Adaptive exact-approximate sequential Monte Carlo

Imke Botha*,†, Robert Kohn†, Leah South*,†, and Christopher Drovandi*†

*School of Mathematical Sciences, Queensland University of Technology (QUT)
†School of Economics, University of New South Wales
‡Australian Research Council Centre of Excellence for Mathematical & Statistical Frontiers (ACEMS)
◊QUT Centre for Data Science

January 28, 2022

Abstract

Exact-approximate sequential Monte Carlo (SMC) methods target the exact posterior of intractable likelihood models by using a non-negative unbiased estimator of the likelihood when the likelihood is computationally intractable. For state-space models, a particle filter estimator can be used to obtain an unbiased estimate of the likelihood. The efficiency of exact-approximate SMC greatly depends on the variance of the likelihood estimator, and therefore on the number of state particles used within the particle filter. We introduce a novel method to adaptively select the number of state particles within exact-approximate SMC. We also utilise the expected squared jumping distance to trigger the adaptation, and modify the exchange importance sampling method of Chopin et al. (2012) to replace the current set of state particles with the new set. The resulting algorithm is fully adaptive, and can significantly improve current methods.

Code for our methods is available at https://github.com/imkebotha/adaptive-exact-approximate-smc.

Keywords— Bayesian inference, State-space models, SMC, Pseudo-marginal, Particle MCMC

1 Introduction

We are interested in performing Bayesian parameter inference for state-space models (SSMs) with intractable likelihoods. SSMs are ubiquitous in the natural sciences, engineering and econometrics; see Cappe et al. (2005) and references therein for an overview. They are used when the process of interest is observed indirectly over time or space, i.e. they consist of a hidden or latent process \( \{X_t\}_{t \geq 1} \) and an observed process \( \{Y_t\}_{t \geq 1} \). Define \( z_{i:j} := \{z_i, z_{i+1}, \ldots, z_j\} \) for \( j \geq i \). A key assumption of state space models is that the process \( \{(x_t, y_t), t \geq 1\} \) is Markov. We will further assume that

\[
p(y_t | x_{t-1}, y_{t-1}, \theta) = g(y_t | x_t, \theta)
\]

and

\[
p(x_t | x_{t-1}, y_{t-1}, \theta) = f(x_t | x_{t-1}, \theta),
\]
where $\theta \in \Theta$ are the model parameters and $t = 1, \ldots, T$ are the observation times. It follows that

$$p(x_t, y_t \mid x_{1:t-1}, y_{1:t-1}, \theta) = g(y_t \mid x_t, \theta)f(x_t \mid x_{t-1}, \theta).$$

The densities $g(y_t \mid x_t, \theta)$ and $f(x_t \mid x_{t-1}, \theta)$ are the observation density and transition density respectively; the initial density of the latent states is $\mu(x_1 \mid \theta)$.

Our interest lies in the posterior distribution of $\theta$,

$$p(\theta \mid y_{1:T}) = \frac{p(\theta)}{p(y_{1:T})} \int_{x_{1:T}} p(x_{1:T}, y_{1:T} \mid \theta) dx_{1:T}, \quad (1)$$

where $p(\theta)$ is the prior distribution, and

$$p(x_{1:T}, y_{1:T} \mid \theta) = \mu(x_1 \mid \theta) \prod_{t=2}^{T} f(x_t \mid x_{t-1}, \theta) \prod_{t=1}^{T} g(y_t \mid x_t, \theta). \quad (2)$$

The integral in (1) is the likelihood function $p(y_{1:T} \mid \theta)$, which is often computationally intractable, but can be estimated unbiasedly by the particle filter. In the general case, particle Markov chain Monte Carlo (MCMC; Andrieu and Roberts, 2009; Andrieu et al., 2010) methods can be used for exact parameter inference. These methods are ‘exact-approximations’ of the ideal MCMC algorithms (Andrieu et al., 2010), i.e. as the number of state particles ($N_x$) used to estimate the likelihood approaches infinity, they target (1) exactly.

Chopin et al. (2012) and Duan and Fulop (2014) extend the idea of ‘exact-approximate’ algorithms to sequential Monte Carlo (SMC) samplers. SMC samplers are a popular alternative to MCMC to simulate from the posterior distribution arising from complex models. Compared to MCMC samplers, they are inherently parallelisable, better equipped to handle multimodal targets and can control the effective sample size (ESS). SMC methods recursively sample through a sequence of distributions using a combination of reweighting, resampling and mutation steps. In the Bayesian setting, this sequence often starts at the prior, and ends at the posterior distribution. Exact-approximate SMC methods for state space models use a particle filter estimate of the likelihood in the reweighting step, and mutate the particles using $R$ particle MCMC iterations. For any fixed number of state particles ($N_x$), exact-approximate SMC targets (1) as the number of parameter particles ($N_\theta$) approaches infinity (Duan and Fulop, 2014).

While they target the exact posterior, the sampling efficiency of exact-approximate methods greatly depends on the variance of the likelihood estimator, and consequently, the number of state particles used within the particle filter. In MCMC, $N_x$ is generally tuned manually, which can be time intensive. The current recommendation (Pitt et al., 2012; Doucet et al., 2015; Sherlock et al., 2015) is to choose $N_x$ such that the variance of the log-likelihood estimator is between 1 and 3 when evaluated at a central value of the parameters, e.g. the posterior mean. This requires at least a pilot run of the algorithm to estimate the posterior mean, and an exploration of the sample variance over multiple values of $N_x$.

Although Chopin et al. (2012, 2015) and Duan and Fulop (2014) propose strategies to automatically tune $N_x$ in exact-approximate SMC, these have a number of drawbacks. Firstly, all three methods fix the number of MCMC iterates $R$, and adapt $N_x$ when the acceptance rate of the mutation step falls below some threshold value. Since the optimal
acceptance rate within particle MCMC is problem-specific, both it and $R$ must be tuned. The value of $N_x$ can also be difficult to choose in practice, and has a significant effect on both the Monte Carlo error of the SMC approximation to the target distribution and the computation time. Current methods require a moderate starting value of $N_x$ to avoid poor values in subsequent iterations, i.e. values that are too low and negatively impact the accuracy of the samples, or unnecessarily high values that increase the computation time. Our article introduces a novel and principled strategy to automatically tune both $N_x$ and $R$, while aiming to keep an optimal balance between statistical and computational efficiency. We also give a modification of the exchange importance sampling method of Chopin et al. (2012) to update the set of state particles once $N_x$ has been adapted. Unlike the exchange importance sampling approach, however, this modified version introduces no extra variability in the parameter particle weights.

The rest of the paper is organized as follows. Section 2 gives the necessary background on sequential Monte Carlo methods, particle filters and exact-approximate SMC. Section 3 describes the current methods for adapting the number of state particles in exact-approximate SMC. Section 4 describes our novel tuning methodology. Section 5 shows the performance of our methods on a Brownian motion model, a stochastic volatility model, a noisy theta-logistic model and a noisy Ricker model. Section 6 concludes.

2 Sequential Monte Carlo

2.1 General SMC and Particle Filters

Sequential Monte Carlo (SMC) recursively samples from a sequence of distributions, starting at one that is easy to sample from and ending at the target distribution, i.e. the posterior \cite{DelMoral2006}. Assuming that the likelihood function is tractable, there are at least two general ways to construct this sequence. The first is likelihood tempering, which gives $\pi_t(\theta \mid y) \propto \eta_t(\theta, y) = p(y_{1:t} \mid \theta)^{\gamma_t} p(\theta)$ for $t = 0, \ldots, D$, where $0 = \gamma_0 \leq \ldots \leq \gamma_D = 1$. The second is data annealing \cite{Chopin2002}, which gives $\pi_t(\theta \mid y) \propto \eta_t(\theta, y) = p(y_{1:t} \mid \theta)p(\theta)$ as the tth density, for $t = 0, \ldots, T$, where $T$ is the number of observations and $D = T$. Both sequences have $\pi_0(\theta \mid y) = p(\theta)$ and $\pi_D(\theta \mid y) = p(\theta \mid y_{1:T})$.

The distributions $\pi_0(\theta \mid y), \ldots, \pi_D(\theta \mid y)$ are traversed using a combination of reweight, resample and mutation steps. Initially, $N_\theta$ samples are drawn from $\pi_0(\theta \mid y)$ and given equal weights $\{\theta_0^i, W_0^i\} = \{1 \over N_\theta\}_{i=1}^{N_\theta}$. For each subsequent distribution, the samples are reweighted as

$$w_t^n = w_{t-1}^n \cdot \frac{\pi_t(\theta_t^n)}{\pi_{t-1}(\theta_{t-1}^n)}, \quad W_t^n = \frac{w_t^n}{\sum_{i=1}^{N_\theta} w_t^i},$$

and then resampled according to their weights, thus removing particles with negligible weights and duplicating high-weight particles. Finally, the particles are diversified using a mutation kernel which ensures that the current target $\pi_t(\theta \mid y)$ remains invariant, e.g. using an MCMC step. At each iteration $t$, the weighted particles $\{\theta_t^n, W_t^n\}_{n=1}^{N_\theta}$ form an approximation of $\pi_t(\theta \mid y)$.

An advantage of SMC methods is that an unbiased estimate of the normalizing constant
of the target distribution can be obtained as follows

\[ \int \eta_t(\theta, y) d\theta \approx \prod_{t=0}^{D} \sum_{n=1}^{N_\theta} w^n_t. \]  

This feature is fundamental to the exact-approximate methods described in Section 2.2

By constructing a data annealing SMC algorithm, targeting

\[ \pi_t(x_{1:t} \mid y_{1:t}, \theta) \propto p(x_1, y_1 \mid \theta) \prod_{j=2}^{t} p(x_j, y_j \mid x_{j-1}, \theta), \quad t = 1, \ldots, T, \]

an unbiased estimate of the likelihood \( p(y_{1:T} \mid \theta) \) can be obtained from the weights as in (3). SMC methods for dynamic models are known as particle filters; Algorithm 1 shows pseudo-code for the bootstrap particle filter (Gordon et al., 1993). Define \( x_{1:T}^{1:N_x} := \{x_1^{1:N_x}, \ldots, x_T^{1:N_x}\} \). The likelihood estimate with \( N_x \) state particles is then

\[ \hat{p}_{N_x}(y_{1:T} \mid \theta, x_{1:T}^{1:N_x}) = \prod_{t=1}^{T} \sum_{n=1}^{N_x} w^n_t = \prod_{t=1}^{T} \left( \frac{1}{N_x} \sum_{j=1}^{N_x} g(y_t \mid x^n_j, \theta) \right). \]  

Let \( \psi(x_{1:T}^{1:N_x}, a_{1:T-1}^{1:N_x}) \) be the joint distribution of all the random variables drawn during the course of the particle filter, i.e. the latent states \( x_{1:T}^{1:N_x} \) and their associated ancestral indices \( a_{1:T-1}^{1:N_x} \) (Andrieu et al., 2010). For brevity, explicit dependence on the ancestral indices is omitted.

By an unbiased estimate of the likelihood we mean \( \mathbb{E}_{\psi(x_{1:T}^{1:N_x})} \left( \hat{p}_{N_x}(y_{1:T} \mid \theta, x_{1:T}^{1:N_x}) \right) = p(y_{1:T} \mid \theta) \) (Section 7.4.1 of Del Moral et al., 2006; see also Pitt et al., 2012). The notation

\[ \hat{p}_{N_x}(y_{1:T} \mid \theta) = \hat{Z}(\theta) = \hat{p}_{N_x}(y_{1:T}, x_{1:T}^{1:N_x} \mid \theta) = \hat{p}_{N_x}(y_{1:T} \mid \theta, x_{1:T}^{1:N_x}) \psi(x_{1:T}^{1:N_x}) \]

\[ = \frac{1}{N_x} \sum_{n=1}^{N_x} \hat{p}_{N_x}(y_{1:T} \mid \theta, x^n_{1:T}), \quad x^n_{1:T} \sim \psi(x_{1:T}^{1:N_x}) \]

is used interchangeably below.

## 2.2 Exact-approximate SMC

Standard SMC methods cannot be applied directly to state-space models if the parameters \( \theta \) are unknown — the exception being when the integral in (11) is analytically tractable. When the likelihood is intractable, exact-approximate methods may be used. Two general methods are the density tempered marginalised SMC algorithm of Duan and Fulop (2014) and the data annealing SMC method of Chopin et al. (2012), which we refer to as EASMC-DT and EASMC-DA respectively.

The sequence of distributions \( \pi_t(\theta) \) for \( t = 0, 1, \ldots, D \) are given by

\[ \pi_t(\theta, x_{1:T}^{1:N_x} \mid y_{1:T}) \propto p(\theta) \left[ \hat{p}_{N_x}(y_{1:T} \mid \theta, x_{1:T}^{1:N_x}) \right]^{\gamma_t} \psi(x_{1:T}^{1:N_x}), \quad 0 = \gamma_0 \leq \ldots \leq \gamma_D = 1 \]

for EASMC-DT and

\[ \pi_t(\theta, x_{1:T}^{1:N_x} \mid y_{1:T}) \propto p(\theta) \hat{p}_{N_x}(y_{1:T} \mid \theta, x_{1:T}^{1:N_x}) \psi(x_{1:T}^{1:N_x}), \quad D = T \]
Algorithm 1: The bootstrap particle filter of Gordon et al. (1993).

**Input**: data $y_{1:T}$, number of state particles $N_x$ and the static parameters $\theta$.

The index $(n)$ means ‘for all $n \in \{1, \ldots, N_x\}$’

**Output**: likelihood estimate $\hat{Z}(\theta)$, set of weighted state particles $\{x_{1:T}^{1:N_x}, W_{1:T}^{1:N_x}\}$

/* Initialise */

1. Initialise $x_1^{1:N_x} \sim \mu(\cdot \mid \theta)$ and calculate the initial weights

$$w_1^{(n)} = \frac{1}{N_x} \cdot g(y_1 \mid x_1^{(n)}, \theta), \quad W_1^{(n)} = \frac{w_1^{(n)}}{\sum_{i=1}^{N_x} w_1^{(i)}}$$

/* Initialise likelihood estimate */

2. Initialise the likelihood estimate $\hat{Z}(\theta) = \sum_{n=1}^{N_x} w_1^{(n)}$

3. for $t = 2$ to $T$ do

   /* Resample */

4. Resample $N_x$ particles from $x_{t-1}^{1:N_x}$ with probability $W_{t-1}^{1:N_x}$

   /* Simulate forward */

5. Simulate the particles forward, $x_t^{(n)} \sim f(\cdot \mid x_{t-1}^{(n)}, \theta)$

   /* Reweight */

6. Re-weight the particles from $\pi_{t-1}(\cdot)$ to $\pi_t(\cdot)$

$$w_t^{(n)} = \frac{1}{N_x} \cdot g(y_t \mid x_t^{(n)}, \theta), \quad W_t^{(n)} = \frac{w_t^{(n)}}{\sum_{i=1}^{N_x} w_t^{(i)}}$$

/* Update likelihood estimate */

7. Update the likelihood estimate $\hat{Z}(\theta) = \hat{Z}(\theta) \cdot \sum_{n=1}^{N_x} w_t^{(n)}$

end
for EASMC-DA. Algorithm 2 shows the pseudo-code for both methods. For conciseness, we denote the set of weighted state particles as \( \tilde{x}_t^{1:N_x,n} = \{ x_t^{1:N_x,n}, s_t^{1:N_x,n} \} \), where \( s_t^{1:n} \) is the normalised weight of the \( j \)th state particle associated with the \( n \)th parameter particle at iteration \( t \), where \( j = 1, \ldots, N_x \) and \( n = 1, \ldots, N_\theta \). The \( n \)th parameter particle with its attached set of weighted state particles is denoted as \( \theta_t^n = \{ \theta_t^n, \tilde{x}_t^{1:N_x,n} \} \), \( n = 1, \ldots, N_\theta \).

The weights for \( \theta_t^n \) are

\[
w_t^n = W_{t-1} \cdot \frac{\pi_t(\theta_{t-1}^n)}{\pi_{t-1}(\theta_{t-1}^n)}, \quad W_t^n = \frac{w_t^n}{\sum_{i=1}^{N_\theta} w_t^i}
\]

More specifically,

\[
w_t^n = \begin{cases} W_{t-1} \cdot \left[ \tilde{p}_{N_x}(y_{1:T} \mid \theta, x_{1:T}) \right]^{\gamma_{t-1} - \gamma_{t-1}}, & \text{EASMC-DT} \\
W_{t-1} \cdot \tilde{p}_{N_x}(y_t \mid y_{1:t-1}, \theta_{t-1}^n), & \text{EASMC-DA} \end{cases}
\]

where \( \tilde{p}_{N_x}(y_t \mid y_{1:t-1}, \theta_{t-1}^n) \) is obtained from iteration \( t \) of a particle filter (see [1] and Algorithm 1). Particles are mutated using a particle MCMC kernel \( K(\cdot, \cdot) \); Section 2.3 describes the particle marginal Metropolis-Hastings (PMMH) algorithm.

Due to the tempering parameter \( \gamma_t \), EASMC-DT is only exact at the final temperature, i.e. \( p(\theta \mid y_{1:T}, \gamma_t) \propto p(\theta)p(y_{1:T} \mid \theta)^{\gamma_t} \) is a marginal distribution of \( \pi_t(\theta, x_{1:T} \mid y_{1:T}) \) only when \( \gamma_t = 1 \). In contrast, EASMC-DA admits \( p(\theta \mid y_{1:t}) \) as a marginal distribution of \( \pi_t(\theta, x_{1:t} \mid y_{1:t}) \) for all \( t = 1, \ldots, T \). Note that the target at \( t = 0 \) is the prior for both methods, which is assumed to be easy to evaluate and sample from.

### Algorithm 2: Exact-approximate SMC

**Input**: data \( y_{1:T} \), number of particles \( N_\theta \). The index \( n \) means ‘for all \( n \in \{1, \ldots, N_\theta\} \)’

**Output**: set of weighted state particles \( \{ \theta_{t:D}^{1:N_\theta}, W_{t:D}^{1:N_\theta} \} \)

1. Initialise \( \theta_0^{1:N_\theta} \) and set \( W_0^{1:N_\theta} = \frac{1}{N_\theta} \)
2. for \( t = 1 \) to \( D \) do
   /* Reweight */
   3. Re-weight the particles from \( \pi_{t-1}(\cdot) \) to \( \pi_t(\cdot) \) using (5)
   /* Resample */
   4. Resample \( N_\theta \) particles from \( \theta_t^{1:N_\theta} \) with probability \( W_t^{1:N_\theta} \)
   /* Mutate */
   5. for \( r = 1 \) to \( R \) do
      6. PMMH mutation \( \vartheta_t^{(n)} \sim K(\vartheta_t^{(n)}, \cdot) \) (See Algorithm 3)
   7. end
6. end

### 2.3 Particle MCMC mutations

The simplest choice to mutate the particles in exact-approximate SMC is a sequence of Markov move steps using the PMMH algorithm; see Gunawan et al. (2021) for alternatives.
The PMMH method is a standard Metropolis-Hastings algorithm where the intractable likelihood is replaced by the particle filter estimate in (4). Algorithm 3 shows a single PMMH iteration.

**Algorithm 3: Particle marginal Metropolis-Hastings iteration**

**Input:** data \( y \), current parameter value \( \theta_t \), current likelihood estimate \( \hat{p}_{N_x}(y \mid \theta_t) \). Optional: current set of weighted state particles \( \tilde{x}_t^{1:N_x} \).

**Output:** new parameter value \( \theta_t \), new likelihood estimate \( \hat{p}_{N_x}(y \mid \theta_t) \). Optional: new set of weighted state particles \( \tilde{x}_t^{1:N_x} \).

1. Sample \( \theta_t^* \sim q(\cdot \mid \theta_t) \).
2. Run Algorithm 1 to obtain \( \hat{p}_{N_x}(y \mid \theta_t^*) \) and \( \tilde{x}_t^{1:N_x,*} \).
3. Calculate acceptance probability
   
   \[ \alpha(\theta_t, \theta_t^*) = \min\left(1, \frac{\hat{p}_{N_x}(y \mid \theta_t^*) p(\theta_t^*) q(\theta_t^* \mid \theta_t)}{\hat{p}_{N_x}(y \mid \theta_t) p(\theta_t) q(\theta_t \mid \theta_t)}\right). \] (6)
4. With probability \( \alpha(\theta_t, \theta_t^*) \), set \( \theta_t = \theta_t^* \), \( \hat{p}_{N_x}(y \mid \theta_t) = \hat{p}_{N_x}(y \mid \theta_t^*) \), \( \tilde{x}_t^{1:N_x} = \tilde{x}_t^{1:N_x,*} \), otherwise keep the current values of \( \theta_t \), \( \hat{p}_{N_x}(y \mid \theta_t) \) and \( \tilde{x}_t^{1:N_x} \).

While a PMMH mutation leaves the current target invariant, its acceptance rate is sensitive to the variance of the likelihood estimator \cite{Andrieu2010}. In practice, this means that if the variance is too high, then some particles may not be mutated during the mutation step — even with a large number of MCMC iterations.

In the context of particle MCMC samplers, \cite{Andrieu2010} show that \( N_x \) must be chosen as \( O(T) \) to achieve reasonable acceptance rates, i.e. reasonable variance of the likelihood estimator. \cite{Pitt2012, Doucet2015} and \cite{Sherlock2015} recommend choosing \( N_x \) such that the variance of the log-likelihood estimator is between 1 and 3 when evaluated at, e.g., the posterior mean. This generally requires a (potentially time-consuming) tuning process for \( N_x \) before running the algorithm.

For EASMC, less particles may be required to achieve reasonable acceptance rates in the early stages of the algorithm; in EASMC-DA, \( N_x = O(t) \) suggests starting with a small \( N_x \), and increasing it with each added observation. Likewise, in EASMC-DT, a small \( \gamma_t \) will reduce the impact of a highly variable log-likelihood estimator. In addition, unlike particle MCMC methods, it is possible to automatically adapt \( N_x \) within exact-approximate SMC.

The next section describes the tuning strategies proposed by \cite{Chopin2012, Chopin2015} and \cite{Duan2014}.

### 3 Existing methods to calibrate \( N_x \)

There are three main stages to adapting \( N_x \): (1) triggering the adaptation, (2) choosing the new number of particles \( N_x^* \), and (3) replacing the current set of state particles \( \tilde{x}_t^{1:N_x,1:N_\theta} \) with the new set \( \tilde{x}_t^{1:N_x^*,1:N_\theta} \). To simplify notation, we write \( \tilde{x}_t^{1:N_x,1:N_\theta} \) as \( \tilde{x}_t^{1:N_x} \).
Stage 1. Triggering the adaptation

It may be necessary to adapt \( N_x \) when the mutation step no longer achieves sufficient particle diversity. Chopin et al. (2012, 2015) and Duan and Fulop (2014) fix the number of MCMC iterations (\( R \)) and change \( N_x \) whenever the acceptance rate of a single MCMC iteration falls below some target value. This approach has two main drawbacks. First, the acceptance rate does not take the jumping distances of the particles into account, and can be made artificially high by making very local proposals. Second, both \( R \) and the target acceptance rate must be tuned — even if the exact likelihood is used, the acceptance rate may naturally be low, depending on the form of the posterior and the proposal function used within the mutation kernel. Ideally, \( N_x \) and \( R \) should be jointly adapted.

Stage 2. Choosing the new number of particles \( N_x^* \)

A new number of state particles (\( N_x^* \)) is determined in the second stage. Chopin et al. (2012) set \( N_x^* = 2 \cdot N_x \) (DOUBLE), while Duan and Fulop (2014) set \( N_x^* = \sigma_{N_x}^2 \cdot N_x \) (RESCALE-VAR), where \( \sigma_{N_x}^2 \) is the variance of the log-likelihood estimator using \( N_x \) state particles. The variance is estimated from \( k \) independent estimates of the log-likelihood (for the current SMC target) based on the sample mean of the parameter particles. This choice is motivated by the results of Pitt et al. (2012), Doucet et al. (2015) and Sherlock et al. (2015), who show that \( \sigma_{N_x}^2 \propto 1/N_x \) for any number of state particles \( N_x \). Setting \( \sigma_{N_x}^2 = \alpha/N_x \) and rearranging gives both \( \alpha = \sigma_{N_x}^2 \cdot N_x \) and \( N_x = \alpha/\sigma_{N_x}^2 \). Given \( N_x \) and \( \sigma_{N_x}^2 \), these expressions can be used to find a new number of state particles \( N_x^* \) such that \( \sigma_{N_x^*}^2 = 1 \), by noting that \( N_x^* = \alpha/\sigma_{N_x^*}^2 = \alpha/1 = \sigma_{N_x}^2 \cdot N_x \).

We find that if the initial \( N_x \) is too small, then the DOUBLE scheme of Chopin et al. (2012) can take a significant number of iterations to set \( N_x \) to a reasonable value. It can also increase \( N_x \) to an unnecessarily high value if the adaptation is triggered when the number of state particles is already large.

While the RESCALE-VAR method of Duan and Fulop (2014) is more principled, as it takes the variance of the log-likelihood estimator into account, we find that it is also sensitive to the initial number of particles. For a poorly chosen initial \( N_x \), the variance of the log-likelihood estimator can be of order \( 10^2 \) or higher. In this case, scaling the current number of particles by \( \sigma_{N_x}^2 \) may give an extremely high value for \( N_x^* \).

Chopin et al. (2015) propose a third method; they set \( N_x^* = \tau/\sigma_{N_x}^2 \), where \( \tau \) is a model-specific tuning parameter, and \( \sigma_{N_x}^2 \) is an estimate of the variance of the log-likelihood estimator with \( N_x \) state particles. This choice is motivated by the results from Doucet et al. (2012) (an earlier version of Doucet et al. (2015)). See Chopin et al. (2015) for further details. This approach is not included in our numerical experiments in Section 5 due to the tuning parameter \( \tau \).

Stage 3. Replacing the particle set

The final stage replaces the current set of state particles \( \tilde{x}_t^1:N_x \) by the new set \( \tilde{x}_t^1:N_x^* \). Chopin et al. (2012) propose a reweighting step (REWEIGHT) using the generalised importance sampling method of Del Moral et al. (2006) to swap \( \tilde{x}_t^1:N_x^* \) with \( \tilde{x}_t^1:N_x^* \). The
The modified sequence of distributions is

\[
\pi_t(\theta, x_{1:T}^{1:N_x^*} | y_{1:T}) \propto \mathcal{Q}(\theta)^{1-\gamma_t} \left[ p(\theta) \overline{p}_{N_x}(y_{1:T} \mid \theta, x_{1:T}^{1:N_x^*}) \right]^{\gamma_t} \psi(x_{1:T}^{1:N_x^*}), \quad 0 = \gamma_0 \leq \ldots \leq \gamma_D = 1.
\]

The REINIT method aims to minimize the variance of the weights, but we find it can be very slow as the algorithm may reinitialise numerous times before completion, each time with a larger number of particles. This approach also assumes that the current set of particles is more informative than the prior, which is not necessarily the case if the adaptation is triggered early.
4 Methods

This section describes our proposed approach for each of the three stages involved in adapting the number of state particles.

4.1 Triggering the adaptation

Instead of using the acceptance rate to measure particle diversity, we use the expected squared jumping distance (ESJD), which accounts for both the acceptance rate (the probability that the particles will move) and the jumping distance (how far they will move). See Pasarica and Gelman (2010), Fearnhead and Taylor (2013), Salomone et al. (2018) and Bon et al. (2021) for examples of this idea outside of the exact-approximate context. The conditional ESJD is defined as

\[ H(\theta, \theta^*) := \mathbb{E} \left[ \|\theta^* - \theta\|^2 \mid (\theta, \theta^*) \right] \]  

which can be estimated as

\[ \hat{H}(\theta, \theta^*) = \|\theta^* - \theta\|^2 \alpha(\theta, \theta^*) = (\theta - \theta^*)^\top \hat{\Sigma}^{-1}(\theta - \theta^*)\alpha(\theta, \theta^*), \]  

where \( \|\theta^* - \theta\| \) is the estimated Mahalanobis distance, \( \hat{\Sigma} \) is the sample covariance of the current parameter particle set, \( \theta \) is the current value of the parameters, \( \theta^* \) is the proposed value, and \( \alpha(\theta, \theta^*) \) is the acceptance probability in (6).

The unconditional ESJD is

\[ \text{ESJD} = \mathbb{E} \left[ \|\theta^* - \theta\|^2 \right] = \mathbb{E}[H(\theta, \theta^*)] \]

which can be estimated using

\[ \overline{\text{ESJD}} = \frac{1}{N_0} \sum_{i=1}^{N_0} \hat{H}(\theta_i, \theta_i^*). \]

We use \( \overline{\text{ESJD}}_{t,r} \) to refer to the estimated unconditional ESJD of the \( r \)th MCMC iteration of the mutation step at iteration \( t \) (steps 5-7 of Algorithm 2). The total estimated unconditional ESJD for iteration \( t \) is \( \text{ESJD}_t = \sum_{r=1}^R \overline{\text{ESJD}}_{t,r} \).

Algorithm 4 outlines how \( N_x \) and \( R \) are adapted. To summarise, the adaptation is triggered in iteration \( t \) if \( \text{ESJD}_{t-1} \) is below some target value (stage 1). Once triggered, the number of particles is adapted (stage 2) and the particle set is updated (stage 3). A single MCMC iteration is then run with the new number of particles, and the results from this step are used to determine how many MCMC iterations are required to reach the target ESJD, i.e. \( R \) is given by dividing the target ESJD by the unconditional ESJD of the single MCMC iteration and rounding up. Once the adaptation is complete, the remaining MCMC iterations are completed. This approach gives a general framework which can be implemented with any of the stage 2 and stage 3 methods described in Section 3 as well as our novel methods in Sections 4.2 and 4.3.

4.2 Choosing the new number of particles \( N_x^* \)

To set the new number of state particles \( N_x^* \), we build on the rescale-var method of Duan and Fulop (2014). Recall, this method sets \( N_x^* = \sigma_{N_x}^2 \cdot N_x \), where \( \sigma_{N_x}^2 \) is the sample
**Algorithm 4: Adaptive mutation step**

**Input**: the total unconditional ESJD from the previous iteration ($\text{ESJD}_{t-1}$), the target total unconditional ESJD for each iteration ($\text{ESJD}_{\text{target}}$) and the current set of particles $\vartheta_t^{1:N_\theta}$

1. \[ \text{adapt} = \text{ESJD}_{t-1} < \text{ESJD}_{\text{target}} \]
2. if adapt then
   3. /* Adapt $N_x$ */
   4. Set new $N_x$ and update the particle set using any combination of the stage 2 and stage 3 methods described in Sections 3.1.2 and 1.3
5. /* Initial mutation step with updated $N_x$ (if applicable) */
6. PMMH mutation $\vartheta_t^{1:N_\theta} \sim K(\vartheta_t^{1:N_\theta}, \cdot)$, calculate $\text{ESJD}_{t,1}$
7. if adapt then
   8. /* Adapt $R$ */
   9. Set $R = \left\lfloor \frac{\text{ESJD}_{\text{target}}}{\text{ESJD}_{t,1}} \right\rfloor$
10. /* Remaining mutation steps */
11. for $r = 2$ to $R$ do
12.   PMMH mutation $\vartheta_{t,r}^{1:N_\theta} \sim K(\vartheta_{t,r-1}^{1:N_\theta}, \cdot)$
13. end
14. Set $\vartheta_t^{1:N_\theta} = \vartheta_t^{1:N_\theta}$
variance of $K$ log-likelihood estimates evaluated at the sample mean of the current set of parameter particles. In practice, we find that \textsc{rescale-var} changes $N_x$ too drastically from one iteration to the next for two reasons. First, the sample mean of the parameter particles changes throughout the iterations, meaning that the number of state particles needed to reach a variance of 1 also changes throughout the iterations. Second, the sample variance itself may be highly variable, especially when $N_x$ is low.

Our first attempt to overcome this problem is to scale the number of state particles by the standard deviation instead of the variance, i.e. we set $N_x^* = \sigma_{N_x} \cdot N_x$ and call this method \textsc{rescale-std}. A variance of 1 is still the overall target, however, more moderate values of $N_x$ are proposed when $\sigma^2_{N_x} \neq 1$; at any given iteration, the new target variance is the current standard deviation, i.e. $N_x^*$ is chosen such that $\sigma^2_{N_x^*} = \sigma_{N_x}$. The main drawback of \textsc{rescale-std} is that the variance at the final iteration may be too high, depending on the initial value of $N_x$ and the variability of the sample variance between iterations, i.e. it may approach a variance of 1 too slowly. In our numerical experiments in Section 5, however, we find that the final variance of the \textsc{rescale-std} method is generally between 1 and $1.2^2$, which is fairly conservative; in their numerical experiments, Doucet et al. (2015) found that the optimal $N_x$ generally gives a variance that is between $1.2^2 = 1.44$ and $1.5^2 = 2.25$.

Our second method (which we refer to as \textsc{novel-var}) aims to improve upon \textsc{rescale-var} by estimating the variance at different values of $N_x$. To obtain our set of candidate values, $N_{x,1:M}$, we scale $N_x$ by different fractional powers of $\sigma^2_{N_x}/\sigma^2_{\text{target}}$, where $\sigma^2_{\text{target}}$ is the target variance. Note that the candidate values $N_{x,1:M}$ will be close to $N_x$ if $\sigma^2_{N_x}$ is close to $\sigma^2_{\text{target}}$; to avoid unnecessary computation, the current $N_x$ is left unchanged if $\sigma^2_{N_x}$ falls within some range $\sigma^2_{\text{min}} < \sigma^2_{\text{target}} < \sigma^2_{\text{max}}$. Similarly, we also round the candidate number of state particles up to the nearest 10, which ensures that there is at least a difference of 10 between each $N_{x,m} \in N_{x,1:M}$. Once $N_{x,1:M}$ has been obtained, we then estimate the variance for each $N_{x,m} \in N_{x,1:M}$, and set the new number of state particles to the $N_{x,m}$ that has the highest variance less than or equal to $\sigma^2_{\text{max}}$.

In our numerical experiments in Section 5, we set

$$N_{x,1:3} = \left[ N_x \cdot \{s^{0.5}, s^{0.75}, s^1\}^T \right], \quad s = \frac{\sigma^2_{N_x}}{\sigma^2_{\text{target}}} ,$$

which gives candidate values ranging from \textsc{rescale-std} ($s^{0.5} \cdot N_x$) to \textsc{rescale-var} ($s^1 \cdot N_x$). The target, minimum and maximum variances are $\sigma^2_{\text{target}} = k \cdot 1$, $\sigma^2_{\text{min}} = k \cdot 0.95^2$ and $\sigma^2_{\text{max}} = k \cdot 1.05^2$ respectively, where $k = 1$ for EASMC-DA and $k = 1/\max(0.6^2, \gamma_t^2)$ for EASMC-DT. These variances are fairly conservative and aims to keep the variance between $0.95^2 \approx 0.9$ and $1.05^2 \approx 1.1$. For EASMC-DT, this takes advantage of the effect of the tempering parameter on the variance, i.e. that $\text{var}(\log(\hat{p}_{N_x}(y | \theta)^{\gamma_t})) = \gamma_t^2 \cdot \text{var}(\log(\hat{p}_{N_x}(y | \theta)))$. Capping the value of $k$ is necessary in practice, since aiming for an excessive variance is difficult due to the variability of the variance estimate when $N_x$ is low. Note that including the tempering parameter in this way is not feasible for \textsc{rescale-var} or \textsc{rescale-std}. For the former, changing the target variance only exacerbates the problem of too drastic changes of $N_x$ between iterations. This is largely due to the increased variability of the sample variance when $\gamma_t < 1$. While the variability of $\sigma^2_{N_x}$ is less of a problem for \textsc{rescale-std}, this method struggles to keep up with the increasing variance target.

Compared to \textsc{rescale-var}, we find that both \textsc{rescale-std} and \textsc{novel-var} are significantly less sensitive to the initial number of state particles, sudden changes in the variance
arising from changes in the sample mean of the parameter particles, and variability in the sample variance of the log-likelihood estimator. The NOVEL-VAR method is also more predictable in what variance is targeted at each iteration compared to RESCALE-STD.

Our final method (NOVEL-ESJD) also compares different values of $N_x$, but using the unconditional ESJD instead of the variance of the log-likelihood estimator. As before, the choice of candidate values $N_{x,1:M}$ is flexible, and in the numerical experiments in Section 5 we set

$$N_{x,1:t} = \left[ N_x \cdot \{1, 2, s^{0.5}, s^1\}^T \right], \quad s = \frac{\sigma_{N_x}^2}{k},$$

where $k = 1$ for EASMC-DA and $k = 1/\max(0.6^2, \gamma_1^2)$ for EASMC-DT. Again, each $N_{x,m} \in N_{x,1:M}$ is rounded up to the nearest 10. A score is calculated for a particular $N_{x,m} \in N_{x,1:M}$ by first doing a mutation step with $N_{x,m}$ state particles, then calculating the number of MCMC iterations ($R_m$) needed to reach the ESJD target; the score for $N_{x,m}$ is $(N_m \cdot R_m)^{-1}$. Algorithm 5 describes the adaptive mutation step when using NOVEL-ESJD. Since the candidate $N_x$ values are tested in ascending order (see step 3 of Algorithm 5), it is unnecessary to continue testing the values once the score starts to decrease (steps 10-19 of Algorithm 5).

This method does not target a particular variance, but instead aims to select the $N_x$ having the cheapest mutation while still achieving the ESJD target. Compared to DOUBLE and the variance-based methods, we find that NOVEL-ESJD is consistent between independent runs, in terms of the run time and the adaptation for $N_x$. It is also relatively insensitive to the initial number of state particles, as well as variability in the variance of the likelihood estimator.

4.3 Replacing the state particle set

The REWEIGHT scheme of Chopin et al. (2012) reweights the parameter particles using the incremental weights $\overline{p_{N_x}^\theta(y_{1:t} \mid \theta, x_{1:N_x}^{1:N_x})}/\overline{p_{N_x}^\theta(y_{1:t} \mid \theta, x_{1:N_x}^{1:N_x})}$. These weights are obtained by replacing $p(y_{1:t} \mid \theta)$ with $p_{N_x}^\theta(y_{1:t} \mid \theta, x_{1:N_x}^{1:N_x})$ to approximate the optimal backward kernel; see Section 5 for details.

Our final contribution (denoted REPLACE) is a variation of REWEIGHT. Instead of using $p(y_{1:t} \mid \theta) \approx p_{N_x}^\theta(y_{1:t} \mid \theta, x_{1:N_x}^{1:N_x})$ to approximate the optimal backward kernel, we use $p(y_{1:t} \mid \theta) \approx p_{N_x}^\theta(y_{1:t} \mid \theta, x_{1:N_x}^{1:N_x})$, which gives the backward kernel

$$L_t(x_{1:N_x}^{1:N_x}, x_{1:N_x}^{1:N_x}) = \frac{\overline{p_{N_x}^\theta(y_{1:t} \mid \theta, x_{1:N_x}^{1:N_x})}/\overline{p_{N_x}^\theta(y_{1:t} \mid \theta)}}{\overline{p_{N_x}^\theta(y_{1:t} \mid \theta, x_{1:N_x}^{1:N_x})}/\overline{p_{N_x}^\theta(y_{1:t} \mid \theta, x_{1:N_x}^{1:N_x})}}.$$

Using this backward kernel, the incremental weights are

$$\frac{\pi_t(\theta, x_{1:N_x}^{1:N_x} \mid y_{1:t}) L_t(x_{1:N_x}^{1:N_x}, x_{1:N_x}^{1:N_x})}{\pi_t(\theta, x_{1:N_x}^{1:N_x} \mid y_{1:t})} = \frac{\overline{p_{N_x}^\theta(y_{1:t} \mid \theta, x_{1:N_x}^{1:N_x})} L_t(x_{1:N_x}^{1:N_x}, x_{1:N_x}^{1:N_x})}{\overline{p_{N_x}^\theta(y_{1:t} \mid \theta, x_{1:N_x}^{1:N_x})} \psi(x_{1:N_x}^{1:N_x})} \frac{\overline{p_{N_x}^\theta(y_{1:t} \mid \theta, x_{1:N_x}^{1:N_x})} \psi(x_{1:N_x}^{1:N_x})}{\overline{p_{N_x}^\theta(y_{1:t} \mid \theta, x_{1:N_x}^{1:N_x})} \psi(x_{1:N_x}^{1:N_x})}$$

$$= 1.$$
Algorithm 5: Adaptive mutation step

Input: the total unconditional ESJD from the previous iteration (ESJD_{t-1}), the target total unconditional ESJD for each iteration (ESJD_{target}) and the current set of particles \( \vartheta_{t}^{1:N_{\theta}} \)

/* Trigger the adaptation */
1 adapt = ESJD_{t-1} < ESJD_{target}

2 if adapt then
    /* Adapt \( N_{x} \) and \( R \) */
3 Calculate the set of candidate values, \( N_{x,1:M} \) (e.g. using (10)), and sort in ascending order, such that \( N_{x,1} < N_{x,2} < \ldots < N_{x,M} \)
4 Set \( m^{*} = M \)
5 for \( N_{x,m} \in N_{x,1:M} \) do
6    Replace the current set of state particles with \( \tilde{x}_{t}^{1:N_{x,m}} \) using the method described in Section 4.3
7 PMMH mutation \( \vartheta_{t,m}^{1:N_{\theta}} \sim K(\vartheta_{t}^{1:N_{\theta}}, \cdot) \), calculate ESJD_{t,m}
8 Calculate \( R_{m} = \left[ \frac{\text{ESJD}_{\text{target}}}{\text{ESJD}_{t,m}} \right] \)
9 Calculate score \( z_{m} = (N_{x,m} \cdot R_{m})^{-1} \)
10 /* If more than one value has been tested */
11 if \( m > 1 \) then
12    /* If the current score is worse than the previous one */
13    if \( z_{m}/z_{m-1} < 1 \) then
14        Set \( m^{*} = m - 1 \)
15        Replace the current set of state particles with \( \tilde{x}_{t}^{1:N_{x,m^{*}}} \) using the method described in Section 4.3
16        break
17 /* If the current score is equal to the previous one */
18 else if \( z_{m}/z_{m-1} = 1 \) then
19    Set \( m^{*} = m \)
20    break
21 end
22 /* Update \( N_{x} \) and \( R \) */
23 Set \( N_{x} = N_{x,m^{*}} \) and \( R = R_{m^{*}} \)
24 else
    /* Initial mutation step */
25 PMMH mutation \( \vartheta_{t,1}^{1:N_{\theta}} \sim K(\vartheta_{t}^{1:N_{\theta}}, \cdot) \), calculate ESJD_{t,1}
26 /* Remaining mutation steps */
27 for \( r = 2 \) to \( R \) do
28    PMMH mutation \( \vartheta_{t,r}^{1:N_{\theta}} \sim K(\vartheta_{t,r-1}^{1:N_{\theta}}, \cdot) \)
29 end
30 Set \( \vartheta_{t}^{1:N_{\theta}} = \vartheta_{t,R}^{1:N_{\theta}} \)
Since the incremental weights reduce to 1, this approach introduces no extra variability in the parameter particle weights.

5 Examples

5.1 Implementation

The methods are evaluated on a simple Brownian motion model, the one-factor stochastic volatility (SV) model in Chopin et al. (2012), and two ecological models: the theta-logistic model (Peters et al., 2010; Drovandi et al., 2021) and the noisy Ricker model (Fasiolo et al., 2016).

All code is implemented in MATLAB. The likelihood estimates are obtained using the bootstrap particle filter (Algorithm 1) with adaptive multinomial resampling, i.e. resampling is done whenever the effective sample size (ESS) drops below \( N_x/2 \). The results for all models, except for the Ricker model, are calculated from 50 independent runs, each with \( N_\theta = 1000 \) parameter samples. Due to time and computational constraints, the Ricker model results are based on 20 independent runs, each with \( N_\theta = 400 \) parameter samples.

For EASMC-DT, the temperatures are set adaptively using the bisection method to aim for an ESS of 0.6 \( \cdot N_\theta \). Similarly, the resample-move step is run for EASMC-DA if the ESS falls below 0.6 \( \cdot N_\theta \). A target ESJD of 6 is used for all methods, i.e. \( \text{ESJD}_{\text{target}} = 6 \); choice of target ESJD is flexible as we find it has little effect on the adaptation of \( N_x \), but controls the value of \( R \) throughout the algorithm. For all methods except \textsc{reinit} and \textsc{double}, we also trigger the adaptation whenever \( \text{ESJD}_{t-1} > 2 \cdot \text{ESJD}_{\text{target}} \) — this allows the algorithm to recover if the values of \( N_x \) and/or \( R \) are set too high at any given iteration, which may occur e.g. if there are outliers with EASMC-DA. When the \textsc{reinit} method is used, a mixture of three Gaussians is fit to the current sample when reinitialising the algorithm. For \textsc{rescale-var}, \textsc{rescale-std}, \textsc{novel-var}, and \textsc{novel-esjd}, the sample variance \( \sigma^2_{N_x} \) is calculated using 100 log-likelihood estimates.

The methods are compared based on the mean squared error (MSE) of the posterior mean of each parameter, where the ground truth is taken as the posterior mean from a PMMH chain of length 1 million. As the gold standard (GS), EASMC-DT and EASMC-DA are also run for each model with a fixed number of particles, while still adapting \( R \). For each of these runs, the number of state particles is tuned such that \( \sigma_{N_x} \approx 1 \) for the full dataset, and the extra tuning time is not included in the results.

To measure the efficiency of a given method, we use the MSE of the method for each parameter multiplied by the total number of log-likelihood evaluations, denoted by TLL; each time the particle filter is run for a particular parameter particle, TLL is incremented by \( N_x \times t \), where \( t \) is the current number of observations. This gives a measure of efficiency for each parameter \( p \) as

\[
z_{p,\text{method}} = (\text{MSE}_{p,\text{method}} \cdot \text{TLL}_{\text{method}})^{-1}, \quad p = 1, \ldots, N_p,
\]

where \( N_p \) is the total number of parameters. The overall performance is determined by the minimum and median efficiencies across the \( N_p \) parameters relative to the gold standard, i.e.

\[
Z_{\text{min,method}} := \frac{z_{\text{min,method}}}{z_{\text{min,GS}}}, \quad Z_{\text{med,method}} := \frac{z_{\text{med,method}}}{z_{\text{med,GS}}},
\]

(12)
where \( Z_{\text{min,method}} \) and \( Z_{\text{med,method}} \) are referred to as the minimum and median scores respectively. Higher values are preferred. When \( Z_{\text{min,method}} > 1 \), the given method has a better minimum efficiency than the gold standard, and similarly for \( Z_{\text{med,method}} \).

The adaptive mutation step in Algorithm 4 is used for all methods except \textsc{novel-esjd}, which uses the adaptive mutation step in Algorithm 5. The options for stage 2 are \textsc{double}, \textsc{rescale-var}, \textsc{rescale-std}, \textsc{novel-var} and \textsc{novel-esjd}. Likewise, the options for stage 3 are \textsc{reweight}, \textsc{reinit}, and our novel method \textsc{replace}. Since the aim of the \textsc{novel-var} method is to regularly increase the number of state particles throughout the iterations, the combination \textsc{novel-var} with \textsc{reinit} is not tested. Similarly, due to the number of times \( N_x \) is updated when using \textsc{novel-esjd}, only the combination \textsc{novel-esjd} with \textsc{replace} is tested. For all combinations (excluding \textsc{double} and \textsc{reinit}), we allow the number of state particles to decrease and we cap the number of state particles at 5 times the number of state particles used for the gold standard method.

### 5.2 Brownian Motion Model

The first example is a stochastic differential equation with constant drift and diffusion coefficients,

\[
dX_t = \left( \beta - \frac{\gamma^2}{2} \right) dt + \gamma dB_t,
\]

where \( B_t \) is a standard Brownian motion process (Øksendal 2003, p. 44). The transition and observation densities are

\[
g(y_t | x_t, \theta) = \mathcal{N}(x_t, \sigma^2)
\]

\[
f(x_t | x_{t-1}, \theta) = \mathcal{N} \left( x_{t-1} + \beta - \frac{\gamma^2}{2}, \gamma^2 \right).
\]

One hundred observations are generated from this model using \( \theta := \{x_0, \beta, \gamma, \sigma\} = \{1, 1.2, 1.5, 1\} \) and the priors assigned are \( \mathcal{N}(x_0 \mid 3, 5^2) \), \( \mathcal{N}(\beta \mid 2, 5^2) \), Half-Normal(\(\gamma \mid 2^2\)), and Half-Normal(\(\sigma \mid 2^2\)), respectively.

Results for all stage 2 and stage 3 combinations are obtained for initial \( N_x \) values of 10 and 100. The variance of the log-likelihood estimator is around 95 for \( N_x = 10 \) and around 2.7 for \( N_x = 100 \). The gold standard method is run with 240 state particles.

Table 1 shows the minimum and median scores (averaged over the two initial values of \( N_x \) and relative to \textsc{reweight}) for the three stage 3 options (\textsc{reweight}, \textsc{reinit} and \textsc{replace}). Apart from \textsc{EASMC-DA} with the \textsc{double} method — which has fairly similar performance for \textsc{reinit} and \textsc{replace} — \textsc{replace} significantly outperforms both \textsc{reweight} and \textsc{reinit}. Interestingly, \textsc{reinit} consistently outperforms \textsc{reweight} with \textsc{EASMC-DA}, but performs poorly with \textsc{EASMC-DT}; the performance of this method greatly depends on the number of times the algorithm is reinitialised and the final number of state particles.

Table 2 shows the minimum and median scores for all the \textsc{replace} combinations. Of \textsc{double} and the variance-based methods (\textsc{rescale-var}, \textsc{rescale-std} and \textsc{novel-var}), \textsc{novel-var} has the best results for \textsc{EASMC-DT}, while \textsc{rescale-var} has the best results for \textsc{EASMC-DA}; \textsc{double} performs well on \textsc{EASMC-DT}, but poorly on \textsc{EASMC-DA}. Interestingly, \textsc{novel-esjd} has the highest minimum score out of all the methods, and a high median score for initial \( N_x = 100 \), but it has one of the lowest median scores for
initial $N_x = 10$. This method tends to adapt $N_x$ to a much lower value than all the other methods, especially when the initial $N_x$ is already low. In this case, the lower median score is mainly due to the parameter $\sigma$, which has a better score when $N_x$ is higher and is one of the two middle scores used in the median score calculation.

Overall, the performance gain (relative to the gold standard) is less for EASMC-DA than for EASMC-DT, which may be due to high variability in the variance of the log-likelihood estimator, and the mean of the parameter particles, during the initial iterations. Since fewer observations are used to estimate the likelihood in these early iterations ($t < T$), the mean of the parameter particles can change drastically from one iteration to the next, leading to similarly drastic changes in the sample variance of the log-likelihood estimator.

| Method           | EASMC-DT | EASMC-DA |
|------------------|----------|----------|
|                  | min      | med      | min      | med      |
| DOUBLE REWEIGHT  | 1.00     | 1.00     | 1.00     | 1.00     |
| DOUBLE REINIT    | 0.10     | 0.03     | 1.52     | 1.25     |
| DOUBLE REPLACE   | 4.09     | 7.76     | 1.94     | 1.08     |
| RESCALE-VAR REWEIGHT | 1.00 | 1.00 | 1.00 | 1.00 |
| RESCALE-VAR REINIT | 5.01   | 0.84     | 11.51    | 11.01    |
| RESCALE-VAR REPLACE | 9.21   | 11.49    | 38.51    | 34.27    |
| RESCALE-STD REWEIGHT | 1.00 | 1.00 | 1.00 | 1.00 |
| RESCALE-STD REINIT | 2.19   | 1.38     | 3.57     | 4.23     |
| RESCALE-STD REPLACE | 21.60  | 34.99    | 18.49    | 15.48    |

Table 1: Minimum (min) and median (med) scores for the stage 3 options for the Brownian motion model — higher values are preferred. The results are averaged over the two starting values of $N_x$ and are relative to the REWEIGHT method.

| Method     | EASMC-DT | EASMC-DA |
|------------|----------|----------|
|            | 10       | 100      | 10       | 100      |
|            | min      | med      | min      | med      |
| GOLD STANDARD | 1.00   | 1.00     | 1.00     | 1.00     |
| DOUBLE     | 15.41    | 86.84    | 4.84     | 9.84     |
| RESCALE-VAR | 5.07   | 20.62    | 5.85     | 19.00    |
| RESCALE-STD | 16.10  | 54.67    | 10.80    | 21.03    |
| NOVEL-VAR  | 16.86    | 87.10    | 11.75    | 56.46    |
| NOVEL-ESJD | 28.52    | 23.10    | 11.75    | 56.46    |

Table 2: Minimum (min) and median (med) scores for the Brownian motion model — higher values are preferred. Results shown are for the REPLACE method.

### 5.3 Stochastic Volatility Model

Our second example is the one-factor stochastic volatility model used in Chopin et al. (2012),

\[
y_t \sim \mathcal{N}(\mu + \beta v_t, v_t)\\
\]

\[
z_t = \exp(-\lambda)z_{t-1} + \sum_{j=1}^{k} \exp(-\lambda(t - c_j))c_j, \quad z_0 \sim \text{Gamma}(\xi^2/\omega^2, \xi/\omega^2)\]

\[
v_t = \frac{1}{\lambda} \left[ z_{t-1} - z_t + \sum_{j=1}^{k} c_j \right], \quad x_t = \{v_t, z_t\}, \]

\[
k \sim \text{Poisson}(\lambda \xi^2/\omega^2), \quad c_{1:k} \overset{iid}{\sim} \text{Uniform}(t - 1, t), \quad e_{1:k} \overset{iid}{\sim} \text{Exponential}(\xi/\omega^2).\]
The transition density of this method cannot be evaluated point-wise, but it can be simulated.

We use a synthetic dataset with 200 observations, which was simulated using \( \theta := \{\xi, \omega^2, \lambda, \beta, \mu\} = \{4, 0.5, 5, 0, 2\} \). The priors are Exponential(\(\xi | 0.2\)), Exponential(\(\omega^2 | 0.2\)), Exponential(\(\lambda | 1\)), \(\mathcal{N}(\beta | 0, 2)\) and \(\mathcal{N}(\mu | 0, 2)\).

Results for all stage 2 and stage 3 combinations are obtained for initial \(N_x\) values of 300 and 600. The variance of the log-likelihood estimator is around 7 for 300 state particles around 3 for 600 state particles. The gold standard method is run with 1650 state particles.

Table 3 shows the minimum and median scores for the three stage 3 options, relative to REWEIGHT and averaged over the two initial \(N_x\) values. As with the previous example, REPLACE generally outperforms REWEIGHT and REINIT.

Table 4 shows the minimum and median scores for all the REPLACE combinations. All methods have fairly similar results for this model. In terms of accuracy (measured by the MSE), the optimal variance of the log-likelihood estimator seems to be smaller for this model than for the others. However, the efficiency of a smaller variance coupled with the increased computation time is fairly similar to the efficiency of a larger variance with cheaper computation. In this example, NOVEL-ESJD has a worse median score than the other methods, due to the more expensive adaptation for \(N_x\).

| Method       | EASMC-DT min | EASMC-DT med | EASMC-DA min | EASMC-DA med |
|--------------|--------------|--------------|--------------|--------------|
| DOUBLE REWEIGHT | 1.00         | 1.00         | 1.00         | 1.00         |
| DOUBLE REPLACE | 4.90         | 3.57         | 1.52         | 1.30         |
| RESCALE-VAR REWEIGHT | 1.00         | 1.00         | 1.00         | 1.00         |
| RESCALE-VAR REPLACE | 2.00         | 1.37         | 29.69        | 8.99         |
| RESCALE-STD REWEIGHT | 1.00         | 1.00         | 1.00         | 1.00         |
| RESCALE-STD REPLACE | 4.95         | 2.88         | 18.24        | 11.48        |

Table 3: Minimum (min) and median (med) scores for the stage 3 options for the stochastic volatility model — higher values are preferred. The results are averaged over the two starting values of \(N_x\) and are relative to the REWEIGHT method.

| Method       | EASMC-DT min | EASMC-DT med | EASMC-DA min | EASMC-DA med |
|--------------|--------------|--------------|--------------|--------------|
| INITIAL N_x | 300 | 600 | 300 | 600 |
| GOLD STANDARD | 1.00 | 1.00 | 1.00 | 1.00 |
| DOUBLE | 2.22 | 3.81 | 1.59 | 2.00 |
| RESCALE-VAR | 1.23 | 2.06 | 1.01 | 2.44 |
| RESCALE-STD | 1.76 | 2.56 | 1.39 | 2.43 |
| NOVEL-VAR | 1.62 | 2.79 | 1.49 | 2.48 |
| NOVEL-ESJD | 2.77 | 0.92 | 1.65 | 1.42 |

Table 4: Minimum (min) and median (med) scores for the stochastic volatility model — higher values are preferred. Results shown are for the REPLACE method.
5.4 Theta-logistic Model

The next example is the theta-logistic ecological model (Peters et al., 2010),

\[
g(y_t \mid x_t, \theta) = \mathcal{N}(y_t \mid a \cdot \log(x_t), \sigma^2) \\
\log(x_{t+1}) = \log(x_t) + \beta_0 + \beta_1 x_t^{\beta_2} + z_t, \quad z_t \sim \mathcal{N}(0, \gamma^2).
\]

We fit the model to the first 100 observations of female nutria populations measured at monthly intervals (Peters et al., 2010; Drovandi et al., 2021), using the priors \( \mathcal{N}(\beta_0 \mid 0, 1), \mathcal{N}(\beta_1 \mid 0, 1), \mathcal{N}(\beta_2 \mid 0, 1), \) Half-Normal(\(x_0 \mid 1000^2\)), Exponential(\(\gamma \mid 1\)), Exponential(\(\sigma \mid 1\)) and \( \mathcal{N}(a \mid 1, 0.5^2) \).

Results for all combinations are obtained for initial \( N_x \) values of 700 and 2400. The variance of the log-likelihood estimator is around 40 for 700 state particles and around 3 for 2400 state particles. The gold standard method is run with 4600 state particles. Due to time constraints, results for the DOUBLE method with REWEIGHT and initial \( N_x = 700 \) is not available for EASMC-DA.

Table 5 shows the minimum and median scores for the three stage 3 options, averaged over the initial \( N_x \) values and relative to REWEIGHT. Except for DOUBLE with EASMC-DT, both REINIT and REPLACE outperform REWEIGHT, but the results for REINIT and REPLACE are mixed. The performance of REINIT greatly depends on how many times the adaptation is triggered. On average, the algorithm is reinitialised fewer times for RESCALE-STD for this example than for the others.

Table 6 shows the minimum and median scores for all the REPLACE combinations. In this example, NOVEL-ESJD outperforms all other methods, followed by NOVEL-VAR and RESCALE-VAR. Unlike the previous examples, DOUBLE and RESCALE-STD perform poorly here.

| Method         | EASMC-DT   | EASMC-DA   |
|----------------|-----------|------------|
|                | min med   | min med    |
| DOUBLE REWEIGHT| 1.00 1.00 | 1.00 1.00  |
| DOUBLE REPLACE | 0.96 0.80 | 0.78 1.93  |
| RESCALE-VAR REWEIGHT | 1.00 1.00 | 1.00 1.00  |
| RESCALE-VAR REINIT   | 2.90 1.79 | 6.33 2.53  |
| RESCALE-VAR REPLACE  | 2.51 5.65 | 5.54 4.56  |
| RESCALE-STD REWEIGHT | 1.00 1.00 | 1.00 1.00  |
| RESCALE-STD REINIT   | 2.41 2.51 | 9.67 3.43  |
| RESCALE-STD REPLACE  | 2.37 8.67 | 3.06 1.17  |

Table 5: Minimum (min) and median (med) scores for the stage 3 options for the theta-logistic model — higher values are preferred. The results are averaged over the two starting values of \( N_x \) and are relative to the REWEIGHT method. Note that DOUBLE with REWEIGHT for EASMC-DA is based only on the results for an initial \( N_x \) of 2400.

5.5 Noisy Ricker Model

Our final example is the noisy Ricker population model (Fasiolo et al., 2016),

\[
g(y_t \mid x_t, \theta) = \text{Poisson}(y_t \mid \phi x_t) \\
x_{t+1} = r \cdot x_t \exp(-x_t + z_{t+1}), \quad z_t \sim \mathcal{N}(0, \sigma^2).
\]
The transition density of the Ricker model cannot be evaluated point-wise; however, it is straightforward to generate $x_t$ from it, conditional on $x_{t-1}$. This model, and its variants, is typically used to represent highly non-linear or near-chaotic ecological systems, e.g. the population dynamics of sheep blowflies (Fasiolo et al., 2016). Fasiolo et al. (2016) show that the likelihood function of the noisy Ricker model exhibits extreme multimodality when the process noise is low, making it difficult to estimate the model.

We draw 700 observations using $\theta := \{\log(\phi), \log(\tau), \log(\sigma)\} = \{\log(10), \log(44.7), \log(0.6)\}$. Following Fasiolo et al. (2016), we assign uniform priors to the log-parameters, $\mathcal{U}(\log(\phi) \mid 1.61, 3)$, $\mathcal{U}(\log(\tau) \mid 2, 5)$ and $\mathcal{U}(\log(\sigma) \mid -1.8, 1)$, respectively.

Results for all combinations are obtained for initial $N_x$ values of 1000 and 20000. The variance of the log-likelihood estimator is around 13 for 1000 state particles and around 2.3 for 20000 state particles. The gold standard method is run with 90000 state particles. Due to time constraints, the ground truth for the posterior mean is based on a PMMH chain of length 200000.

Computation was stopped if the run time exceeded 9 days. As a result, a full comparison of the stage 3 options cannot be made. Of the ones that finished, REPLACE gave the best results. In a number of cases, the gold standard and REPLACE were the only methods to finish within the time frame. Table 7 shows the minimum and median scores for all the REPLACE combinations. NOVEL-VAR and NOVEL-ESJD have the best overall results across both EASMC-DT and EASMC-DA. RESCALE-STD and RESCALE-VAR perform similarly on this example.

### Table 6: Minimum (min) and median (med) scores for the theta-logistic model — higher values are preferred. Results shown are for the REPLACE method.

| Method        | EASMC-DT | EASMC-DA |
|---------------|----------|----------|
|               | 700      | 2400     | 700      | 2400     |
|               | min      | med      | min      | med      |
| GOLD STANDARD | 1.00     | 1.00     | 1.00     | 1.00     |
| DOUBLE        | 0.61     | 0.48     | 0.49     | 0.57     |
| RESCALE-VAR   | 0.62     | 9.01     | 0.58     | 4.59     |
| RESCALE-STD   | 0.82     | 7.76     | 0.42     | 3.85     |
| NOVEL-VAR     | 1.00     | 9.44     | 0.53     | 9.62     |
| NOVEL-ESJD    | 1.13     | 26.16    | 0.61     | 17.93    |

### Table 7: Minimum (min) and median (med) scores for the noisy Ricker model — higher values are preferred. Results shown are for the REPLACE method.

| Method        | EASMC-DT | EASMC-DA |
|---------------|----------|----------|
|               | 1000     | 20000    | 1000     | 20000    |
|               | min      | med      | min      | med      |
| GOLD STANDARD | 1.00     | 1.00     | 1.00     | 1.00     |
| DOUBLE        | 3.35     | 3.76     | -        | -        |
| RESCALE-VAR   | 2.44     | 1.63     | 3.06     | 2.36     |
| RESCALE-STD   | 5.49     | 3.45     | 2.86     | 1.80     |
| NOVEL-VAR     | 3.67     | 4.48     | 2.52     | 3.45     |
| NOVEL-ESJD    | 4.54     | 8.15     | 2.65     | 2.47     |

6 Discussion

We introduce a fully adaptive exact-approximate SMC algorithm for parameter inference of intractable-likelihood state-space models. This method has three hyper-parameters that
must be set: the target ESJD for the mutation step, the target ESS for the parameter
particles and the initial number of state particles. Empirically, the results are fairly
insensitive to the target ESJD and ESS, suggesting that good default values should be
sufficient in practice, e.g. using a target ESJD of 6 and a target ESS of 0.5 \cdot N_θ. While
any initial number of state particles \( N_x \) can be used, a small value yields the most
efficient results. Compared to the currently available methods, the new approach requires
no tuning, gives consistent results and is straightforward to use with both data annealing
and density tempering EASMC.

Of the methods used to select the new number of state particles, NOVEL-ESJD gave the
most consistent results across all models, choice of initial \( N_x \) and between EASMC-DT
and EASMC-DA; it either outperformed the other methods, or gave relatively similar re-
sults. A significant advantage of NOVEL-ESJD is that the adaptation of \( N_x \) is consistent
across independent runs of the algorithm (i.e. when starting at different random seeds),
substantially more so than the other methods. Similarly, the REPLACE method typically
shows great improvement over REWEIGHT and REINIT. Unlike REWEIGHT, REPLACE in-
troduces no extra variability in the parameter particle weights, and it is more consistent
than REINIT. The fully adaptive methods also generally outperforms the gold standard
method, despite the latter being pre-tuned.

An interesting extension to the current work would be to assess the effect of the target
ESJD, the target ESS and the target variance of the log-likelihood estimator when EASMC
is used for model selection. Another area of future work is extending the method for
application to mixed effects models \cite{Botha_2020}; for these models, it may be
possible to obtain significant gains in efficiency by allowing the number of particles to
(adaptively) vary between subjects. The new method can also be used as the proposal
function within importance sampling squared \cite{Tran_2020}.

7 Acknowledgments

Imke Botha was supported by an Australian Research Training Program Stipend and
a QUT Centre for Data Science Top-Up Scholarship. We gratefully acknowledge the
computational resources provided by QUT’s High Performance Computing and Research
Support Group (HPC).

References

Andrieu, C., Doucet, A., and Holenstein, R. (2010). Particle Markov chain Monte Carlo
methods. Journal of the Royal Statistical Society: Series B (Statistical Methodology),
72(3):269–342.

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

Bon, J. J., Lee, A., and Drovandi, C. (2021). Accelerating sequential Monte Carlo with
surrogate likelihoods. Statistics and Computing, 31(5).

Botha, I., Kohn, R., and Drovandi, C. (2020). Particle methods for stochastic differential
equation mixed effects models. Bayesian Analysis.
Cappé, O., Moulines, E., and Rydén, T. (2005). *Inference in Hidden Markov Models*. Springer New York.

Chopin, N. (2002). A sequential particle filter method for static models. *Biometrika*, 89(3):539–552.

Chopin, N., Jacob, P. E., and Papaspiliopoulos, O. (2012). SMC2: an efficient algorithm for sequential analysis of state space models. *Journal of the Royal Statistical Society: Series B (Statistical Methodology)*, 75(3):397–426.

Chopin, N., Ridgway, J., Gerber, M., and Papaspiliopoulos, O. (2015). Towards automatic calibration of the number of state particles within the SMC² algorithm. *arXiv preprint arXiv:1506.00570*.

Del Moral, P., Doucet, A., and Jasra, A. (2006). Sequential Monte Carlo samplers. *Journal of the Royal Statistical Society: Series B (Statistical Methodology)*, 68(3):411–436.

Doucet, A., Pitt, M. K., Deligiannidis, G., and Kohn, R. (2015). Efficient implementation of Markov chain Monte Carlo when using an unbiased likelihood estimator. *Biometrika*, 102(2):295–313.

Doucet, A., Pitt, M. K., and Kohn, R. (2012). Efficient implementation of Markov chain Monte Carlo when using an unbiased likelihood estimator. *arXiv preprint*, page arXiv:1210.1871v2.

Drovandi, C., Everitt, R. G., Golightly, A., and Prangle, D. (2021). Ensemble MCMC: Accelerating Pseudo-Marginal MCMC for State Space Models using the Ensemble Kalman Filter. *Bayesian Analysis*.

Duan, J.-C. and Fulop, A. (2014). Density-Tempered Marginalized Sequential Monte Carlo Samplers. *Journal of Business & Economic Statistics*, 33(2):192–202.

Fasiolo, M., Pya, N., and Wood, S. N. (2016). A Comparison of Inferential Methods for Highly Nonlinear State Space Models in Ecology and Epidemiology. *Statistical Science*, 31(1):96–118.

Fearnhead, P. and Taylor, B. M. (2013). An Adaptive Sequential Monte Carlo Sampler. *Bayesian Analysis*, 8(2):411–438.

Gordon, N. J., Salmond, D. J., and Smith, A. F. M. (1993). Novel approach to nonlinear/non-Gaussian Bayesian state estimation. *IEE Proceedings F Radar and Signal Processing*, 140(2):107.

Gunawan, D., Kohn, R., and Tran, M. N. (2021). Robust Particle Density Tempering for State Space Models. *arXiv preprint*, page arXiv:1805.00649.

Jacob, P. E., Murray, L. M., and Rubenthaler, S. (2015). Path storage in the particle filter. *Statistics and Computing*, 25(2):487–496.

Øksendal, B. (2003). *Stochastic differential equations: an introduction with applications*. Springer.

Pasarica, C. and Gelman, A. (2010). Adaptively Scaling the Metropolis Algorithm Using Expected Squared Jumped Distance. *Statistica Sinica*, 20(1):343–364.
Peters, G. W., Hosack, G. R., and Hayes, K. R. (2010). Ecological non-linear state space model selection via adaptive particle Markov chain Monte Carlo (AdPMCMC). *arXiv preprints*, page arXiv:1005.2238.

Pitt, M. K., dos Santos Silva, R., Giordani, P., and Kohn, R. (2012). On some properties of Markov chain Monte Carlo simulation methods based on the particle filter. *Journal of Econometrics*, 171(2):134–151.

Salomone, R., South, L. F., Drovandi, C. C., and Kroese, D. P. (2018). Unbiased and Consistent Nested Sampling via Sequential Monte Carlo. *Arxiv preprint arXiv:1805.03924*.

Sherlock, C., Thiery, A. H., Roberts, G. O., and Rosenthal, J. S. (2015). On the efficiency of pseudo-marginal random walk Metropolis algorithms. *The Annals of Statistics*, 43(1):238–275.

Tran, M.-N., Scharth, M., Gunawan, D., Kohn, R., Brown, S. D., and Hawkins, G. E. (2020). Robustly estimating the marginal likelihood for cognitive models via importance sampling. *Behavior Research Methods*. 23