_{1:T-1}, \theta \right). \quad (2.20) \]

Algorithm 3 (Particle Gibbs)

Step 1 For \( t = 1, \ldots, T - 1 \)

Step 1.1 generate \( B_t \sim \text{Uniform } \{1, \ldots, N_t\} \),
Step 1.2 generate \( A_{t-B_t}^t \) and \( X_{t-B_t}^t \) using the Sequential Monte Carlo Algorithm 1,
Step 1.3 set \( \bar{X}_t^{old} = \bar{x}_t^C \),
Step 1.4 for \( j = C_t - 1, \ldots, 1 \)

Step 1.4.1 generate \( \bar{X}_j^t \) from
\[ K_t \left( \bar{X}_t^{old}, \bar{x}_1:t-1, X_{t-B_t}^{t}, \bar{x}_{t+1}^{C_{t+1}}, \bar{a}_{1:t-2}, A_{t-1}^{B_t}, \theta \right), \]
Step 1.4.2 set \( \bar{X}_j^{old} = \bar{X}_j^t \),
Step 1.5 generate \( X_{t}^{B_t} \) from
\[ K_t \left( \bar{X}_t^{old}, \bar{x}_1:t-1, X_{t}^{B_t}, \bar{x}_{t+1}^{C_{t+1}}, \bar{a}_{1:t-2}, A_{t-1}^{B_t}, \theta \right), \]
Step 1.6 if \( t > 1 \) then generate \( A_{t-1}^{B_t} \) as follows

Step 1.6.1 compute and normalize the weights
\[ v_{t-1}^i = w_{t-1}^i f_t \left( X_{t}^{B_t} | X_{t-1}^{i}, \theta \right), \]
\[ V_{t-1}^i = \frac{v_{t-1}^i}{\sum_{j=1}^{N_{t-1}} v_{t}^j}, \]
Step 1.6.2 generate \( A_{t-1}^{B_t} \sim \mathcal{F} (\cdot | V_{t-1}) \).
Step 2 For $t = T$, generate $A^B_{T-1}$ as follows

**Step 2.1** compute and normalize the weights

$$v^i_{T-1} = w^i_{T-1} f_T \left( X^B_T | X^i_{T-1}, \theta \right)$$

$$V^i_{T-1} = \frac{v^i_{T-1}}{\sum_{j=1}^{N_T} v^j_{T-1}}$$

**Step 2.2** generate $A^B_{T-1} \sim F(\cdot | V_{T-1})$.

Step 3 For $t = T$, generate $A^{-B}_{T-1}$ and $X^{-B}_T$ using the Sequential Monte Carlo Algorithm 1.

Lemma 4 gives the properties of the algorithm described above. Its proof is given in the Appendix.

**Lemma 4** Algorithm 3 generates a sample from the distribution given in (2.20).

## 3 Estimation for State Space Models

This section shows how to use the algorithms and distributions in Section 2 to carry out smoothing and inference for state space models. We first consider the smoothing case and then consider several approaches to parameter estimation. We also consider ergodicity results for the methods.

### 3.1 Smoothing approaches

The simplest application of the results in Section 2 is the smoothing problem where the parameter $\theta$ is regarded as fixed and known and we wish to generate a sample from the density $\pi(x_{1:T} | \theta)$ defined in (2.16). There are several possible smoothing approaches. We first describe a particle independent Metropolis-Hastings approach using the following sampling scheme that describes one sweep of a Markov chain Monte Carlo algorithm.

**Sampling Scheme 1 (PMMH Smoothing)** Given $U_{1:T}$ and $\theta$

**Step 1** Sample $U'_{1:T} \sim \Psi(\cdot | \theta)$ using Algorithms 1 and 2.

**Step 2** Accept $U'_{1:T}$ with probability

$$\min \left[ 1, \frac{\prod_{t=1}^{T} \left\{ \sum_{i=1}^{N_t} \left( w^i_t \right)^{N_t} \right\}}{\prod_{t=1}^{T} \left\{ \sum_{i=1}^{N_t} w^i_t \right\}} \right]. \tag{3.1}$$

**Remark 1** The acceptance probability (3.1) only requires the output from Algorithm 1 so it is possible to run Algorithm 1 in Step 1 and only run Algorithm 2 if the Metropolis-Hasting proposal is accepted in Step 2.
Remark 2 The acceptance probability (3.1) is the same expression as obtained for the particle independent Metropolis-Hasting methods described in Andrieu et al. (2010) and Olsson and Ryden (2011). The advantage of our method is that Algorithm 2 generates new values of the states that are not restricted to the values from the sequential Monte Carlo output from Algorithm 1.

It is also possible to use a particle Gibbs sampler to generate a sample from the density $\pi(x_{1:T|}\theta)$. We use the following sampling scheme that describes one sweep of a Markov chain Monte Carlo algorithm.

Sampling Scheme 2 (Particle Gibbs Smoothing) Given $\tilde{X}_1^{C_1}, \ldots, \tilde{X}_{T-1}^{C_{T-1}}, X_T^{B_T}, B_T, \theta$

Step 1 Run the particle Gibbs Algorithm 3 to sample $X_1^{T-1}, X_T^{B_T}, A_1^{T-1}, \tilde{X}_1^{C_1}, \ldots, \tilde{X}_{T-1}^{C_{T-1}}$ from $\Pi \{dX_1^{T-1}, dX_T^{B_T}, A_1^{T-1}, d\tilde{X}_1^{C_1}, \ldots, d\tilde{X}_{T-1}^{C_{T-1}} | \tilde{X}_1^{C_1}, \ldots, \tilde{X}_{T-1}^{C_{T-1}}, X_T^{B_T}, B_T, \theta \}$.

Step 2 Sample $B_1^{T}, \tilde{X}_1^{T-1}$ from $\Pi \left( B_1^{T}, d\tilde{X}_1^{T-1} | X_1^{T}, A_1^{T-1}, \theta \right)$, using Algorithm 2.

The potential advantage of Sampling Scheme 2 is that it is a Gibbs sampler and hence avoids the inefficiency involved in rejecting proposed moves. A potential disadvantage of Sampling Scheme 2 is that it is computationally more expensive than Sampling Scheme 1.

Remark 3 A random scan version of Sampling Scheme 2 may be more efficient since Step 1 can be sampled with low probability to avoid the computational cost of running the particle Gibbs Algorithm 3 for each iterate.

3.2 Inference using general sampling schemes

This section considers full Bayesian inference where both the auxiliary variables and the parameters are generated. There are three possible approaches to generating the parameters: particle Marginal Metropolis-Hasting, particle Gibbs and particle Metropolis within Gibbs steps. We illustrate the method with an example where the parameters are partitioned into $p$ components $\theta = (\theta_1, \ldots, \theta_p)$, where each component may be a vector. Let $\Theta = \Theta_1 \times \ldots \times \Theta_p$ be the corresponding partition of the parameter space. We will use the notation $\theta_{-i} = (\theta_1, \ldots, \theta_{i-1}, \theta_{i+1}, \ldots, \theta_p)$.

We denote the prior density for $\theta$ by $p(\theta)$ and the posterior density by $\pi(\theta)$ and we assume that both densities are strictly positive.
Let $0 \leq p_1 \leq p$. The following sampling scheme generates the parameters $\theta_1, \ldots, \theta_p$ using particle Marginal Metropolis-Hasting steps and the parameters $\theta_{p_1+1}, \ldots, \theta_p$ using particle Gibbs or particle Metropolis within Gibbs steps. We call this a general sampler as described in Mendes et al. (2014).

**Sampling Scheme 3**

Given $U_{1:T}$ and $\theta$

**Part 1 (PMMH sampling)** For $i = 1, \ldots, p_1$

Step $i$:

(a) sample

$$\theta'_i \sim q_i(\cdot | U_{1:T}, \theta_{-i}, \theta_i)$$

(b) sample

$$U'_{i:T} \sim \Psi(\cdot | \theta_{-i}, \theta'_i)$$

using Algorithms 1 and 2.

(c) accept $U'_{1:T}, \theta'_i$ with probability equal to

$$
1 \wedge \frac{\prod_{t=1}^{T} \left\{ \sum_{i=1}^{N_t} (w_i)' \right\} p(\theta'_i | \theta_{-i}) q_i(\theta_i | U'_{1:T}, \theta_{-i}, \theta'_i)}{\prod_{t=1}^{T} \left\{ \sum_{i=1}^{N_t} w_i \right\} p(\theta_i | \theta_{-i}) q_i(\theta'_i | U_{1:T}, \theta_{-i}, \theta_i)}.
$$

**Part 2 (PG or PMwG sampling)** For $i = p_1 + 1, \ldots, p$

Step $i$:

(a) sample $\theta'_i \sim q_i(\cdot | \tilde{X}_1^1, \ldots, \tilde{X}_{T-1}^{C_{T-1}}, X_T^{B_T}, B_T, \theta_{-i}, \theta_i)$,

(b) run the Particle Gibbs Algorithm 3 to sample

$$\tilde{X}'_{1:T-1}, \left( X_T^{b_T} \right)', \tilde{A}'_{1:T-1}, B'_{1:T-1}, \left( \tilde{X}_1^{C_1} \right)', \ldots, \left( \tilde{X}_{T-1}^{C_{T-1}} \right)'$$

from

$$
\Pi \left( d\tilde{X}_{1:T-1}, dX_T^{b_T}, \tilde{A}_{1:T-1}, B_{1:T-1}, d\tilde{X}_1^{C_1}, \ldots, d\tilde{X}_{T-1}^{C_{T-1}} | \tilde{X}_1^1, \ldots, \tilde{X}_{T-1}^{C_{T-1}}, X_T^{B_T}, B_T, \theta_{-i}, \theta_i \right),
$$

(c) accept the proposed values $\tilde{X}'_{1:T-1}, \left( X_T^{b_T} \right)', \tilde{A}'_{1:T-1}, B'_{1:T-1}, \left( \tilde{X}_1^{C_1} \right)', \ldots, \left( \tilde{X}_{T-1}^{C_{T-1}} \right)'$ and $\theta'_i$ with probability

$$
1 \wedge \frac{\pi(\theta_i | \tilde{X}_1^1, \ldots, \tilde{X}_{T-1}^{C_{T-1}}, X_T^{B_T}, B_T, \theta_{-i}) q_i(\theta_i | \tilde{X}_1^1, \ldots, \tilde{X}_{T-1}^{C_{T-1}}, X_T^{B_T}, B_T, \theta_{-i}, \theta'_i)}{\pi(\theta'_i | \tilde{X}_1^1, \ldots, \tilde{X}_{T-1}^{C_{T-1}}, X_T^{B_T}, B_T, \theta_{-i}) q_i(\theta'_i | \tilde{X}_1^1, \ldots, \tilde{X}_{T-1}^{C_{T-1}}, X_T^{B_T}, B_T, \theta_{-i}, \theta_i)}.
$$

(d) sample $B_{1:T}, \tilde{X}_{1:T-1}$ from

$$
\Pi \left( B_{1:T}, d\tilde{X}_{1:T-1} | \tilde{X}_{1:T}, \tilde{A}_{1:T-1}, \theta \right).
$$
We will assume that the Metropolis-Hasting proposals \( q_i(\cdot|U_{1:T}, \theta_{-i}, \theta_i) \) for \( i = 1, \ldots, p_1 \) and \( q_i(\cdot|\tilde{X}_1^{C_1}, \ldots, \tilde{X}_{T-1}^{C_{T-1}}, X_T^{B_T}, B_T, \theta_{-i}, \theta_i) \) for \( i = p_1 + 1, \ldots, p \) are strictly positive densities.

**Remark 4** A similar sampling scheme is given in Mendes et al. (2014) for the augmented models from Andrieu et al. (2010) and Olsson and Ryden (2011). Mendes et al. (2014) show that more general sampling schemes perform better than the particle Marginal Metropolis-Hastings approach in Andrieu et al. (2010) and the particle Gibbs approach in Lindsten et al. (2014) for some applications.

**Remark 5** Similar comments apply between Sampling Scheme 1 and Part 1 of Sampling Scheme 3. Similarly to Sampling Scheme 1 only the terms in the acceptance probabilities (3.3) are required in Part 1, Step \( i(a) \). We have shown the most general case for the Metropolis-Hastings proposal (3.3) which requires both Algorithms 1 and 2 to be run. Simpler Metropolis-Hasting proposals of the form
\[
q_i(\cdot|\tilde{X}_1^{1:T}, \tilde{A}_1^{1:T-1}, \theta)
\]
would only require Algorithm 2 to be run if the Metropolis-Hasting proposal is accepted in Part 1 Step \( i(c) \).

**Remark 6** In Part 2 of Sampling Scheme 3, it is only necessary to generate the values in Step \( i(b) \) if the Metropolis-Hasting proposal is accepted in Step \( i(c) \).

**Remark 7** In Part 2 of Sampling Scheme 3 it is possible to remove Step \( i(d) \) for \( i = p_1 + 1, \ldots, p - 1 \).

### 3.3 Ergodicity

This section gives sufficient conditions for Sampling Schemes 1 to 3 to converge to their stationary distributions in total variation norm and uniform convergence.

Note that, by construction, Sampling Schemes 1 to 3 have correct invariant distributions, so to prove convergence in total variation norm it is sufficient to prove that the corresponding Markov chains are irreducible and aperiodic and then use standard Markov chain convergence results – see, for example, Theorem 4 in Roberts and Rosenthal (2004).

Theorem 1 gives sufficient conditions for Sampling Scheme 1 to converge to \( \Pi \) in total variation norm.

**Theorem 1** If Assumptions 1 and 2 hold, then for all \( \theta \in \Theta \) Sampling Scheme 1 generates a sequence \( \{U_{1:T}(j)\} \), whose distributions \( \{\mathcal{L}\{U_{1:T}(j) \in \cdot\}\} \) satisfy
\[
|\mathcal{L}\{U_{1:T}(j) \in \cdot\} - \Pi(\cdot|\theta)|_{TV} \to 0 \quad \text{as } j \to \infty.
\]

Its proof follows directly from Lemma 2 and standard convergence results for Markov chains. Part (iii) of Lemma 2 shows that Sampling Scheme 1 is an independent Metropolis-Hasting algorithm with target distribution \( \Pi(\cdot) \) and Part (ii) of Lemma 2 shows that the Markov chain is irreducible and aperiodic.
Theorem 2 uses Assumption 3 to give sufficient conditions for the convergence in total variation norm of Sampling Scheme 2.

Assumption 3 For \( t = 1, \ldots, T - 1 \), the product kernel

\[
K_t^{C_t} \left( x_t, dx'_t | \tilde{x}_t^{-b_t}, \bar{x}_t^{C_t+1}, \tilde{\bar{x}}_{t+1}, \bar{a}_t^{-b_t}, \bar{a}_{t+1}^{-1}, \theta \right) \gg dx'_t
\]

for all values of \( x_t, \tilde{x}_t^{-b_t}, \bar{x}_t^{C_t+1}, \tilde{\bar{x}}_{t+1}, \bar{a}_t^{-b_t}, \bar{a}_{t+1}^{-1} \) and all \( \theta \in \Theta \).

Theorem 2 If Assumptions 1 to 3 hold, then for all \( \theta \in \Theta \) Sampling Scheme 2 generates a sequence \( \{U_{1:T}(j)\} \), whose distributions \( \{L(U_{1:T}(j) \in \cdot)\} \) satisfy

\[
|L(U_{1:T}(j) \in \cdot) - \Pi(\cdot|\theta)|_{TV} \to 0 \quad \text{as } j \to \infty.
\]

The proof is given in the appendix.

Theorem 3 gives sufficient conditions for the convergence in total variation norm of Sampling Scheme 3. We use the following notation. Let \( \{V(n), n = 1, 2, \ldots\} \) denote the iterates of the Markov chains on the state space \( V = U_{1:T} \times \Theta \).

Theorem 3 If Assumptions 1 to 3 hold, then Sampling Scheme 3 generates a sequence \( \{V(j)\} \), whose distributions \( \{L(V(j) \in \cdot)\} \) satisfy

\[
|L(V(j) \in \cdot) - \Pi(\cdot|\theta)|_{TV} \to 0 \quad \text{as } j \to \infty.
\]

The proof is given in the Appendix.

To derive results on uniform convergence we use a similar approach to Andrieu and Roberts (2009), Andrieu and Vihola (2012), Lindsten and Schönbjerg (2012) and Mendes et al. (2014) and relate Sampling Scheme 3 to the ideal sampling scheme defined below. The extension from Mendes et al. (2014) to Sampling Scheme 3 is straightforward, but we include the results for completeness. Similarly to Mendes et al. (2014), we define the ideal sampling scheme:

**Sampling Scheme 4** Given \( U_{1:T} \) and \( \theta \)

**Part 1** (PMMH sampling) For \( i = 1, \ldots, p_1 \)

Step i:

(a) sample

\[
\theta'_i \sim q_i(\cdot|U_{1:T}, \theta_{-i}),
\]

(b) sample \( U'_{1:T} \) from

\[
\Pi(\cdot|\theta_{-i}, \theta'_i),
\]

(c) accept \( U'_{1:T}, \theta'_i \) with probability equal to

\[
1 \wedge \frac{\pi(\theta'_i|\theta_{-i}) q_i(\theta'_i|U'_{1:T}, \theta_{-i}, \theta'_i)}{\pi(\theta_i|\theta_{-i}) q_i(\theta_i|U_{1:T}, \theta_{-i}, \theta_i)}. \tag{3.5}
\]
Part 2 (PG or PMwG sampling) For $i = p_1 + 1, \ldots, p$

Step $i$:

(a) sample

$$
\theta_i' \sim q_i(\cdot|\bar{X}_1^{C_1}, \ldots, \bar{X}_{T-1}^{C_{T-1}}, X_T^{B_T}, B_T, \theta_{-i}, \theta_i),
$$

(b) run the Particle Gibbs Algorithm $[3]$ to sample

$$
\bar{X}_{1:T-1}^{b'}, (X_T^{b'})', \bar{A}_{1:T-1}^{c'}, (\bar{X}_1^{c_1})', \ldots, (\bar{X}_{T-1}^{C_{T-1}})'
$$

from

$$
\Pi\left\{d\bar{X}_{1:T-1}^{b'}, dX_T^{b'}, \bar{A}_{1:T-1}^{c'}, d\bar{X}_1^{C_1}, \ldots, d\bar{X}_{T-1}^{C_{T-1}} | \bar{X}_1^{C_1}, \ldots, \bar{X}_{T-1}^{C_{T-1}}, X_T^{B_T}, B_T, \theta_{-i}, \theta_i'\right\},
$$

(c) accept the proposed values $\bar{X}_{1:T-1}^{b'}, (X_T^{b'})', \bar{A}_{1:T-1}^{c'}, (\bar{X}_1^{c_1})', \ldots, (\bar{X}_{T-1}^{C_{T-1}})'$ and $\theta_i'$ with probability

$$
1 \wedge \frac{\pi(\theta_i'|\bar{X}_1^{C_1}, \ldots, \bar{X}_{T-1}^{C_{T-1}}, X_T^{B_T}, B_T, \theta_{-i}) q_i(\theta_i|\bar{X}_1^{C_1}, \ldots, \bar{X}_{T-1}^{C_{T-1}}, X_T^{B_T}, B_T, \theta_{-i}, \theta_i')}{\pi(\theta_i'|\bar{X}_1^{C_1}, \ldots, \bar{X}_{T-1}^{C_{T-1}}, X_T^{B_T}, B_T, \theta_{-i}) q_i(\theta_i'|\bar{X}_1^{C_1}, \ldots, \bar{X}_{T-1}^{C_{T-1}}, X_T^{B_T}, B_T, \theta_{-i}, \theta_i')},
$$

(d) sample $B_{1:T}, \bar{X}_{1:T-1}$ from

$$
\Pi\left(B_{1:T}, d\bar{X}_{1:T-1} | \bar{X}_{1:T}, \bar{A}_{1:T-1}, \bar{X}_{1:T-1}, \theta_i\right).
$$

We call Sampling Scheme $[4]$ an ideal sampling scheme because in Step $i(b)$ of Part 1 we sample the auxiliary variables $U_{1:T}$ from their conditional distribution $\Pi(\cdot | \theta)$, whereas Sampling Scheme $[3]$ Step $i(b)$ of Part 1 uses the Metropolis-Hasting proposal $\Psi (\cdot | \theta)$. Thus, comparing the two Sampling Schemes allows us to study the effect of this Metropolis-Hastings proposal on the convergence of the sampler. Let $P(v; \cdot)$ be the substochastic transition kernel of Sampling Scheme $[3]$ that defines the probabilities for accepted Metropolis-Hastings moves and let $P(v; \cdot)$ be the corresponding substochastic kernel for Sampling Scheme $[4]$. The following theorem gives sufficient conditions for the existence of minorization conditions for Sampling Scheme $[3]$ which, from Roberts and Rosenthal (2004) are equivalent to uniform ergodicity.

**Theorem 4** Suppose that

(i) **Sampling Scheme $[4]$** satisfies the following minorization condition: there exists a constant $\epsilon > 0$, a number $n_0 \geq 1$, and a probability measure $\nu$ on $\mathcal{V}$ such that $\bar{P}^{n_0}(v; A) \geq \epsilon \nu(A)$ for all $v \in \mathcal{V}, A \in \mathcal{B}(\mathcal{V})$.

(ii) $h(u_{1:T} | \theta) = \frac{\Pi(dU_{1:T} | \theta)}{\Psi(dU_{1:T} | \theta)} \leq \gamma < \infty.$
Then, Sampling Scheme 3 satisfies the minorization condition

\[ \mathbb{P}(v; A) \geq \gamma^{-n_0} \mathbb{P}_1(v; A), \]

and for all starting values for the Markov chain

\[ \left| \mathcal{L} \{ V^{(n)} \in \cdot \} - \Pi \{ \cdot \} \right|_TV \leq (1 - \delta)^{\lfloor n/n_0 \rfloor}, \]

where \( 0 < \delta < 1 \) and \( \lfloor n/n_0 \rfloor \) is the greatest integer not exceeding \( n/n_0 \).

The proof is similar to Theorem 6 of Mendes et al. (2014) and is omitted.

Sufficient conditions for the condition in Theorem 4 to be satisfied are given in Lemma 7 of Mendes et al. (2014).

4 Examples

4.1 Proposal densities for the backward MCMC steps

An important issue in implementing the method is the choice of the transition kernels (2.10) and (2.11). The user specifies proposal distributions denoted by

\[ Q_t \left( x_t, dx'_t | \tilde{x}_{t-1}, x_{t-1}^{b_{t-1}}, \tilde{x}_{t+1}^{C_{t+1}}, \tilde{a}_{t-2}, a_{t-1}, \theta \right), \]

for \( t = 1, \ldots, T - 2 \) and

\[ Q_T \left( x_{T-1}, dx'_{T-1} | \tilde{x}_{T-2}, x_{T-2}^{b_{T-2}}, x_T^{b_T}, \tilde{a}_{T-3}, \tilde{a}_{T-2}, \theta \right), \]

which are used with the target distributions (2.5) and (2.9) to calculate the acceptance probabilities of the Metropolis-Hastings steps in Algorithms 2 and 3. Denote these acceptance probabilities by

\[ \alpha_t \left( x_t, x'_t | \tilde{x}_{t-1}, x_{t-1}^{b_{t-1}}, \tilde{x}_{t+1}^{C_{t+1}}, \tilde{a}_{t-2}, a_{t-1}, \theta \right) = 1 \wedge \]

\[ \frac{p \left( dx' | \tilde{x}_{t-1}, x_{t-1}^{b_{t-1}}, \tilde{x}_{t+1}^{C_{t+1}}, \tilde{a}_{t-2}, \tilde{a}_{t-1}, \theta \right) Q_t \left( x_t, dx'_t | \tilde{x}_{t-1}, x_{t-1}^{b_{t-1}}, \tilde{x}_{t+1}^{C_{t+1}}, \tilde{a}_{t-2}, \tilde{a}_{t-1}, \theta \right)}{p \left( dx | \tilde{x}_{t-1}, x_{t-1}^{b_{t-1}}, \tilde{x}_{t+1}^{C_{t+1}}, \tilde{a}_{t-2}, \tilde{a}_{t-1}, \theta \right) Q_t \left( x_t, dx' | \tilde{x}_{t-1}, x_{t-1}^{b_{t-1}}, \tilde{x}_{t+1}^{C_{t+1}}, \tilde{a}_{t-2}, \tilde{a}_{t-1}, \theta \right)} \]

for \( t = 1, \ldots, T - 2 \) and

\[ \alpha_{T-1} \left( x_{T-1}, dx'_{T-1} | \tilde{x}_{T-2}, x_{T-2}^{b_{T-2}}, x_T^{b_T}, \tilde{a}_{T-3}, a_{T-2}, \theta \right) = 1 \wedge \]

\[ \frac{p \left( dx'_{T-1} | \tilde{x}_{T-2}, x_{T-2}^{b_{T-2}}, \tilde{x}_T^{b_T}, \tilde{a}_{T-3}, \tilde{a}_{T-2}, \theta \right) Q_t \left( x_{T-1}, dx'_{T-1} | \tilde{x}_{T-2}, x_{T-2}^{b_{T-2}}, \tilde{x}_T^{b_T}, \tilde{a}_{T-3}, \tilde{a}_{T-2}, \theta \right)}{p \left( dx_{T-1} | \tilde{x}_{T-2}, x_{T-2}^{b_{T-2}}, \tilde{x}_T^{b_T}, \tilde{a}_{T-3}, \tilde{a}_{T-2}, \theta \right) Q_t \left( x_{T-1}, dx'_{T-1} | \tilde{x}_{T-2}, x_{T-2}^{b_{T-2}}, \tilde{x}_T^{b_T}, \tilde{a}_{T-3}, \tilde{a}_{T-2}, \theta \right)}. \]

This section illustrates some possible choices. To simplify notation dependence on the parameter \( \theta \) will be omitted and the conditioning states \( \tilde{x}_{t+1}^{C_{t+1}} \) for \( t = 1, \ldots, T - 2 \) and \( x_T^{b_T} \) will be denoted by
\( \tilde{x}_{t+1} \) for \( t = 1, \ldots, T - 1 \). We first consider estimates of the mean and variance of the smoothing density \( p(x_t|y_{1:t}, \tilde{x}_{t+1}) \).

**Backward weights:** The Markov transition kernel is conditional on the particles \( x_t^{−b_t} \), sampled in the filtering step. These particles provide an approximation

\[
p(x|y_{1:t}, \tilde{x}_{t+1}) = \frac{\sum_{i \neq b_t} w_t^i f_t(\tilde{x}_{t+1}|x_t^i) \delta(x - x_t^i)}{\sum_{i \neq b_t} w_t^i f_t(\tilde{x}_{t+1}|x_t^i)}. \tag{4.5}
\]

for \( t = 1, \ldots, T - 1 \) to the smoothing density \( p(x_t|y_{1:t}, \tilde{x}_{t+1}) \) and can be used for constructing proposal densities. This method works well if the particles \( x_t^{−b_t} \) provide a good approximation to the smoothing density. The estimates for the smoothing mean \( \tilde{x}_{t|T} \) and smoothing covariance matrix \( \tilde{S}_{t|T} \) are

\[
\tilde{x}_{t|T} = \frac{\sum_{i \neq b_t} w_t^i x_t^i}{\sum_{i \neq b_t} w_t^i} \quad \text{and} \quad \tilde{S}_{t|T} = \frac{\sum_{i \neq b_t} w_t^i (x_t^i - \tilde{x}_{t|t})(x_t^i - \tilde{x}_{t|T})'}{\sum_{i \neq b_t} w_t^i}.
\]

**Linearization:** This constructs a Gaussian linear approximation to the state evolution density. Write the approximate state evolution equation as

\[
x_{t+1} = h_{t+1} + H_{t+1} x_t + u_{t+1},
\]

where \( u_t \sim N(0, \Sigma_{t+1}) \). Estimate the filtered mean, \( \tilde{x}_{t|t} \), and covariance matrix, \( \tilde{S}_{t|t} \), using the particles \( x_t^{−b_t} \) and the forward weights \( w_t^{−b_t} \):

\[
\tilde{x}_{t|t} = \frac{\sum_{i \neq b_t} w_t^i x_t^i}{\sum_{i \neq b_t} w_t^i} \quad \text{and} \quad \tilde{S}_{t|t} = \frac{\sum_{i \neq b_t} w_t^i (x_t^i - \tilde{x}_{t|t})(x_t^i - \tilde{x}_{t|t})'}{\sum_{i \neq b_t} w_t^i}.
\]

The mean \( x_{t|T} \) and variance \( S_{t|T} \) for \( t = 1, \ldots, T - 1 \) of the proposals for (4.1) and (4.2) are

\[
x_{t|T} = \tilde{x}_{t|t} + \tilde{S}_{t|t} H_{t+1} R_{t+1}^{-1} e_{t+1} \quad \text{(4.6)}
\]

\[
S_{t|T} = \tilde{S}_{t|t} - \tilde{S}_{t|t} H_{t+1} R_{t+1}^{-1} H_{t+1} \tilde{S}_{t|t} \quad \text{(4.7)}
\]

where \( R_{t+1} = H_{t+1} S_{t|t} H_{t+1} + \Sigma_{t+1} \) and \( e_{t+1} = \tilde{x}_{t+1} - h_{t+1} - H_{t+1} \tilde{x}_{t|t} \). A similar algorithm may be used if the state evolution equation is approximated by a Gaussian mixture.

Although less flexible, this approach is preferred if the state evolution density is linear and Gaussian or can be approximated arbitrarily well by a mixture Gaussian density. An advantage of this method over the first one is that it does not require calculating the backward weights and, therefore, can be applied to state space models in which (4.5) does not provide a good approximation to \( p(x_t|y_{1:t}, \tilde{x}_{t+1}) \).

**Random walk proposal:** The two previous approaches to estimating the variance of the smoothing density may be used to construct a random walk proposal. In the random walk proposal we use the estimate of variance and multiply it by a factor of 2.38\( d_x / d_x \), where \( d_x \) is the dimension of the state vector \( x_t \).

**Independent elliptical proposal:** For the independent elliptical proposal, traditional choices of densities are a non-central Student \( t \) distribution or a Gaussian distribution, where the scale and
mean are calculated using the previous methods. The computational cost for constructing these proposal densities increases linearly with the number of particles.

**Bootstrap proposal:** The third alternative is similar in spirit to the bootstrap filter. The most expensive part of the MCMC moves is evaluating $\sum_i w_i^{t-1} f(x_{i,t-1}^i)$, present in the acceptance probabilities (4.3) and (4.4). We suggest using the proposal density

$$q(x|x_{t-1}) = \sum_{i=1}^{N_{t-1}} W_i^{t-1} f_t(x_{i,t-1}^i). \tag{4.8}$$

for $t = 1, \ldots, T - 1$. For two distinct values $x$ and $x'$, the Metropolis-Hastings ratio is

$$1 \wedge \frac{f_t(\tilde{x}_{t+1}|x) \, g_t(y_t|x)}{f_t(\tilde{x}_{t+1}|x') \, g_t(y_t|x')}$$

as the proposal density (4.8) and the sum in the target densities (2.8) and (2.9) cancel out.

This method is faster than the previous ones, but it does not take into account $\tilde{x}_{t+1}$ or $y_t$ to construct the proposal. Furthermore, the only assumption about the state evolution equation is that it can be sampled from and evaluated up to a normalizing constant.

### 4.2 Nonlinear state space model

The goal of this example is to evaluate the performance of the algorithm for several combinations of the number of particles $N$ and MCMC iterations $C$. We consider the following nonlinear state-space model used by many authors including Gordon et al. (1993), Kitagawa (1996), and Andrieu et al. (2010):

$$y_t = \frac{x_t^2}{20} + \sigma \varepsilon_t$$

$$x_{t+1} = \frac{x_t}{2} + 25 \frac{x_t}{1 + x_t^2} + 8 \cos(1.2 t) + \tau \eta_{t+1},$$

where $\varepsilon_t$ and $\eta_t$ are standard Gaussian random variables and $x_1 \sim N(0, 5)$. We choose an inverse Gamma prior for both $\sigma^2$ and $\tau^2$ with shape 1 and scale 0.1.

We simulate 50 observations with parameters $\sigma^2 = 1$ and $\tau^2 = 10$. The bootstrap filter samples the particles from the state evolution equation, while the bootstrap MCMC proposal samples the states from (4.8). The variance term in the random walk proposal is calculated using (4.5) and scaled by the factor 2.38. Despite being sub-optimal, these choices are very general and only require that one can sample from the state density and can evaluate both the observation and state densities. We avoid using a Gaussian independent proposal as it provides a poor approximation to the bimodal target.

We generate 100,000 iterations and discard the initial 10,000 as warm up. The performance of each method is measured as the maximum IACT of the $\sigma$ and $\tau$ iterates, i.e., $\max(\text{IACT}(\tau), \text{IACT}(\sigma))$ where $\text{IACT}(\theta)$ is the integrated autocorrelation time estimate of a parameter $\theta$. In the simulations, we take $N = 5, 10, 20, 50$ and $C = 2, 5, 10$. Figures 1a and 1b show the results for the particle Gibbs
sampler using a bootstrap proposal and a random walk proposal, respectively. Both results are compared with the particle Gibbs with backward simulation method proposed by Lindsten and Schön (2012). To distinguish between the methods we will refer to our approach as the extended space particle Gibbs sampler. The IACTs are calculated using overlapping batch means (see, e.g. Jones et al. 2006) using 90,000 samples and block size 300.

![Image](a)

![Image](b)

Figure 1: Nonlinear state space model. Maximum of the IACT of $\sigma$ and $\tau$ for different choices of number of particles ($N=5,10,20,50$) and MCMC steps ($C=2,5,10$) for the extended space particle Gibbs sampler (ES). Also shown is the performance of the backward simulation approach in Lindsten and Schön (2012) (BSi). Panels (a) and (b) show the result for the “bootstrap” proposal and the random walk proposal with backward weights, respectively.

The performance of the samplers improves as the number of particles and number of MCMC moves increase. The bootstrap proposal performs worse than the random walk proposal for a fixed number of particles and MCMC steps. In practice, the difference between the IACTs is negligible as the number of particles increases. In this simulation study, the random walk proposal is between 2.3
and 6.7 times slower than the bootstrap proposal, depending on the number of particles and MCMC moves.

### 4.3 Stochastic Volatility Model

In this example we fit a stochastic volatility (SV) model for the Pound/Dollar daily exchange rates from 1-Oct-1981 to 26-Jun-1985 (see Durbin and Koopman [2001], Sec. 14.4). The observation and state transition equations are

$$y_t = e^{h_t/2} \epsilon_t \quad \text{and} \quad h_{t+1} = \mu + \phi (h_t - \mu) + \tau \eta_{t+1},$$

with $(\epsilon_t, \eta_t)$ independently distributed standard Gaussian random variables. In this model, $h_t$ is the log-volatility at time $t$, $\mu$ is the mean of the log-volatility, $\tau$ its standard deviation and $\phi$ the autoregressive parameter. The specification of the SV model is completed by assuming the distribution of the initial state $h_1 \sim N(\mu, \tau^2/(1-\phi^2))$. We are interested in performing Bayesian inference for the parameters of this model. To complete the Bayesian specification, we use the following priors. The autocorrelation parameter $\phi$ is uniform on $(-1, 1)$, the state standard deviation $\tau$ has a half-$t$ distribution with degrees of freedom $d = 4$ (Gelman [2006]), and the log-volatility mean $\mu \sim N(0, 2^2)$.

We reparametrize the model as $y_t = \exp\{\mu + \tau x_t\} \epsilon_t$ where $x_t = (h_t - \mu)/\tau$ and $x_{t+1} = \phi x_t + \eta_{t+1}$ with $x_1 \sim N(0, 1/(1-\phi^2))$, using independent Metropolis steps within the Gibbs sampler to draw from $p(\mu, \tau|x_1:T, y_1:T)$ and $p(\phi|x_1:T)$. The independent proposals are calculated using the Laplace approximation of the conditional densities and yield an acceptance rate close to 90%.

We consider an adapted particle filter using the optimal importance densities described in Doucet et al. (2000) and five different proposal densities for the MCMC step: a random walk with variance calculated using (4.5), a random walk with variance calculated using (4.7), a Gaussian independent proposal with mean and variances calculated using (4.5), a Gaussian independent proposal with mean and variance calculated using (4.6) and (4.7), and the independent proposal (4.8). We compare the performance of the proposals for several different combinations of the number of particles $N$ and MCMC iterations $C$.

We run the extended space particle Gibbs sampler for 50,000 iterations using the first 5,000 as warmup and calculate the IACT (inefficiency factor) using the overlapping batch means method with a bandwidth of 213 samples. In all the simulations, the posterior means and variances are consistent with values previously found in the literature (see, e.g. Durbin and Koopman [2001], Sec. 14.4). The posterior means for $\mu$, $\tau$ and $\phi$ are respectively $-.952$, $.180$ and $.971$, while the posterior standard deviations are $.1997$, $.0351$ and $.0126$, respectively. Table 1 shows the IACT and relative time to run each algorithm for each combination of $N$ and $C$. We display the relative time to run each of the algorithms compared to the bootstrap MCMC proposal. The bootstrap proposal is used as the baseline for time because it is fastest; it avoids $C \times N \times T$ state evolution density evaluations when compared to the independent sampler or the random walk sampler.

Table 1 shows that in this example all the algorithms perform similarly, given the number of particles and MCMC steps. As the number of particles increases the efficiencies of the methods decrease steadily. Increasing the number of MCMC steps, however, does not have a significant impact on the IACT. One possible explanation is that only a few iterations are enough to break the
dependence structure of the conditional sequential Monte Carlo and increasing the number of steps is irrelevant. Finally, a bootstrap MCMC proposal with $N=400$ and $C=5$ yields $\text{IACT}(\mu) = 51$, $\text{IACT}(\tau) = 29$ and $\text{IACT}(\phi) = 23$, showing that even increasing the number of particles eight-fold does not decrease the inefficiencies much.

### 4.4 Binomial regression model with time-varying coefficients

Consider the state space model with binomial observations

\[
Y_t | x_t \sim \text{Binomial}(n_t, p_t), \quad \log \frac{p_t}{1 - p_t} = \beta_0 + \beta_{1,t}z_{1,t} + \cdots + \beta_{m,t}z_{m,t} \tag{4.9}
\]

where $z_t = (z_{1,t}, \ldots, z_{m,t})'$ is vector of covariates. We take the intercept $\beta_0$ to be fixed for all $t$ with a prior $N(0, 5^2)$, but allow the coefficients $\beta_t = (\beta_{1,t}, \ldots, \beta_{m,t})'$ to evolve over time by using the random walk prior $\beta_t = \beta_{t-1} + \tau \eta_t$ for $t = 1, \ldots, T$, with $\eta_t \sim N(0, I_m)$ and $\tau = \text{diag}(\tau_1, \ldots, \tau_m)$.

We use the prior $\tau^2_i \sim IG(1, 5)$ for $i = 1, \ldots, m$, with the $\tau_i$ independent apriori. We also generate independent values of $n_t \sim \text{Binomial}(100, 0.5)$ for $t = 1, \ldots, T$, which gave values of $n_t$ lying in the interval (35, 65). We generate independent values of the covariates $z_{i,t} \sim U(-1, 1)$ for $i = 1, \ldots, m$ and $t = 1, \ldots, T$. We generate $T = 200$ observations from model (4.9), setting $\beta_0 = 0.5$ and $\tau_i = 0.6$ and $\beta_{i,0} = 0$ for $i = 1, \ldots, m$, and we take the number of covariates $m = 4$. The minimum generated values of $p_t$ were close to zero and the maximum values were close to one.

The extended space particle Gibbs specification uses a bootstrap particle filter with the bootstrap MCMC proposal for the states. We vary the number of particles and MCMC moves and estimate the largest IACT among the $\tau_i$'s ($\text{max}_{i=1,\ldots,p} \text{IACT}(\tau_i)$). We run 100,000 iterations of the Gibbs sampler and discard the initial 5,000 as warm up. The remaining 95,000 samples are used to calculate the IACT using the overlapping batch means method, using a window size of 309 samples.

Figure 2a displays the IACTs for our method using $N = 5, 10, 20, 30, 40$ and $C = 10, 20, 30$ and compares it with the backward simulation algorithm of [Lindsten and Schön (2012)](https://link.springer.com/article/10.1007%2Fs10950-012-0368-7) using the same number of particles. Figure 2b shows the IACTs for the backward simulation method for $N = 5, 10, 20, 30, 40, 50, 75, 100, 150, 200, 250, 300$ and compares with the results using the new approach. The inefficiency factors for the new approach converge to a minimum faster than backward simulation. The extended support approach yields a minimal IACT with $N = 40$ and $C = 30$, while the backward simulation takes around $N = 250$ particles to achieve this value and twice the time in our particular, general, specification using the Julia programming language.

### References

C. Andrieu and G. O. Roberts. The pseudo-marginal approach for efficient Monte Carlo computations. *The Annals of Statistics*, 37(2):697–725, 2009.

C. Andrieu and M. Vihola. Convergence properties of pseudo-marginal Markov chain Monte Carlo algorithms. arXiv preprint arXiv:1210.1484, 2012.

C. Andrieu, A. Doucet, and R. Holenstein. Particle Markov chain Monte Carlo methods. *Journal of the Royal Statistical Society, Series B*, 72:269–342, 2010.
| N  | C  | Method | IACT(\(\mu\)) | IACT(\(\phi\)) | IACT(\(\tau\)) | Relative Time |
|----|----|--------|----------------|----------------|----------------|---------------|
|    |    | Boot   | 132.9         | 82.2           | 66.9           | 1.00          |
|    |    | RW1    | 122.3         | 82.0           | 63.3           | 2.81          |
| 5  |    | RW2    | 116.6         | 77.3           | 61.4           | 2.36          |
|    |    | Ind1   | 141.3         | 85.1           | 72.1           | 3.10          |
|    |    | Ind2   | 111.7         | 67.3           | 55.5           | 2.55          |
|    |    | Boot   | 139.3         | 74.7           | 65.8           | 1.00          |
|    | 10 | RW1    | 108.3         | 71.3           | 54.4           | 3.29          |
|    |    | RW2    | 140.3         | 75.7           | 64.2           | 3.06          |
|    |    | Ind1   | 122.4         | 77.9           | 60.7           | 3.65          |
|    |    | Ind2   | 119.2         | 82.0           | 66.1           | 3.20          |
|    | 20 | Boot   | 105.1         | 75.2           | 58.5           | 1.00          |
|    |    | RW1    | 125.7         | 80.1           | 63.5           | 4.84          |
|    |    | RW2    | 116.8         | 71.9           | 56.8           | 4.68          |
|    |    | Ind1   | 121.8         | 80.7           | 63.2           | 5.44          |
|    |    | Ind2   | 116.5         | 69.4           | 58.5           | 5.22          |
|    | 20 | Boot   | 102.3         | 63.3           | 52.9           | 1.00          |
|    |    | RW1    | 113.2         | 56.9           | 47.9           | 3.36          |
|    |    | RW2    | 98.0          | 50.9           | 44.8           | 2.74          |
|    |    | Ind1   | 90.3          | 56.4           | 44.8           | 3.70          |
|    |    | Ind2   | 82.4          | 50.3           | 39.2           | 2.99          |
|    | 20 | Boot   | 91.8          | 60.7           | 49.5           | 1.00          |
|    |    | RW1    | 116.5         | 62.9           | 55.9           | 4.24          |
|    |    | RW2    | 96.1          | 54.3           | 45.5           | 3.81          |
|    |    | Ind1   | 111.8         | 65.1           | 53.7           | 4.62          |
|    |    | Ind2   | 100.9         | 51.1           | 49.5           | 4.10          |
|    | 50 | Boot   | 95.79         | 56.0           | 44.48          | 1.00          |
|    |    | RW1    | 115.9         | 58.1           | 49.5           | 6.81          |
|    |    | RW2    | 116.7         | 58.0           | 48.4           | 6.59          |
|    |    | Ind1   | 89.8          | 54.7           | 44.3           | 7.36          |
|    |    | Ind2   | 90.4          | 53.4           | 43.2           | 6.89          |
|    | 50 | Boot   | 74.9          | 46.5           | 37.5           | 1.00          |
|    |    | RW1    | 73.2          | 43.1           | 36.2           | 4.62          |
|    |    | RW2    | 93.6          | 48.1           | 41.6           | 3.25          |
|    |    | Ind1   | 73.1          | 41.9           | 33.7           | 5.02          |
|    |    | Ind2   | 59.9          | 45.0           | 35.3           | 3.39          |
|    | 50 | Boot   | 78.6          | 57.2           | 41.4           | 1.00          |
|    |    | RW1    | 77.5          | 43.4           | 35.3           | 5.21          |
|    |    | RW2    | 68.7          | 41.4           | 32.4           | 4.74          |
|    |    | Ind1   | 97.3          | 52.0           | 45.9           | 6.04          |
|    |    | Ind2   | 86.2          | 39.0           | 34.7           | 5.13          |
|    | 20 | Boot   | 72.2          | 48.9           | 38.3           | 1.00          |
|    |    | RW1    | 73.2          | 43.0           | 34.5           | 9.32          |
|    |    | RW2    | 94.8          | 44.8           | 38.6           | 8.48          |
|    |    | Ind1   | 76.7          | 44.9           | 37.0           | 9.47          |
|    |    | Ind2   | 70.0          | 43.5           | 36.2           | 8.84          |

Table 1: Stochastic volatility model. Inefficiency factors (IACT) for the extended space particle Gibbs sampler, using five different proposals for the MCMC for the states and different number of particles \(N\) and number of MCMC moves \(C\). The MCMC proposals are random walk with scale calculated using the particles (RW1), random walk with scale calculated using linearization (RW2), Gaussian proposal with mean and variance calculated using the particles (Ind1), Gaussian proposal with mean and variance calculated using linearization (Ind2), and the bootstrap proposal (Boot). Relative Time shows the relative time to run each proposal when compared to the bootstrap (Boot), given the number of particles and MCMC moves.
M. A. Beaumont. Estimation of population growth or decline in genetically monitored populations. *Genetics*, 164:1139–1160, 2003.

P. Bunch and S. Godsill. Improved particle approximations to the joint smoothing distribution using Markov chain Monte Carlo. *IEEE Transactions on Signal Processing*, 61(4):956–963, 2013.

B. P. Carlin, N. G. Polson, and D. S. Stoffer. A Monte Carlo approach to nonnormal and nonlinear state-space modeling. *Journal of the American Statistical Association*, 87(418):493–500, 1992.

C. K. Carter and R. Kohn. On Gibbs sampling for state space models. *Biometrika*, 81(3):541–553, 1994.

N. Chopin and S. S. Singh. On the particle Gibbs sampler. arXiv preprint arXiv:1304.1887, 2013.

A. Doucet, S. Godsill, and C. Andrieu. On sequential Monte Carlo sampling methods for Bayesian filtering. *Statistics and Computing*, 10(3):197–208, 2000.

C. Dubarry and R. Douc. Particle approximation improvement of the joint smoothing distribution with on-the-fly variance estimation. arXiv:1107.5524v1, 2011.

J. Durbin and S. Koopman. *Time series analysis of state space methods*. Oxford University Press, 2001.

P. Fearnhead, D. Wyncoll, and J. Tawn. A sequential smoothing algorithm with linear computational cost. *Biometrika*, 97(2):447–464, 2010.

S. Frühwirth-Schnatter. Data augmentation and dynamic linear models. *Journal of Time Series Analysis*, 15(2):183–202, 1994.

S. Frühwirth-Schnatter. *Finite Mixture and Markov Switching Models*. New York, NY: Springer Science+ Business Media, LLC, 2006.

A. Gelman. Prior distributions for variance parameters in hierarchical models. *Bayesian Analysis*, 1(3):515–533, 2006.

R. Gerlach, C. Carter, and R. Kohn. Efficient Bayesian inference for dynamic mixture models. *Journal of the American Statistical Association*, 95(451):819–828, 2000.

S. Godsill, A. Doucet, and M. West. Monte Carlo smoothing for nonlinear time series. *Journal of the American Statistical Association*, 99(465):156–168, 2004.

N. J. Gordon, D. J. Salmond, and A. F. Smith. Novel approach to nonlinear/non-Gaussian Bayesian state estimation. In *IEE Proceedings F (Radar and Signal Processing)*, volume 140, pages 107–113. IET, 1993.

G. L. Jones, M. Haran, B. S. Caffo, and R. Neath. Fixed-width output analysis for Markov chain Monte Carlo. *Journal of the American Statistical Association*, 101(476):1537–1547, 2006.

G. Kitagawa. Monte Carlo filter and smoother for non-Gaussian nonlinear state space models. *Journal of computational and graphical statistics*, 5(1):1–25, 1996.
A Proofs of lemmas

Proof of Lemma 2
To prove Part (i), integrate \( \Pi(du_{1:T}|\theta) \) over \( x_{1:T}^{y_{1:T}} \) and sum over \( \pi_{T-1} \) to get

\[
\Pi \left( d\bar{x}_{1:T-1}, dx_{T}^{y_{T}}, \bar{a}_{1:T-2}, b_{1:T}, d\bar{x}_{1:T-1}|\theta \right) = \pi \left( \bar{x}_{1}^{C_{1}}, \ldots, \bar{x}_{T-1}^{C_{T-1}}, x_{T}^{y_{T}}|\theta \right) dx_{1}^{C_{1}} \cdots dx_{T-1}^{C_{T-1}} dx_{T}^{y_{T}} \left( \frac{1}{N_{T}} \right) \\
\Psi \left( d\bar{x}_{1:T-1}, \bar{a}_{1:T-2} |\theta \right) M_{1} \left( dx_{1}^{b_{1}}|y_{1}, \theta \right) \prod_{t=2}^{T-1} \left\{ W_{t-1}^{a_{t-1}} M_{t} \left( dx_{t}^{b_{t}}|y_{t}, x_{t-1}^{a_{t-1}}, \theta \right) \right\} \left( \frac{1}{N_{T-1}} \right) \\
\prod_{t=2}^{T-1} \left\{ w_{t-1}^{b_{t}} f_{t} \left( x_{t}^{a_{t}}, x_{t-1}^{b_{t}}, \theta \right) \right\} \left( \frac{1}{N_{T-1}} \right) \\
C_{T-1} \prod_{j=2}^{T-1} K_{T-1} \left( \bar{x}_{j}^{j}, dx_{j-1}^{j}|x_{1:t-1}, x_{j-1}^{b_{j}}, \bar{x}_{j-1}^{a_{j-1}}, x_{j-1}^{b_{j}}, a_{j-1}^{b_{j}} \right) \\
K_{T-1} \left( \bar{x}_{1:T-1}^{1}, dx_{1:T-1}^{y_{1:T-1}}|x_{1:t-1}, x_{1:T-1}^{b_{1:T}}, a_{1:T-2}^{b_{1:T-2}} \right) \\
\prod_{t=1}^{T-2} \left\{ \left( \frac{1}{N_{t}} \right) C_{t} \prod_{j=2}^{T-1} K_{t} \left( \bar{x}_{t}^{j}, dx_{t}^{j}|x_{1:t-1}, x_{t}^{b_{t}}, \bar{x}_{t+1}^{a_{t+1}}, x_{t+1}^{b_{t}}, a_{t+1}^{b_{t}} \right) \right\} . \quad (A.1)
\]
Now sum over $a_{T-2}^{by_1}$, integrate over $x_{T-1}^{by_1}, \ldots, x_{T-1}^{by_1}$, integrate over $x_{T-1}^{-by_1}$, sum over $a_{T-2}^{-by_1}$, and sum over $b_{T-1}$ to get

$$
\Pi \left( d\bar{x}_{1:T-2}, dx_{T-2}^{by_1}, \bar{a}_{1:T-3}, b_{1:T-2}, b_T, d\bar{x}_{1:T-2}, dx_{T-1}^{by_1} \right)
\begin{align*}
&= \pi \left( \bar{x}_1^{C_1}, \ldots, \bar{x}_{T-1}^{by_1}, x_{T-1}^{by_1} | \theta \right) dx_1^{C_1} \ldots dx_{T-1}^{by_1} \left( \frac{1}{N_T} \right) \\
&\quad \times \frac{\psi \left( \bar{x}_1, \ldots, \bar{x}_{T-2}, \bar{a}_1, \ldots, \bar{a}_{T-3} | \theta \right) d\bar{x}_1 \ldots d\bar{x}_{T-2}}{M_1 \left( x_1^{by_1} | y_1, \theta \right) \prod_{t=2}^{T-2} \left\{ \frac{\alpha_{t-1}}{w_{t-1}^{y_1}} M_t \left( x_t^{by_1} | y_t, x_{t-1}^{by_1} \right) \right\}} \\
&\quad \times \frac{\prod_{t=2}^{T-2} \sum_{i=1}^{N_t-1} w_{t-1}^{y_1} f_t \left( x_t^{by_1} | x_{t-1}^{by_1}, \theta \right)}{\prod_{t=1}^{T-2} \left\{ \left( \frac{1}{N_t} \right) \prod_{j=2}^{C_t} K_t \left( \bar{x}_t^{j-1}, dx_t^{j-1} | \bar{x}_1, \ldots, \bar{x}_{t-1}, x_t^{-by_1}, \bar{x}_{t+1}^{C_{t+1}}, \bar{a}_1, \ldots, \bar{a}_{t-2}, a_{t-1}^{-by_1}, \theta \right) \right\}}. 
\end{align*}
$$

(A.2)

The expression in (A.2) shows that we can repeatedly for $t = T - 2, \ldots, 2$ do the following: sum over $a_{t-1}^{by_1}$, integrate over $x_t^{by_1}, \bar{x}_t^{by_1}, \ldots, \bar{x}_{t-1}^{by_1}$, integrate over $x_t^{-by_1}$, sum over $a_{t-1}^{-by_1}$, and sum over $b_t$ to get

$$
\Pi \left( d\bar{x}_{1:t-1}, dx_{t-1}^{by_1}, \bar{a}_{1:t-2}, b_{1:t-1}, b_T, d\bar{x}_{1:t-1}, dx_{t-1}^{by_1} \right)
\begin{align*}
&= \pi \left( \bar{x}_1^{C_1}, \ldots, \bar{x}_{t-1}^{by_1}, x_{t-1}^{by_1} | \theta \right) dx_1^{C_1} \ldots dx_{t-1}^{by_1} \left( \frac{1}{N_T} \right) \\
&\quad \times \frac{\psi \left( \bar{x}_1, \ldots, \bar{x}_{t-1}, \bar{a}_1, \ldots, \bar{a}_{t-2} | \theta \right) d\bar{x}_1 \ldots d\bar{x}_{t-1}}{M_1 \left( x_1^{by_1} | y_1, \theta \right) \prod_{s=2}^{t-1} \left\{ \frac{\alpha_{s-1}}{w_{s-1}^{y_1}} M_{s} \left( dx_s^{by_1} | y_s, x_{s-1}^{by_1} \right) \right\}} \\
&\quad \times \frac{\prod_{s=2}^{t-1} \sum_{i=1}^{N_s-1} w_{s-1}^{y_1} f_t \left( x_s^{by_1} | x_{s-1}^{by_1}, \theta \right)}{\prod_{s=1}^{t-1} \left\{ \left( \frac{1}{N_s} \right) \prod_{j=2}^{C_s} K_s \left( \bar{x}_s^{j-1}, dx_s^{j-1} | \bar{x}_1:t-1, x_s^{-by_1}, \bar{x}_{s+1}^{C_{s+1}}, \bar{a}_1, \ldots, \bar{a}_{t-2}, a_{s-1}^{-by_1}, \theta \right) \right\}}. 
\end{align*}
$$

(A.3)
For $t = 1$ this simplifies to
\[
\Pi \left( d\mathbf{x}_1, dx_T^{b_T}, b_T, d\mathbf{x}_1, d\mathbf{x}_2^{C_2}, \ldots, d\mathbf{x}_{T-1}^{C_{T-1}} | \theta \right)
\]
\[= \pi \left( \mathbf{x}_1^{C_1}, \ldots, \mathbf{x}_{T-1}^{C_{T-1}}, x_T^{b_T} | \theta \right) d\mathbf{x}_1^{C_1} \ldots d\mathbf{x}_{T-1}^{C_{T-1}} dx_T^{b_T} \left( \frac{1}{N_T} \right) \tag{A.4}
\]
\[
\psi (\mathbf{x}_1 | \theta) \frac{\prod_{j=2}^{C_1} K_1 (\tilde{x}_1, d\tilde{x}_1^{j-1}, x_1^{b_1}, x_2^{C_2}, \theta)}{M_1 (\mathbf{x}_1, y_1, \theta) \prod_{j=2}^{C_1} K_1 (\tilde{x}_1, d\tilde{x}_1^{j-1} | x_1^{b_1}, x_2^{C_2}, \theta)} K_1 (\tilde{x}_1, dx_1^{b_1} | x_1^{b_1}, x_{t+1}^{C_{t+1}}, \theta).
\]

Now integrate over $x_1^{b_1}$, $x_1^1$, ..., $x_1^{C_{t-1}}$, integrate over $x_1^{b_1}$, and sum over $b_1$ to get
\[
\Pi \left( dx_T^{b_T}, b_T, d\mathbf{x}_1, d\mathbf{x}_2^{C_2}, \ldots, d\mathbf{x}_{T-1}^{C_{T-1}} | \theta \right)
\]
\[= \pi \left( \mathbf{x}_1^{C_1}, \ldots, \mathbf{x}_{T-1}^{C_{T-1}}, x_T^{b_T} | \theta \right) d\mathbf{x}_1^{C_1} \ldots d\mathbf{x}_{T-1}^{C_{T-1}} dx_T^{b_T} \left( \frac{1}{N_T} \right),
\]
as required.

For Part (ii), we first note that from Assumption[1] the probability measure $\Pi \left( d\mathbf{u}_{1:T} | \theta \right)$ is equivalent to the probability measure
\[
\Pi^* \left( d\mathbf{u}_{1:T} | \theta \right) := \pi \left( d\mathbf{x}_1^{C_1} | \mathbf{x}_2^{C_2}, \theta \right) \prod_{t=2}^{T-1} \pi \left( dx_t^{C_t} | \mathbf{x}_{1:t-1}, \mathbf{x}_{t+1}^{C_{t+1}}, \mathbf{a}_{1:t-2}, \theta \right) \pi \left( dx_T^{b_T} | \theta \right) \left( \frac{1}{N_T} \right)
\]
\[
\psi \left( d\mathbf{x}_{1:T}, \mathbf{a}_{1:T-1} | \theta \right) \prod_{t=2}^{T} \left\{ W_{t-1}^{a_t^{b_t}} \prod_{t=2}^{T} M_t \left( dx_t^{b_t} | y_t, \mathbf{x}_{t-1}^{a_t^{b_t}}, \mathbf{a}_{t-1}^{a_t^{b_t}}, \theta \right) \right\}
\]
\[
\prod_{t=2}^{T} \sum_{i=1}^{N_{t-1}} w_{t-1}^{a_t^{b_t}} f_t \left( x_t^{b_t} | x_{t-1}^{a_{t-1}}, \theta \right)
\]
\[
\left( \frac{1}{N_{T-1}} \right) \prod_{j=2}^{C_{T-1}} K_{T-1} \left( \tilde{x}_j, d\tilde{x}_j^{j-1} | \mathbf{x}_{1:T-2}, \mathbf{x}_{T-1}^{b_{T-1}}, x_T^{b_T}, \mathbf{a}_{1:T-3}, \mathbf{a}_{T-2}^{b_{T-1}}, \theta \right)
\]
\[
\prod_{t=1}^{T-2} \left\{ \frac{1}{N_t} \prod_{j=2}^{C_t} K_t \left( \tilde{x}_j, d\tilde{x}_j^{j-1} | \mathbf{x}_{1:t-1}, \mathbf{x}_j^{b_j}, \mathbf{x}_{t+1}^{C_{t+1}}, \mathbf{a}_{1:t-2}, \mathbf{a}_{t-1}^{b_t}, \theta \right) \right\}.
\]
Applying the detailed balance condition in Assumption 2 repeatedly gives

\[ \Pi^* (du_{1:T}|\theta) = \]

\[ \pi \left( dx_{1:T}^b | \tilde{x}_2^C, \theta \right) \prod_{t=2}^{T-1} \hat{p} \left( dx_t^b | \tilde{x}_{t-1}^C, \tilde{x}_{t+1}^C, \tilde{a}_{1:t-2}, \theta \right) \pi \left( dx_T^b | \theta \right) \left( \frac{1}{N_T} \right) \]

\[ \Psi \left( d\tilde{x}_{1:T}, \tilde{a}_{1:T-1} | \theta \right) \]

\[ M_1 \left( dx_1^b | y_1, \theta \right) \prod_{t=2}^{T} \left\{ W_{t-1}^{a_{t-1}} M_t \left( dx_t^b | y_t, x_{t-1}^a, \theta \right) \right\} \]

\[ \prod_{t=2}^{T} \sum_{i=1}^{N_t-1} w_{t-1}^i f_t \left( x_t^b | x_{t-1}^a, \theta \right) \]

\[ \left( \frac{1}{N_{T-1}} \right) \prod_{j=2}^{C_{T-1}} K_{T-1} \left( \tilde{x}_{T-1}^j, dx_{T-1}^j | \tilde{x}_{1:T-2}, x_{T-1}^a, x_T^b, \tilde{a}_{1:T-3}, \tilde{a}_{T-2}^a, \theta \right) \]

\[ K_{T-1} \left( \tilde{x}_{T-1}^j, dx_{T-1}^j | \tilde{x}_{1:T-2}, x_{T-1}^a, x_T^b, \tilde{a}_{1:T-3}, \tilde{a}_{T-2}^a, \theta \right) \]

\[ \prod_{t=1}^{T-2} \left\{ \left( \frac{1}{N_t} \right) \prod_{j=2}^{C_t} K_t \left( \tilde{x}_{t-1}^j, dx_t^j | \tilde{x}_{1:t-1}, x_t^a, x_{t+1}^a, \tilde{a}_{1:t-2}, a_{t-1}^b, \theta \right) \right\} \]

\[ K_t \left( x_t^b, dx_t | \tilde{x}_{1:t-1}, x_t^a, x_{t+1}^a, \tilde{a}_{1:t-2}, a_{t-1}^b, \theta \right) \]

which is an equivalent measure to \( \Psi (du_{1:T}|\theta) \) defined by (2.14) and (2.15).
To prove Part (iii), we first note that (2.14), (2.15) and (2.17) gives

\[
\frac{\prod (dx_{1:T}, \bar{a}_{1:T-1}, b_{1:T}, dx_{1:T-1}|\theta)}{\Psi (dx_{1:T}, \bar{a}_{1:T-1}, b_{1:T}, dx_{1:T-1}|\theta)} = \left[ \prod \left( d\bar{x}^{C_1}_1, \ldots, d\bar{x}^{C_{T-1}}_{T-1}, dx_T|\theta \right) \left( \frac{1}{N_T} \right) \right]
\]

\[
\Psi (dx_{1:T}, \bar{a}_{1:T-1}|\theta)
\]

\[
M_1 \left( dx_{1|y_1, \theta} T \prod_{t=2}^{T} \left\{ W_{t+1}^{a_{b_t}} M_t \left( dx_t^{b_t}|y_t, x_{t-1} \right) \right\} \right)
\]

\[
\prod_{t=2}^{T} \sum_{i=1}^{N_{t-1}} \frac{w_{i-1}^{a_{b_t}}}{M_t} f_t \left( x_t^{b_t}|a_{b_{t-1}}, \theta \right) \]

\[
\left( \frac{1}{N_{T-1}} \right) \prod_{j=2}^{C_{T-1}} K_{T-1} \left( \bar{x}^{j}_{T-1}, d\bar{x}^{j-1}_{T-1}|\bar{x}_{1:T-2}, \bar{x}_{T-1}^{b_{T-1}}, a_{T-1}, \theta \right)
\]

\[
K_{T-1} \left( \bar{x}^{1}_{T-1}, d\bar{x}^{b_{T-1}}_{T-1}|\bar{x}_{1:T-2}, \bar{x}_{T-1}^{b_{T-1}}, a_{T-1}, \theta \right)
\]

\[
\prod_{t=1}^{T-2} \left\{ \left( \frac{1}{N_t} \right) \prod_{i=1}^{C_t} K_t \left( \bar{x}^{1}_{t}, d\bar{x}^{i-1}_{t}|\bar{x}_{1:t-1}, \bar{x}_{t}^{b_{t}}, a_{t-1}, \theta \right) \right\} / \left[ \Psi (dx_{1:T}, \bar{a}_{1:T-1}|\theta) \right]
\]

\[
W_{T}^{b_{T}} \bar{W}_{T-1}^{b_{T-1}}
\]

\[
K_{T-1} \left( \bar{x}^{T-1}_{T-1}, d\bar{x}^{1}_{T-1}|\bar{x}_{1:T-2}, \bar{x}_{T-1}^{b_{T-1}}, a_{T-1}, \theta \right)
\]

\[
\prod_{j=2}^{C_{T-1}} K_{T-1} \left( \bar{x}^{j}_{T-1}, d\bar{x}^{j-1}_{T-1}|\bar{x}_{1:T-2}, \bar{x}_{T-1}^{b_{T-1}}, a_{T-1}, \theta \right)
\]

\[
\prod_{t=1}^{T-2} \left\{ \left( \frac{1}{N_t} \right) \prod_{i=1}^{C_t} K_t \left( \bar{x}^{1}_{t}, d\bar{x}^{i-1}_{t}|\bar{x}_{1:t-1}, \bar{x}_{t}^{b_{t}}, a_{t-1}, \theta \right) \right\} / \left[ \Psi (dx_{1:T}, \bar{a}_{1:T-1}|\theta) \right]
\]

\[
W_{T}^{b_{T}} \bar{W}_{T-1}^{b_{T-1}}
\]

To simplify the expression in (A.5) we note that from the detailed balance Assumption 2

\[
\frac{K_1 \left( dx'_1|x_1^{b_1}, x_1, \bar{x}_2^{C_2}, \theta \right)}{K_1 \left( dx|x_1^{b_1}, x_1, \bar{x}_2^{C_2}, \theta \right)} = \frac{p \left( dx'_1|y_1, \bar{x}_2^{C_2}, \theta \right)}{p \left( dx|y_1, \bar{x}_2^{C_2}, \theta \right)}
\]
\[
\prod_{j=2}^{C_1} K_1 \left( \frac{\tilde{x}_{1,j}}{d\tilde{x}_{1,j}^{-1}} | x_{1,j}^{-b_1}, \tilde{x}_{2,j}^C, \theta \right) 
\prod_{j=2}^{C_1} K_1 \left( \frac{x_{1,j}^{-b_1}}{d\tilde{x}_{1,j}} | x_{1,j}^{-b_1}, \tilde{x}_{2,j}^C, \theta \right)
\]

\[
= \frac{p \left( dx_{1,t}^b | \tilde{x}_{2,t}^C, \theta \right)}{p \left( dx_{1,t}^{C_{1,t+1}} | \tilde{x}_{2,t}^C, \theta \right)}
\]

\[
= g_1 \left( y_1 | x_{1,t}^b, \theta \right) f_2 \left( \tilde{x}_{2,t}^C | x_{1,t}^b, \theta \right) f_1 \left( x_{1,t}^b | \theta \right) dx_{1,t}^b
\]

\[
g_1 \left( x_1^C_{t+1}, \theta \right) f_2 \left( \tilde{x}_{2,t}^C | x_1^C_{t+1}, \theta \right) f_1 \left( x_1^C_{t+1} | \theta \right) d\tilde{x}_{1,t}^C.
\]

(A.6)

For \( t = 2, \ldots, T - 2 \)

\[
K_t \left( x_t, dx_t | x_{t-1}^{C_{t-1}}, x_{t-1}^{-b_1}, \tilde{x}_{t-1}^{C_{t-1}}, \tilde{x}_{t-1}^{-b_1}, \tilde{a}_{t-1}, \theta \right)
\]

\[
= \frac{\hat{p} \left( dx_t | x_{t-1}^{C_{t-1}}, \tilde{x}_{t-1}^{C_{t-1}}, \tilde{a}_{t-1}, \theta \right)}{\hat{p} \left( dx_t | x_{t-1}^{C_{t-1}}, \tilde{x}_{t-1}^{C_{t-1}}, \tilde{a}_{t-1}, \theta \right)}
\]

so using (2.8)

\[
\left\{ \prod_{j=2}^{C_t} K_t \left( \frac{\tilde{x}_{1,t,j}}{d\tilde{x}_{1,t,j}^{-1}} | x_{1,t-1}^{C_{t-1}}, x_{t,j}^{-b_1}, \tilde{x}_{t,j}^{C_{t+1}}, \tilde{a}_{t-1}^{C_{t-1}}, \tilde{a}_{t-1}^{-b_1}, \theta \right) \right\}
\]

\[
= \frac{\hat{p} \left( dx_t^b | x_{t-1}^{C_{t-1}}, \tilde{x}_{t+1}^{C_{t+1}}, \tilde{a}_{t-1}^{C_{t-1}}, \tilde{a}_{t-1}^{-b_1}, \theta \right)}{\hat{p} \left( dx_t^{C_t} | x_{t-1}^{C_{t-1}}, \tilde{x}_{t+1}^{C_{t+1}}, \tilde{a}_{t-1}^{C_{t-1}}, \tilde{a}_{t-1}^{-b_1}, \theta \right)}
\]

\[
= g_t \left( y_t | x_{t}^b, \theta \right) f_{t+1} \left( \frac{\tilde{x}_{t+1}}{d\tilde{x}_{t+1}^{-1}} | x_{t+1}^{-b_1}, \theta \right) \sum_{i=1}^{N_{t-1}} w_{t-1}^i f_t \left( x_{t}^b | x_{t-1}^i, \theta \right) dx_{t}^b
\]

\[
= g_t \left( y_t | x_{t}^C, \theta \right) f_{t+1} \left( \frac{\tilde{x}_{t+1}}{d\tilde{x}_{t+1}} | x_{t}^C, \theta \right) \sum_{i=1}^{N_{t-1}} w_{t-1}^i f_t \left( x_{t}^b | x_{t-1}^i, \theta \right) d\tilde{x}_{t}^C
\]

\[
= g_t \left( y_t | x_{t}^C, \theta \right) f_{t+1} \left( \frac{\tilde{x}_{t+1}}{d\tilde{x}_{t+1}} | x_{t}^C, \theta \right) \sum_{i=1}^{N_{t-1}} w_{t-1}^i f_t \left( x_{t}^b | x_{t-1}^i, \theta \right) d\tilde{x}_{t}^C.
\]

(A.7)
For $t = T - 1$

$$
K_{T-1} \left( x_{T-1}, dx'_{T-1} | x_{1:T-2}, x_{T-1}^{-b_{T-1}}, x_{T}^{b_{T}}, \bar{a}_{1}, \ldots, \bar{a}_{T-3}, a_{T-2}^{-b_{T-1}}, \theta \right)
\frac{K_{T-1} \left( x'_{T-1}, dx_{T-1} | x_{1:T-2}, x_{T-1}^{-b_{T-1}}, x_{T}^{b_{T}}, \bar{a}_{1}, \ldots, \bar{a}_{T-3}, a_{T-2}^{-b_{T-1}}, \theta \right)}{\hat{p} \left( dx'_{T-1} | x_{1:T-2}, x_{T-1}^{-b_{T-1}}, x_{T}^{b_{T}}, \bar{a}_{1}, \ldots, \bar{a}_{T-3}, a_{T-2}^{-b_{T-1}}, \theta \right)}
= \frac{\hat{p} \left( dx'_{T-1} | x_{1:T-2}, x_{T-1}^{-b_{T-1}}, x_{T}^{b_{T}}, \bar{a}_{1}, \ldots, \bar{a}_{T-3}, a_{T-2}^{-b_{T-1}}, \theta \right)}{\hat{p} \left( dx_{T-1} | x_{1:T-2}, x_{T-1}^{-b_{T-1}}, x_{T}^{b_{T}}, \bar{a}_{1}, \ldots, \bar{a}_{T-3}, a_{T-2}^{-b_{T-1}}, \theta \right)}.
$$
so using (2.9)

$$
\begin{align*}
\prod_{j=2}^{C_{T-1}} K_{T-1} \left( \frac{\bar{x}_{T-1}^{j}}{x_{T-1}}, \frac{dx_{T-1}^{j}}{dx_{T-1}} | \bar{x}_{1:T-2}, x_{T-1}^{-b_{T-1}}, x_{T}^{b_{T}}, \bar{a}_{1:T-3}, a_{T-2}^{-b_{T-1}}, \theta \right)
&\frac{K_{T-1} \left( \frac{\bar{x}_{T-1}^{j}}{x_{T-1}}, \frac{dx_{T-1}^{j}}{dx_{T-1}} | \bar{x}_{1:T-2}, x_{T-1}^{-b_{T-1}}, x_{T}^{b_{T}}, \bar{a}_{1:T-3}, a_{T-2}^{-b_{T-1}}, \theta \right)}{\hat{p} \left( dx_{T-1}^{j} | \bar{x}_{1:T-2}, x_{T-1}^{b_{T}}, \bar{a}_{1:T-3}, \theta \right)}
\end{align*}
$$

(A.8)

$$
= \frac{g_{T-1} (y_{T-1} | x_{T-1}^{b_{T-1}}, \theta) f_{T} (x_{T}^{b_{T}} | x_{T-1}^{-b_{T-1}}, \theta) \sum_{i=1}^{N_{T-2}} W_{T-2} f_{T-1} (x_{T-1}^{b_{T-1}} | x_{T-2}^{b_{T}}, \theta) d x_{T-1}^{b_{T-1}}}{g_{T-1} (y_{T-1} | \bar{x}_{T-1}^{C_{T-1}}, \theta) f_{T} (x_{T}^{b_{T}} | \bar{x}_{T-1}^{C_{T-1}}, \theta) \sum_{i=1}^{N_{T-2}} W_{T-2} f_{T-1} (\bar{x}_{T-1}^{C_{T-1}} | x_{T-2}^{b_{T}}, \theta) d \bar{x}_{T-1}^{C_{T-1}}}
$$

$$
= \frac{g_{T-1} (y_{T-1} | x_{T-1}^{b_{T-1}}, \theta) f_{T} (x_{T}^{b_{T}} | x_{T-1}^{-b_{T-1}}, \theta) \sum_{i=1}^{N_{T-2}} w_{T-2} f_{T-1} (x_{T-1}^{b_{T-1}} | x_{T-2}^{b_{T}}, \theta) d x_{T-1}^{b_{T-1}}}{g_{T-1} (y_{T-1} | \bar{x}_{T-1}^{C_{T-1}}, \theta) f_{T} (x_{T}^{b_{T}} | \bar{x}_{T-1}^{C_{T-1}}, \theta) \sum_{i=1}^{N_{T-2}} w_{T-2} f_{T-1} (\bar{x}_{T-1}^{C_{T-1}} | x_{T-2}^{b_{T}}, \theta) d \bar{x}_{T-1}^{C_{T-1}}}
$$

Substituting (A.6), (A.7) and (A.8) into (A.5), expanding the terms involving the normalized
weights and rearranging and cancelling the term $\Psi (d\mathbf{x}_{1:T}, \mathbf{x}_{1:T-1} | \theta)$ gives

\[
\begin{align*}
\Pi \left( d\mathbf{x}_{1:T}, \mathbf{y}_{1:T-1}, \mathbf{b}_{1:T}, d\mathbf{x}_{1:T-1} | \theta \right) \\
\Psi \left( d\mathbf{x}_{1:T}, \mathbf{y}_{1:T-1}, \mathbf{b}_{1:T}, d\mathbf{x}_{1:T-1} | \theta \right) \\
= \pi \left( \mathbf{x}_{1}^{C_{1}}, \ldots, \mathbf{x}_{T-1}^{C_{T-1}}, \mathbf{x}_{T}^{b_{T}} | \theta \right) \prod_{t=1}^{T} \left\{ \left( \sum_{i=1}^{N_{t}} w_{i}^{t} \right) \left( \frac{1}{N_{t}} \right) \right\} \\
\prod_{t=2}^{T} \left( \sum_{i=1}^{N_{t}} w_{i-1}^{t} \right) f_{t} \left( x_{t}^{b_{t}} | x_{t-1}^{a_{t-1}} | \theta \right)
\end{align*}
\]

(A.9)

Equation (2.6) implies that

\[
w_{t}^{b_{t}} M_{t} \left( x_{t}^{b_{t}} | y_{t}, x_{t-1}^{a_{t-1}} | \theta \right) = g_{t} \left( y_{t} | x_{t}^{b_{t}} | \theta \right) f_{t} \left( x_{t}^{b_{t}} | x_{t-1}^{a_{t-1}} | \theta \right),
\]

(A.10)

and (2.7) implies that for $t = 2, \ldots, T$

\[
w_{t}^{b_{t}} M_{t} \left( x_{t}^{b_{t}} | y_{t}, x_{t-1}^{a_{t-1}} | \theta \right) = g_{t} \left( y_{t} | x_{t}^{b_{t}} | \theta \right) f_{t} \left( x_{t}^{b_{t}} | x_{t-1}^{a_{t-1}} | \theta \right).
\]

(A.11)
Substituting (A.10) and (A.11) into (A.9) gives

\[
\Pi (d\mathbf{x}_{1:T}, \mathbf{a}_{1:T-1}, b_{1:T}, d\mathbf{x}_{1:T-1}\mid \theta) \\
\frac{\Psi (d\mathbf{x}_{1:T}, \mathbf{a}_{1:T-1}, b_{1:T}, d\mathbf{x}_{1:T-1}\mid \theta)}{\pi (x_{C_1}, \ldots, x_{C_{T-1}}, x_T^B \mid \theta) \prod_{t=1}^T \left\{ \left( \sum_{i=1}^{N_t} w_i^t \right) \left( \frac{1}{N_t} \right) \right\}}
\]

as required.

**Proof of Lemma 3**

Let

\[
h^* (\mathbf{x}_{1:T}, \mathbf{a}_{1:T-1} \mid \theta) = \frac{\prod_{t=1}^T \left\{ \left( \sum_{i=1}^{N_t} w_i^t \right) \left( \frac{1}{N_t} \right) \right\}}{p(y_{1:T} \mid \theta)}
\]

From (2.18),

\[
\Pi (d\mathbf{x}_{1:T}, \mathbf{a}_{1:T-1}, b_{1:T}, d\mathbf{x}_{1:T-1}\mid \theta) = h^* (\mathbf{x}_{1:T}, \mathbf{a}_{1:T-1} \mid \theta) \Psi (d\mathbf{x}_{1:T}, \mathbf{a}_{1:T-1}, b_{1:T}, d\mathbf{x}_{1:T-1}\mid \theta).
\] (A.12)

Integrating (A.12) over \(b_{1:T}, \mathbf{x}_{1:T-1}\) shows that the marginal distributions of \(\Pi (d\mathbf{x}_{1:T}, \mathbf{a}_{1:T-1})\) and \(\Psi (d\mathbf{x}_{1:T}, \mathbf{a}_{1:T-1})\) satisfy

\[
\Pi (d\mathbf{x}_{1:T}, \mathbf{a}_{1:T-1}\mid \theta) = h^* (\mathbf{x}_{1:T}, \mathbf{a}_{1:T-1} \mid \theta) \Psi (d\mathbf{x}_{1:T}, \mathbf{a}_{1:T-1}\mid \theta).
\]

Hence the conditional distribution of \(\Pi (b_{1:T}, d\mathbf{x}_{1:T-1} \mid \mathbf{x}_{1:T}, \mathbf{a}_{1:T-1}, \theta)\) is given by

\[
\Pi (b_{1:T}, d\mathbf{x}_{1:T-1} \mid \mathbf{x}_{1:T}, \mathbf{a}_{1:T-1}, \theta) = \frac{\Pi (d\mathbf{x}_{1:T}, \mathbf{a}_{1:T-1}, b_{1:T}, d\mathbf{x}_{1:T-1}\mid \theta)}{\Pi (d\mathbf{x}_{1:T}, \mathbf{a}_{1:T-1}\mid \theta)}
\]

\[
= \frac{\Psi (d\mathbf{x}_{1:T}, \mathbf{a}_{1:T-1}, b_{1:T}, d\mathbf{x}_{1:T-1}\mid \theta)}{\Psi (d\mathbf{x}_{1:T}, \mathbf{a}_{1:T-1}\mid \theta)},
\]

which shows that

\[
\Pi (b_{1:T}, d\mathbf{x}_{1:T-1} \mid \mathbf{x}_{1:T}, \mathbf{a}_{1:T-1}, \theta) = \Psi (b_{1:T}, d\mathbf{x}_{1:T-1} \mid \mathbf{x}_{1:T}, \mathbf{a}_{1:T-1}, \theta),
\]

as required.

**Proof of Lemma 4**

The proof is similar to the proof of Part (i) of Lemma 2. Note, however, that the order is reversed since the algorithm starts by generating from the simplest marginal distributions and then adds variables by generating from their conditional distributions.
Equation (A.4) in the proof of Lemma 2 derives the expressions in Step 1 for the case when \( t = 1 \). Similarly, equations (A.2) and (A.3) derive the expressions in Step 1 for the cases when \( t = 2, \ldots, T - 1 \). Finally, equation (A.1) derives the expressions in Steps 2 and 3.

Proof of Theorem 2

Sampling Scheme 2 is a Gibbs sampler targeting \( \Pi(dU_{1:T}|\theta) \) by construction, so it is sufficient to show irreducibility and aperiodicity of the Markov chain.

From Step 2, the marginal process involving \( \tilde{X}_{1:T}, \tilde{A}_{1:T-1}, B_{1:T} \) is a Markov chain. From Assumption 3, the accessible sets of this marginal chain are the same as the assessible sets of the Particle Gibbs sampler of Lindsten and Schön (2012) with fixed parameters \( \theta \). From Assumption 1, Theorem 1 of Lindsten and Schön (2012) applies with fixed parameters \( \theta \), and hence the marginal chain involving \( \tilde{X}_{1:T}, \tilde{A}_{1:T-1}, B_{1:T} \) is irreducible and aperiodic.

From Step 2 of Sampling Scheme 2, \( \tilde{X}_{1:T-1} \) is generated from \( \Pi(d\tilde{X}_{1:T-1}|\tilde{X}_{1:T}, \tilde{A}_{1:T-1}, B_{1:T}, \theta) \) and hence the full chain involving \( X_{1:T}, \tilde{A}_{1:T-1}, B_{1:T}, \tilde{X}_{1:T-1} \) is also irreducible and aperiodic.

Proof of Theorem 3

We first note that if there are PMMH steps in Part 1 of Sampling Scheme 3 then irreducibility and aperiodicity follows from Lemma 2 (ii).

Suppose there are no PMMH steps in Part 1 of Sampling Scheme 3 and the resulting Markov chain is reducible or periodic. This implies that for any fixed value of \( \theta \in \Theta \) the Markov chain for the particle Gibbs smoother in Sampling Scheme 2 is also reducible or periodic, contradicting Theorem 2.
Figure 2: Binomial regression model. Maximum IACT among the $\tau_i$s ($i = 1, 2, 3, 4$) for different choices of number of particles ($N=5,10,20,40$) and MCMC steps ($C=10,20,30$) for the extended space particle Gibbs sampler (ES). Also shown is the performance of the backward simulation approach in Lindsten and Schön (2012) (BSi). We also consider $N = 50, 75, 100, 150, 200, 250$ for the backward simulation approach (BSi) in panel (b). The results for the extended space particle Gibbs sampler is displayed in panel (a). Panel (b) shows the results for the backward simulation algorithm, compared with our new approach. The IACT is calculated using overlap batch means with 95,000 samples and window size 309.