Ensemble Rejection Sampling

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Abstract

We introduce Ensemble Rejection Sampling, a scheme for exact simulation from the posterior distribution of the latent states of a class of non-linear non-Gaussian state-space models. Ensemble Rejection Sampling relies on a proposal for the high-dimensional state sequence built using ensembles of state samples. Although this algorithm can be interpreted as a rejection sampling scheme acting on an extended space, we show under regularity conditions that the expected computational cost to obtain an exact sample increases cubically with the length of the state sequence instead of exponentially for standard rejection sampling. We demonstrate this methodology by sampling exactly state sequences according to the posterior distribution of a stochastic volatility model and a non-linear autoregressive process. We also present an application to rare event simulation.

Keywords: Exact simulation; Feynman–Kac models; Hidden Markov models; Rare event simulation; Rejection sampling; State-space models.

1 Introduction

Rejection sampling (RS) is a standard algorithm introduced by John von Neumann to sample exactly from distributions only known up to a normalizing constant. This is achieved by thinning samples from a suitable proposal distribution; see, e.g., \cite[Chapter 2]{9}. However, RS is deemed inefficient to sample high-dimensional distributions as the computational cost required to obtain an exact sample increases typically exponentially with the dimension. This serious limitation has partly motivated the development of Markov chain Monte Carlo (MCMC) and particle methods.

We are interested here in sampling from the posterior distribution of a sequence of latent states of length $T$ of a non-linear state-space model. As $T$ is large in most applications of interest, RS is inefficient in this context even when the dimension of a single state is small. Consequently, one typically relies instead on particle smoothing schemes \cite{13} or MCMC techniques such as Embedded Hidden Markov Model (EHMM) \cite{17, 18} or particle MCMC \cite{2}. However, particle
smoothing schemes only return approximate samples from the posterior. Similarly, as any MCMC scheme initialized out-of-equilibrium, EHMM and particle MCMC algorithms provide biased samples after a finite number of iterations. While many MCMC-based algorithms to sample exactly from complex probability distributions have been developed following the introduction of coupling from the past [21] - see, e.g., [14] and [16] -, none of the procedures developed in these contributions appear applicable to posterior simulation in state-space models. To our knowledge, the only exact simulation procedure available for such models has been recently proposed in [5] and relies on a combination of dominated coupling from the past and an original version of particle MCMC based on branching processes. We follow here an alternative approach based on RS. Contrary to the methodology proposed in [5], it is only applicable to models where the target distribution satisfies a backward Markovian decomposition (see, e.g., [13] and [Proposition 9.14 9]) but it is significantly easier to analyze and implement. Additionally, this algorithm does not suffer from the “user-impatience” bias problem of procedures based on the coupling-from-the-past protocol [14].

We show that it is indeed possible to leverage the structural properties of state-space models to perform exact simulation using RS ideas. This is achieved by introducing a novel RS scheme which we call Ensemble Rejection Sampling (ERS) as it builds a proposal for the high-dimensional state sequence based on ensembles of state samples which can be sampled efficiently using dynamic programming techniques. This proposal is similar to the one used in a MCMC algorithm recently introduced in [12, Section 3.2] which relies on EHMM ideas. For the corresponding acceptance probability not to vanish exponentially fast with $T$, we introduce a novel auxiliary target distribution which admits a marginal distribution coinciding with the posterior distribution of interest while being “close” to the proposal distribution. This auxiliary target distribution differs from the one introduced in [17, 18] and used in [12, 23] to establish the validity of the MCMC algorithms based on EHMM ideas proposed therein.

Under a strong regularity assumption in the spirit of the assumptions used in the literature to establish quantitative bounds for particle methods [6, Chapter 4], we show that the expected computational cost to obtain one exact sample from the posterior increases only cubically with $T$ using ERS instead of exponentially using standard RS. We demonstrate the algorithm on two state-space models and a rare event problem.

The rest of the paper is organized as follows. For pedagogical reasons, we first introduce the ERS methodology in a simple ‘static’ scenario in Section 2. In this scenario, ERS is of no practical interest but this allows us to introduce the main ideas behind our construction. Section 3 presents and analyzes ERS for the more complex scenario of (dynamic) state-space models. We present a few applications of ERS in Section 4.

# 2 Ensemble Rejection Sampling: Static Case

## 2.1 Set-up and algorithm

In this section, we are interested in sampling exactly from a distribution on a measurable space $(\mathcal{X}, \mathcal{X})$ admitting a density of the form

$$
\pi(x) = \frac{\gamma(x)}{Z}
$$

w.r.t. a suitable dominating measure denoted $dx$. We assume that one can evaluate $\gamma : \mathcal{X} \rightarrow \mathbb{R}^+$ pointwise while the normalizing constant $Z = \int_{\mathcal{X}} \gamma(x) dx$ is typically not available. We also
assume that we have access to a proposal distribution admitting a density \( q(x) \) w.r.t. \( dx \) such that
\[
\sup_{x \in X} w(x) \leq \overline{w} < \infty, \quad \text{where} \quad w(x) := \frac{\gamma(x)}{q(x)},
\]
the bound \( \overline{w} \) being known.

When performing RS to sample from \( \pi \) using \( q \), the average acceptance probability of a proposal is \( p_{RS} = \frac{Z}{\overline{w}} \); see, e.g., [8, Chapter 2]. If one has access to an ensemble of \( N \) proposals \( X^1, \ldots, X^N \overset{i.i.d.}{\sim} q \), we show here that we can use this ensemble to obtain a new proposal \( X \) which will have a higher average acceptance probability. This is achieved by computing the following normalized importance sampling approximation of \( \pi \)
\[
\hat{\pi}(\cdot) = \sum_{i=1}^{N} W^i \delta_{X^i}(\cdot),
\]
(2)
where
\[
W^i = \frac{w(X^i)}{NZ}, \quad \hat{Z} = \frac{1}{N} \sum_{i=1}^{N} w(X^i),
\]
(3)
then sampling from this approximation, \( X \sim \hat{\pi} \), as in sampling importance resampling [22, 24]. Note that \( \hat{Z} \) is an unbiased estimate of \( Z \). If we denote \( X := (X_1, \ldots, X_N) \), the probability distribution of the proposal \( X \) has a density given by
\[
\overline{\pi}(\cdot) = \mathbb{E}_X[\hat{\pi}(\cdot)].
\]
(4)
However, we cannot compute the corresponding density pointwise as it is given by an intractable expectation. The ERS scheme described in Algorithm 1 bypasses this issue by accepting the proposal \( X \) with probability \( \frac{\hat{Z}}{Z} \) where \( Z \) is an upper bound on \( \hat{Z} \) built using all the samples except the one selected as the proposal. To avoid unnecessary complications, we also assume here that \( w(x) > 0 \) -almost surely

Algorithm 1 Ensemble Rejection Sampling: Static Case

1. Sample \( X^1, \ldots, X^N \overset{i.i.d.}{\sim} q \).
2. Sample \( X \sim \hat{\pi} \) given by (2) and compute \( \hat{Z} \) given by (3).
3. Compute the upper bound \( Z = \hat{Z} + \frac{1}{N} (\overline{w} - w(X)) \) on \( \hat{Z} \).
4. With probability \( \frac{\hat{Z}}{Z} \)

output \( X \). Otherwise, return to Step 1.

2.2 Proof of correctness

The ERS scheme described in Algorithm 1 satisfies the following property.

\footnotetext{1}{If this assumption is not satisfied and \( w(X^1) = \cdots = w(X^N) = 0 \), then we cannot build \( \hat{\pi} \) in Step 2 and return to Step 1.}
**Proposition 1.** For any $N \geq 1$, Algorithm 1 returns an exact sample from the distribution $\pi$ defined in (1) and the average acceptance probability $p_{\text{ERS}}$ of a proposal satisfies

$$p_{\text{ERS}} \geq \frac{N_{\text{RS}}}{1 + (N - 1)_{\text{RS}}}.$$ 

In particular, one has $p_{\text{ERS}} \to 1$ as $N \to \infty$.

**Proof.** For $N = 1$, the result is trivial as ERS coincides with the standard RS algorithm. To establish this result for $N \geq 2$, we show that Algorithm 1 is a standard RS scheme sampling a target distribution defined on an extended space; this extended target distribution admitting a marginal distribution equal to $\pi$. Sampling from the proposal in Step 2 of Algorithm 1 can be rewritten as sampling from the distribution

$$q(k,x,x) = \left\{ \prod_{i=1}^{N} q(x^i) \right\} \frac{w(x^k)}{\sum_{i=1}^{N} w(x^i)} \delta_{x^k}(x),$$

(6)

where $x := (x^1, ..., x^N)$; i.e. sample $X^1, ..., X^N \sim q$ then sample an index $K \in \{1, ..., N\}$ where $P(K = k) \propto w(x^k)$ and set $X = X^K$. To simplify notation, we avoid here measure-theoretic notation for the Dirac measure. We can indeed easily check that the distribution of $X$ under (6) is equal to (4). As this proposal is accepted with probability (5), accepted samples are distributed according to a distribution $\pi(k,x,x)$ satisfying

$$\pi(k,x,x) \propto q(k,x,x) \frac{Z}{\sum_{i=1}^{N} q(x^i) \delta_{x^k}(x)},$$

(7)

Elementary calculations show that

$$\frac{\pi(k,x,x)}{Z} = \frac{\pi(x^k)}{N} \delta_{x^k}(x) \prod_{i=1, i \neq k}^{N} q(x^i) := \tilde{\pi}(k,x,x).$$

(8)

The identity (8) has been used for example in [2, Theorem 1]. By using (8), we can rewrite (7) as

$$\pi(k,x,x) \propto \pi(x^k) \delta_{x^k}(x) \frac{\prod_{i=1, i \neq k}^{N} q(x^i)}{Z}.$$  

(9)

The last term on the right hand side of (9) does not indeed depend on $x = x^k$ as $Z = \frac{1}{\tilde{\pi}}(\pi + \sum_{i=1, i \neq k}^{N} w(x^i))$. From (9), it follows directly that the marginal distribution of $X$ under $\pi$ satisfies

$$\pi(x) := \sum_{k=1}^{N} \int \cdots \int_{X^N} \pi(k,x,x) dx$$

$$= \pi(x).$$

Hence we have shown that Algorithm 1 is a RS algorithm targeting $\pi(k,x,x)$ using the proposal $\pi(k,x,x)$. As $\pi(x) = \pi(x)$, this returns in particular a sample from $\pi$. 

4
The average acceptance probability of a proposal for ERS is given by

\[ p_{ERS} = \mathbb{E}_\pi \left[ \frac{\hat{Z}}{Z} \right] = Z \mathbb{E}_\tilde{\pi} \left[ \frac{1}{Z} \right] \]

\[ \geq \frac{Z}{\mathbb{E}_\pi \left[ \frac{1}{Z} \right]} \]

\[ = \frac{NZ}{(N-1)Z + \pi} \]

\[ = \frac{Np_{RS}}{(N-1)p_{RS} + 1} \]

where we have exploited, in turn, the identity (8), Jensen’s inequality and the fact that \( X_i \sim q \) under \( \tilde{\pi} \) for \( i \neq K \) and that \( Z \) only depends on \( X \setminus \{X^K\} \).

An obvious competitor to ERS consists of simply running \( N \) independent standard RS algorithms, this has approximately the same computational complexity and the probability of obtaining at least one sample from \( \pi \) is \( 1 - (1 - p_{RS})^N \). In our experiments ERS never outperforms this simple procedure in terms of expected computational efforts required to obtain an exact sample from \( \pi \). Algorithm 1 is thus of limited practical interest. However, we will see in the next section that the main ideas behind this algorithm can be extended to propose a useful exact simulation algorithm for state-space models.

### 3 Ensemble Rejection Sampling: Dynamic Case

#### 3.1 Algorithm

Let \( z_{i:j} := (z_i, z_{i+1}, ..., z_j) \) for \( i \leq j \) and \( [m] := \{1, 2, ..., m\} \) for any integer \( m \geq 1 \). We now consider the case where we are interested in sampling the posterior distribution of the latent states \( X_{1:T} \in \mathcal{X}^T \) of a state-space model given a realization \( Y_{1:T} = y_{1:T} \) of the observations, i.e. we consider a target distribution of density

\[ \pi(x_{1:T}) = \frac{\gamma(x_{1:T})}{Z}, \]

where

\[ \gamma(x_{1:T}) = p(x_{1:T}; y_{1:T}) = \mu(x_1)g(y_1|x_1)\prod_{t=2}^{T} f(x_t|x_{t-1})g(y_t|x_t), \]

\( \mu \) being the initial prior density of the latent Markov process, \( f \) its homogeneous transition density and \( g \) defining the conditional density of the observations; all these densities being defined w.r.t. to suitable dominating measures. The normalizing constant is thus given by

\[ Z = p(y_{1:T}) = \int_{\mathcal{X}^T} \cdots \int_{\mathcal{X}^T} p(x_{1:T}, y_{1:T})dx_{1:T}. \]

The algorithm detailed below is more generally applicable to a class of Feynman-Kac models [6], i.e. replace \( g(y_i|x_i) \) in (11) by a non-negative function \( G_t(x_t) \); see Section 4 for an application to rare event simulation.
As in Section 2, we will sample from the target using a RS mechanism based on a proposal built using an importance sampling approximation of $\pi$. This approximation is obtained as follows. We draw $X_{1:t}^1, \ldots, X_{1:t}^N \overset{i.i.d.}{\sim} q_t$ for $t \in [T]$, these samples define a random grid in $X^T$. From these ensembles of samples, we can build $\pi^T$ paths $X_{1:T}^{i_1:T} := (X_{1}^{i_1}, \ldots, X_{T}^{i_T})$ where $i_{1:T} \in [N]^T$ and each such path is marginally distributed according to $\prod_{t=1}^T q_t(x_t)$. Thus a self-normalized importance sampling approximation of $\pi$ is given by

$$\hat{\pi}(\cdot) = \sum_{i_{1:T} \in [N]^T} W^{i_{1:T}} \delta_{X_{1:T}^{i_{1:T}}} (\cdot),$$

where

$$W^{i_{1:T}} = \frac{w(X_{1:T}^{i_{1:T}})}{N^T Z}, \quad \hat{Z} = \frac{1}{N^T} \sum_{i_{1:T} \in [N]^T} w(X_{1:T}^{i_{1:T}}).$$

Here the unnormalized importance weights are given by

$$w(x_{1:T}^{i_{1:T}}) = \frac{p(x_{1:T}^{i_{1:T}}, y_{1:T})}{\prod_{t=1}^T q_t(x_t^{i_t})} = w_1(x_1^{i_1}) \prod_{t=2}^T w_t(x_{t-1}^{i_{t-1}}, x_t^{i_t}),$$

where the ‘incremental’ importance weights satisfy

$$w_1(x_1) := \frac{\mu(x_1) g(y_1|x_1)}{q_1(x_1)}, \quad w_t(x_{t-1}, x_t) := \frac{f(x_t|x_{t-1}) g(y_t|x_t)}{q_t(x_t)} \text{ for } t \geq 2.$$

Note that $\hat{Z}$ is an unbiased estimator of $Z$. Even if $\pi$ is defined on the high-dimensional space $X^T$, importance sampling can be expected to provide a decent approximation to $\pi$ as $\hat{\pi}$ relies on an exponentially large number $N^T$ of (dependent) samples. Once the random grid has been sampled, our proposal is simply obtained by sampling $X_{1:T} \sim \hat{\pi}$ given in (12). If we denote $X_t = (X_1^t, \ldots, X_T^t)$ the random samples generated at time $t$, the marginal distribution of the proposal $X_{1:T}$ is thus given by

$$\hat{\pi}(\cdot) = E_{X_{1:T}} [\hat{\pi}(\cdot)].$$

This proposal has been introduced in an independent Metropolis–Hastings scheme in [12, Section 3.2] and it is a slight variation over the approach proposed in [17]².

We will assume from now on that

$$\sup_{x_1} w_1(x_1) \leq \overline{w}_1 < \infty, \quad \sup_{x_{t-1}, x_t} w_t(x_{t-1}, x_t) \leq \overline{w}_t < \infty \text{ for } t \geq 2,$$

where these supremums only have to be taken over the support of the corresponding marginals of $\pi$ and $\overline{w}_1, \ldots, \overline{w}_T$ are known. We might have also access to some upper bounding functions for $t \geq 2$

$$\sup_{x_t} w_t(x_{t-1}, x_t) \leq \overline{\overline{w}}_t(x_{t-1}), \quad \sup_{x_{t-1}} w_t(x_{t-1}, x_t) \leq \overline{\overline{w}}_t(x_t).$$

We can always select $\overline{\overline{w}}_1(x_{t-1}) = \overline{w}_t$ and $\overline{\overline{w}}_2(x_t) = \overline{w}_t$ if tighter bounding functions are not available.

² In [17], a MCMC scheme is proposed to sample $\pi$. At each iteration, $N - 1$ particles $X_1^t, \ldots, X_N^t$ are sampled for each $t \in [T]$ using two MCMC kernels of invariant distribution $q_t$ initialized using the component $X_t$ of a reference path. At equilibrium, the reference path is distributed according to $\pi$. 

6
As observed in [17], a key point is that it is possible to sample exactly from proposals of the form (20) in \(O(N^2T)\) operations despite the fact that it is a discrete distribution defined on a space of cardinality \(N^T\). This can be achieved by using a HMM-type recursion detailed in Algorithm 3 for the ‘embedded’ \(N\)-state Markov chain of state space \(\{X^1_t, \ldots, X^N_T\}\) at time \(t\), initial probability proportional to \(w_0(X^1_t)\), transition probabilities proportional to \(f(X^i_{t-1} | X^i_{t-1})\) and emission probabilities proportional to \(g(y_t | X^i_t)/\bar{q}_{i}(X^i_t)\) at time \(t \geq 2\). Indeed sampling from \(\hat{\pi}\) is equivalent to sampling from the posterior distribution of this embedded HMM defined as

\[
\hat{p}(x_{1:T}|y_{1:T}) := \frac{w(x_{1:T})}{N^T \bar{Z}}.
\]

It is well-known that one can sample from this discrete distribution using a forward filtering-backward sampling algorithm exploiting the decomposition\(^3\)

\[
\hat{p}(x_{1:T}|y_{1:T}) = \hat{p}(x_T|y_{1:T}) \prod_{t=1}^{T-1} \hat{p}(x_t|y_{1:t}, x_{t+1}),
\]

where

\[
\hat{p}(x_t|y_{1:t}, x_{t+1}) := \frac{f(x_{t+1}|x_t)\hat{p}(x_t|y_{1:t})}{\sum_{i=1}^{N} f(x_{t+1}|X^i_t)\hat{p}(X^i_t|y_{1:t})}
\]

As a byproduct of the HMM forward recursion for the embedded chain, we also compute \(\hat{Z}\) in \(O(N^2T)\) operations; see Algorithm 3 for details.

As in Section 2, ERS requires being able to compute an upper bound \(\bar{Z}\) on \(\hat{Z}\) built using all the samples \(X_{1:T}\) except the ones selected as the proposal \(X_{1:T}\). This proposal is of the form \(X_{1:T} = (X^K_{1:T}, \ldots, X^K_{1:T})\) for \((K, \ldots, K) \in [N]^T\) such that \(Pr((K, \ldots, K) = (k, \ldots, k_T)) = \hat{p}(x^{k_1}_{1:T}|y_{1:T})\).

From (13), \(\hat{Z}\) is an average of \(N^T\) products of \(T\) terms of the form \(w_1(X_{t+1}^{i_1})\prod_{t=2}^{T} w_t(X_{t-1}^{i_{t-1}} | X_{t}^{i_{t}})\).

We obtain \(\bar{Z}\) by upper bounding any term \(w_1(X_{t+1}^{i_1})\) by \(\bar{w}_1\), \(w_t(X_{t-1}^{i_{t-1}} | X_{t}^{i_{t}})\) by \(\bar{w}_t\) for \(i_t \neq K_t\) and \(w_t(X_{t-1}^{i_{t-1}} | X_{t}^{i_{t}})\) by \(\bar{w}_t\) for \(t = 2, \ldots, T\).

This bound can be computed in \(O(N^2T)\) operations using a simple modification of the HMM recursion presented in Algorithm 3; this is detailed in Algorithm 4. Algorithm 2 summarizes the ERS scheme. For \(T = 1\), this algorithm corresponds to Algorithm 1 applied to \(\mu(x) = \mu(x)g(y_1|x)\) using \(g(x) = q_1(x)\). We also assume that \(w(x_{1:T}) > 0 \prod_{t=1}^{T} q_{i_t}\) almost surely to simplify presentation.

**Algorithm 2 Ensemble Rejection Sampling: Dynamic Case**

1. For \(t \in [T]\), sample \(X^1_t, \ldots, X^N_t \sim_{i.i.d.} q_t\).
2. Sample \(X_{1:T} \sim \hat{\pi}\) given by (12) and compute \(\hat{Z}\) given by (13) using Algorithm 3.
3. Compute an upper bound \(\bar{Z}\) on \(\hat{Z}\) using Algorithm 4.
4. With probability

\[
\frac{\hat{Z}}{\bar{Z}},
\]

output \(X_{1:T}\). Otherwise, return to Step 1.

\(^3\)This decomposition has also been used to sample exactly from the posterior distribution of linear Gaussian state-space models by leveraging Kalman recursions [3].
Algorithm 3 Hidden Markov Model recursion

1. At time $t = 1$
   (a) For $i \in [N]$, set $\tilde{p}(X_1^i, y_1) = w_1(X_1^i)$.
   (b) Compute $\tilde{p}(y_1) = \sum_{i=1}^{N} w_1(X_1^i)$.
   (c) For $i \in [N]$, compute $\tilde{p}(X_1^i | y_1) = \tilde{p}(X_1^i, y_1) / \tilde{p}(y_1)$.

2. For $t = 2, ..., T$
   (a) For $i \in [N]$, compute $\tilde{p}(X_t^i, y_t | y_{1:t-1}) = \sum_{j=1}^{N} \tilde{p}(X_{t-1}^j | y_{1:t-1}) w_t(X_t^i, X_{t-1}^j)$.
   (b) Compute $\tilde{p}(y_t | y_{1:t-1}) = \sum_{i=1}^{N} \tilde{p}(X_t^i, y_t | y_{1:t-1})$ and $\tilde{p}(y_{1:t}) = \tilde{p}(y_{1:t-1}) \tilde{p}(y_t | y_{1:t-1})$.
   (c) For $i \in [N]$, compute $\tilde{p}(X_t^i | y_{1:t}) = \tilde{p}(X_t^i, y_t | y_{1:t-1}) / \tilde{p}(y_{1:t})$.

3. Sample $X_{1:T}^{K_{t-1}} \sim \tilde{p}(- | y_{1:T})$.

4. For $t = T - 1, ..., 1$, sample $X_t^{K_{t-1}} \sim \tilde{p}(| y_{1:t}, X_{t+1}^{K_{t+1}})$ (see equation (18)).

5. Output $X_{1:T} := X_{1:T}^{K_{t-1}}, K_{1:T}$ and $\tilde{Z} = \tilde{p}(y_{1:T}) / N_T$.

Algorithm 4 Bounding Hidden Markov Model recursion

1. At time $t = 1$
   (a) Set $\overline{p}(X_1^{K_1}, y_1) = \overline{w}_1$ and for $i \in [N] \setminus \{K_1\}$, set $\overline{p}(X_1^i, y_1) = w_1(X_1^i)$.
   (b) Compute $\overline{p}(y_1) = \sum_{i=1}^{N} \overline{p}(X_1^i, y_1)$.
   (c) For $i \in [N]$, compute $\overline{p}(X_1^i | y_1) = \overline{p}(X_1^i, y_1) / \overline{p}(y_1)$.

2. For $t = 2, ..., T$
   (a) For $i \in [N] \setminus \{K_t\}$, compute
      $$\overline{p}(X_t^i, y_t | y_{1:t-1}) = \sum_{j \neq K_{t-1}} \overline{p}(X_{t-1}^j | y_{1:t-1}) w_t(X_t^i, X_{t-1}^j) + \overline{p}(X_{t-1}^{K_{t-1}} | y_{1:t-1}) \overline{w}_t(X_t^i).$$
   (b) For $i = K_t$, compute
      $$\overline{p}(X_t^{K_t}, y_t | y_{1:t-1}) = \sum_{j \neq K_{t-1}} \overline{p}(X_{t-1}^j | y_{1:t-1}) \overline{w}_t(X_t^j) + \overline{p}(X_{t-1}^{K_{t-1}} | y_{1:t-1}) \overline{w}_t.$$
   (c) Compute $\overline{p}(y_t | y_{1:t-1}) = \sum_{i=1}^{N} \overline{p}(X_t^i, y_t | y_{1:t-1})$ and $\overline{p}(y_{1:t}) = \overline{p}(y_{1:t-1}) \overline{p}(y_t | y_{1:t-1})$.
   (d) For $i \in [N]$, compute $\overline{p}(X_t^i | y_{1:t}) = \overline{p}(X_t^i, y_t | y_{1:t-1}) / \overline{p}(y_{1:t-1})$.

3. Output $\overline{Z} = \overline{p}(y_{1:T}) / N_T$. 
3.2 Theoretical results

We establish here the validity of the ERS scheme described in Algorithm 2.

**Proposition 2.** For any \( N \geq 1 \), Algorithm 2 returns an exact sample from the distribution \( \pi \) defined in (10) and its corresponding average acceptance probability satisfies \( p_{ERS} \to 1 \) as \( N \to \infty \).

**Proof.** For \( N = 1 \), ERS is a standard RS scheme so it returns samples from \( \pi \). The first part of the proof is essentially identical to the first part of the proof of Proposition 1. Sampling from the proposal in Step 2 of Algorithm 2 can be rewritten as sampling from the distribution

\[
\mathcal{V}(k_{1:T}, x_{1:T}, x_{1:T}) = \left\{ \prod_{t=1}^{T} \prod_{i=1}^{N} q_t(x_i) \right\} \frac{w(x_{1:T})}{\sum_{i_{1:T} \in [N]^T} w(x_{1:T})} \delta_{x_{1:T}}(x_{1:T}),
\]

(20)

where \( x_i := (x_1^i, ..., x_N^i) \). Indeed, it is easy to check that the marginal distribution of \( X_{1:T} \) under \( \mathcal{V} \) satisfies (14).

The distribution of the samples accepted by Algorithm 2 is thus given by

\[
\pi(k_{1:T}, x_{1:T}, x_{1:T}) \propto \mathcal{V}(k_{1:T}, x_{1:T}, x_{1:T}) \hat{Z},
\]

(21)

where we recall that \( \hat{Z} \) is a function of \( x_{1:T} \) while, by construction, \( \mathcal{Z} \) is only a function of \( x_{1:T} \setminus \{ x_{1:T} \} \). One can verify that

\[
\mathcal{V}(k_{1:T}, x_{1:T}, x_{1:T}) \hat{Z} = \frac{\pi(x_{1:T})}{N^T} \delta_{x_{1:T}}(x_{1:T}) \prod_{t=1}^{T} \prod_{i=1, i \neq k_t} q_t(x_i)
\]

(22)

\[
:= \tilde{\pi}(k_{1:T}, x_{1:T}, x_{1:T}).
\]

The probability distribution \( \tilde{\pi}(k_{1:T}, x_{1:T}, x_{1:T}) \) was introduced in [17] and the identity relating \( \tilde{\pi} \) to \( \mathcal{V}, \mathcal{Z}, Z \) has been established in [12, Section 3.2]. By using (22), we can rewrite (21) as

\[
\pi(k_{1:T}, x_{1:T}, x_{1:T}) \propto \pi(x_{1:T}) \delta_{x_{1:T}}(x_{1:T}) \prod_{t=1}^{T} \prod_{i=1, i \neq k_t} q_t(x_i)
\]

(23)

\[
\text{term independent of } x_{1:T} = x_{1:T}^{k_T}.
\]

From (23), it follows directly that

\[
\pi(x_{1:T}) := \sum_{k_{1:T} \in [N]^T} \int \cdots \int_{X_{1:T}} \pi(k_{1:T}, x_{1:T}, x_{1:T}) dx_{1:T}
\]

\[
= \pi(x_{1:T}).
\]

Hence we have shown that Algorithm 2 is a RS algorithm targeting \( \pi(k_{1:T}, x_{1:T}, x_{1:T}) \) using the proposal \( \mathcal{V}(k_{1:T}, x_{1:T}, x_{1:T}) \). As \( \pi(x_{1:T}) = \pi(x_{1:T}) \), this returns in particular a sample from \( \pi \).

Using arguments similar to the ones used in the proof of Proposition 1, we can show that the average acceptance probability \( p_{ERS} \) of a proposal for ERS satisfies

\[
p_{ERS} = \mathbb{E}_\pi \left[ \frac{\hat{Z}}{Z} \right] \geq \frac{Z}{\mathbb{E}_\pi \left[ \mathcal{Z} \right]},
\]

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where \( \tilde{\pi} \) is defined in (22). By bounding any term of the sum appearing in \( Z \) involving at least one index such that \( i_t = K_t \) for \( t \in [T] \) by \( \prod_{t=1}^{T} w_i \), we obtain the following upper bound

\[
\mathbb{E}_\pi [Z] \leq \left( 1 - \frac{1}{N} \right)^T Z + \left( 1 - \frac{1}{N^2} \right)^T \prod_{t=1}^{T} w_i
\]

(24)
as \( X_t^\pi \sim q_i \) for \( t \in [T] \) and \( i \neq K_t \) under \( \pi \). Hence the r.h.s. of (24) converges to \( Z \) as \( N \to \infty \) and thus \( p_{ERS} \to 1 \) as \( N \to \infty \). □

Proposition 2 does not guarantee that at fixed computational efforts the proposed algorithm ERS is competitive compared to a standard RS algorithm using the proposal \( \prod_{t=1}^{T} q_t(x_i) \). For \( T = 1 \), we have seen in Section 2 that this is not the case. However the following toy example suggests that ERS exhibits desirable properties for large \( T \) if we scale \( N \) with \( T \) appropriately.

**Example 3.** Consider a scenario where \( y_{1:T} = (y, \ldots, y) \),

\[
\gamma(x_{1:T}) = p(x_{1:T} | y_{1:T}) = \prod_{t=1}^{T} \mu(x_t | y_t),
\]

so

\[
Z = Z^T, \quad \text{where} \quad Z = \int \mu(x)g(y|x)dx.
\]

Obviously the corresponding target distribution \( \pi \) factorizes in \( T \) independent terms in this case. However, for the sake of illustration, we ignore this fact and apply directly ERS to \( \pi \). Standard RS using a proposal \( \prod_{t=1}^{T} q_t(x_t) \) has an average acceptance probability \( p_{RS} = \frac{Z}{Z^T} \), where \( p_A = \frac{Z}{Z^T} \). As long as \( q_t(x) \) is not equal to \( \mu(x)g(y|x)/Z \) almost everywhere, then \( p_A < 1 \) and so \( p_{RS} \) decreases exponentially fast with \( T \). In the same scenario, simple calculations shows that ERS has an average acceptance probability satisfying

\[
p_{ERS} \geq \frac{(NZ)^T}{((N-1)Z + w_i)^T} = \frac{1}{(1 + \frac{1}{N} (p_A^{-1} - 1))^T}
\]

(25)

If we select \( N = \lceil \beta T \rceil \) where \( \beta > 0 \), then the r.h.s. of (25) converges to \( \exp \{ \beta^{-1}(1 - p_A^{-1}) \} \) as \( T \to \infty \); i.e. we can control \( p_{ERS} \) by only increasing \( N \) linearly with \( T \).

We now establish a similar result for the more realistic scenario where the target distribution does not factorize. Our result relies on a strong regularity condition in the spirit of the assumptions commonly used in the particle filtering literature to establish quantitative bounds [6, Chapter 4]. It will typically hold for a compact state-space \( \mathcal{X} \) or when the support of the target is given by a compact subspace of \( \mathcal{X}^T \).

**Proposition 4.** Assume that there exist \( w, \overline{w} > 0 \) such that \( w < w_t(x) \leq \overline{w} \) and \( w \leq w_t(x, x') \leq \overline{w} \) for all \( x, x' \in \mathcal{X} \times \mathcal{X} \) and \( t \geq 2 \) and let \( \delta = (\overline{w}/w)^2 \), then the average acceptance probability \( p_{ERS} \) of Algorithm 2 satisfies

\[
p_{ERS} \geq \frac{1}{(1 + \frac{1}{N} \delta^{-1})^T}
\]

In particular, for \( N = \lceil \beta T \rceil \) where \( \beta > 0 \), we have

\[
\liminf_{T \to \infty} p_{ERS} \geq \exp \{ \beta^{-1}(1 - \delta) \}.
\]
Proof. To lower bound $p_{ERS}$, we use again the inequality

$$p_{ERS} \geq \frac{Z}{E_{\tilde{\pi}} \left[ \frac{Z}{T} \right]}$$

where $\tilde{\pi}$ is defined in (22) and then we exploit the assumption on the incremental weights to compute an upper bound on $E_{\tilde{\pi}} \left[ \frac{Z}{T} \right]$ that is tighter than the bound (24) used in the proof of Proposition 2.

The term $Z$ is given by a sum over the indices $i_1:T \in [N]^T$. Of the total $N^T$ terms, $(N - 1)^T$ of these terms are such that such $i_1 \neq K_1, i_2 \neq K_2, ..., i_T \neq K_T$ and each such term has expectation $Z$ under $\tilde{\pi}$. Among the remaining $N^T - (N - 1)^T$ terms, $T(N - 1)^{T-1}$ have exactly one index $t_1 \in [T]$ such that $i_{t_1} = K_{t_1}$ and more generally $(T^m)(N - 1)^{T-n}$ terms have exactly $n$ distinct indices $t_1, t_2, ..., t_n \in [T]^n$ such that $i_{t_m} = K_{t_m}$ for $m \in [n]$. For each such term, we have to bound the corresponding product of the $T$ incremental weights. Each index $i_{t_m} = K_{t_m}$ can impact at most two terms in the product, e.g., $w_{t_m}^1(x_{t_m-1}^{i_{t_m-1}})w_{t_m+1}^2(x_{t_m+1}^{i_{t_m+1}})$ if one considers a sequence $i_1:T$ such that $i_{t_m-1} \not= K_{t_m-1}$ and $i_{t_m+1} \not= K_{t_m+1}$. However, the assumption on the incremental weights yields

$$\frac{\sum_{m=1}^T \left[ w_{t_m}^1(x_{t_m-1}^{i_{t_m-1}})w_{t_m+1}^2(x_{t_m+1}^{i_{t_m+1}}) \right]}{\sum_{m=1}^T \left[ w_{t_m}^1(x_{t_m-1}^{i_{t_m-1}})w_{t_m+1}^2(x_{t_m+1}^{i_{t_m+1}}) \right]} \leq \left( \frac{\delta}{N} \right)^{2} w_{t_m}^1(x_{t_m-1}^{i_{t_m-1}})w_{t_m+1}^2(x_{t_m+1}^{i_{t_m+1}}) \leq \delta w_{t_m}^1(x_{t_m-1}^{i_{t_m-1}})w_{t_m+1}^2(x_{t_m+1}^{i_{t_m+1}})$$

Hence, we have

$$E_{\tilde{\pi}} \left[ \frac{Z}{T} \right] \leq \frac{Z}{N^T} \sum_{n=0}^T \binom{T}{n} (N - 1)^{T-n} \delta^n = Z \sum_{n=0}^T \binom{T}{n} \left( 1 - \frac{1}{N} \right)^{T-n} \left( \frac{\delta}{N} \right)^n = Z \left( 1 + \frac{\delta - 1}{N} \right)^T$$

The result now follows directly.

Proposition 4 ensures that the average acceptance probability $p_{ERS}$ does not vanish as long as $N$ increases linearly with $T$. As the computational complexity to sample from the proposal distribution is $O(N^2T)$, this shows that the expected computational cost to obtain an exact sample is of order $O(T^3)$.

3.3 Settings and Extensions

We discuss here how to select the proposal distributions and propose various extensions of Algorithm 2.

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3.3.1 Selection of the proposal distributions

The need for bounded importance weights, see (15), limits the range of applicability of ERS but can be satisfied for a useful class of non-linear state-space models. For example, consider a model such that

$$\sup_x \mu(x) \leq \overline{\mu} < \infty, \quad \sup_{x,x'} f(x'|x) \leq \overline{f} < \infty, \quad g(y_t) := \int_X g(y_t|x)dx < \infty,$$

for all t. If we use the proposals given by

$$q_t(x_t) \propto g(y_t|x_t),$$

ERS applies with $w_1(x_1) = \mu(x_1), \overline{\mu}_1 = \overline{\mu}$ and $w_t(x_{t-1}, x_t) = f(x_{t-1}, x_t), \overline{\mu}_t = \overline{f}$ for $t \geq 2^t$. Such proposals have been used in the particle filtering literature in [15].

We might also have a model such that

$$f(x'|x) \leq c\nu(x')$$

where $\nu$ is a probability density function. In this case, it is possible to use a proposal of the form

$$q_t(x_t) \propto \nu(x_t) g(y_t|x_t)$$

for $t \geq 2$ and $q_t(x_t) \propto \mu(x_t)g(y_t|x_t)$. In this case, ERS applies with $w_1(x_1) = \overline{\mu}_1 = 1$ and $w_t(x_{t-1}, x_t) = f(x_t|x_{t-1})/\nu(x_t), \overline{\mu}_t = c$ for $t \geq 2$.

3.3.2 Intractable weights

Consider a scenario where the incremental weights are not tractable as $\mu(x), f(x'|x)$ or $g(y|x)$ cannot be evaluated pointwise. If one has access to a non-negative unbiased estimator of the intractable quantity that is upper bounded almost surely by a known finite constant, then ERS can be applied directly without any modification. The correctness of this procedure follows from a standard auxiliary variable construction. This shows for example that ERS can be applied to simulate exactly from the posterior distribution of the class of diffusions considered in [10] whose state is observed at discrete times in some additive Gaussian noise.

3.3.3 Non-integrability of $g(y|x)$ w.r.t. $x$ and missing data

Consider a scenario where $\int g(y|x)dx < \infty$ but $\int g(y_{t+1}|x)dx = \infty$. We can thus use a proposal $q(x|y) \propto g(y|x)$ at time $t$ but not at time $t+1$. To bypass this problem, we can consider instead using an incremental weight at time $t$ of the form

$$w_t(x_{t-1}, x_t) := \frac{f(x_t|x_{t-1})g(y_t|x_t)p(y_{t+1}|x_t)}{q_t(x_t)},$$

where $p(y_{t+1}|x_t) = \int f(x_{t+1}|x_t)g(y_{t+1}|x_{t+1})dx_{t+1}$. A non-negative estimate of this quantity can be obtained if it cannot be calculated in closed-form; e.g., sample $X_{t+1} \sim f(\cdot|x_t)$ and return $g(y_{t+1}|X_{t+1})$. This can be directly extended to scenarios where $\int g(y|x)dx = \infty$ for

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4The target is not modified by replacing $g(y|x)$ by $g(y|x)/g(y)$ so $g(y)$ does not appear in the bounds $\overline{\mu}_t$. 12
Table 1: Estimated average acceptance probability $p_{ERS}$ in % computed using 500 samples as a function of $T$ and $N$

| $\hat{p}_{ERS}$ | $N = T$ | $N = 2T$ | $N = 5T$ |
|-----------------|---------|---------|---------|
| $T = 100$       | 3.19    | 17.29   | 49.00   |
| $T = 250$       | 2.91    | 16.92   | 47.75   |
| $T = 500$       | 2.82    | 16.64   | 48.50   |

$k = t + 1, \ldots, t + \Delta$ for $\Delta \geq 1$. Hence we can also use ERS in this scenario to sample the posterior distribution of the states $x_t$ such that $\int g(y_t|x)dx < \infty$ and then sampling the remaining states according to their full conditionals of the form $p(x_{t+\Delta+1}|x_t, x_{t+\Delta+1}, y_{t+1:t+\Delta})$ using standard RS. Obviously, this method becomes inefficient if $\Delta$ is large.

Similarly, we might be in a scenario where $x_t = (z_t, \ldots, z_{t-\Delta+1})$ and, slightly abusing notation, $g(y_t|x_t) = g(y_t|z_t)$ with $\int g(y_t|z_t)dz_t < \infty$. In this case, we can also pull observations together by blocks of length $\Delta$ to sample the latent state $z_t$ through a distribution proportional to the product of $g(y_t|z_t)$ over a block.

### 3.3.4 Other extensions

There are many other possible extensions of interest. We only briefly mention two of them here. For example, we can make the number of particles depends on the time index to address scenarios where one has outliers. We can also extend the ERS procedures to sample exactly from the posterior distribution of the continuous latent states of a tree-structure directed graphical model as a generalized version of the key forward-backward recursion is available in these scenarios; see, e.g., [4, 25].

### 4 Examples

All the simulations have been performed in Matlab on a standard desktop PC. The code and data will be soon made publicly available.

#### 4.1 Conditioned random walks

To demonstrate our methodology on a rare event problem, we consider here the problem of simulating conditioned random walks discussed in [1, 7] where $\mathcal{X} = \mathbb{R}$, $\mu(x) = \mathcal{U}(x; S)$ is the uniform distribution on $S$, $f(x'|x) = \mathcal{N}(x'; \psi(x), \sigma^2)$ and $G_t(x) = 1_S(x)$ for some bounded set $S \subset \mathbb{X}$. This models the evolution of a particle in an absorbing medium, the particle being absorbed whenever it steps outside $S$. Here the non-negative function $G_t(x)$ replaces $g(y_t|x_t)$ in equation (11). In this case, the distribution $\pi$ corresponds to the distribution of the paths of the particle conditional upon not having been absorbed by time $T$. A method to sample exactly from this distribution has been proposed in [1] but it is only applicable to very specific dynamics and sets $S$. ERS is particularly well-suited to such problems. To implement ERS, we use $q_t(x) = \mathcal{U}(x; S)$ for all $t \geq 1$ so that $\overline{w}_t = 1$ and $\overline{w}_t = 1/\sqrt{2\pi\sigma^2}$ for $t \geq 2$. The assumptions of Proposition 4 are satisfied. In our simulations, we consider $S = [0, 1]$, $\psi(x) = x$, and $\sigma = 0.2$. 

We consider different values for \( T \) as well as corresponding values for \( N \). We estimate \( p_{\text{ERS}} = \mathbb{E}_{q_0}[\hat{Z} / \bar{Z}] \) by Monte Carlo using 500 samples from \( \mathcal{F} \). In this scenario and other examples considered here, the relative variance of the corresponding estimator is small as \( \hat{Z} \) and \( \bar{Z} \) are strongly positively correlated by construction. The results are summarized in Table 1. For this time-homogeneous model, the average acceptance probability is, as expected, fairly stable across \( T \) for a fixed ratio \( N/T \).

4.2 Non-linear autoregressive process

Consider the following non-linear autoregressive model where \( \mathcal{X} = \mathbb{R}, \mu(x) = \mathcal{N}(x; 0, 1), f(x'|x) = \mathcal{N}(x'; \phi \tanh(x), \sigma^2) \) and \( g(y|x) = \mathcal{N}(y; x, \sigma_0^2) \) with \( \phi = 0.9, \sigma_v = 0.3 \) and \( \sigma_w = 0.1 \). We select \( q_t(x_t|y_t) \propto g(y_t|x_t) \) and the corresponding bounds are \( \bar{\pi}_t = 1/\sqrt{2\pi} \) and \( \underline{\pi}_t = 1/\sqrt{2\pi\sigma^2} \) for \( t \geq 2 \). For a given realization of \( T = 500 \) data points, the estimated average acceptance probability \( p_{\text{ERS}} \) using 500 samples is \( p_{\text{ERS}} \) is 0.79\% for \( N = 500 \), 7.34\% for \( N = 1000 \) and 24.34\% using \( N = 2000 \).

4.3 Stochastic volatility model

Consider the following univariate stochastic volatility model where \( \mathcal{X} = \mathbb{R}, \mu(x) = \mathcal{N}(x; 0, 1), f(x'|x) = \mathcal{N}(x'; \phi x, \sigma^2) \) and \( g(y|x) = \mathcal{N}(y; 0, \beta \exp(x/2)) \); see, e.g., [19]. We have \( \log Y_t^2 = X_t + \log \beta^2 + W_t \) where \( \exp(W_t) \sim \chi^2(1) \). This suggests using for \( q_t(x_t|y_t) \) the distribution obtained by sampling \( X_t \) using \( \log y_t^2 - \log \beta^2 - W_t \) where \( \exp(W_t) \sim \chi^2(1) \). The corresponding bounds are given by \( \bar{\pi}_t = \sqrt{(1 - \phi^2)/2\pi} \) and \( \underline{\pi}_t = 1/\sqrt{2\pi\sigma^2} \) for \( t \geq 2 \). We apply ERS to the S&P 500 index daily data using parameters \( \phi = 0.95, \beta = 0.7 \) and \( \sigma = 0.3 \) as in [20] for \( T = 200 \) data points corresponding to the period 09/08/1990 to 24/05/1991. For \( N = 6000 \), the estimated average acceptance probability \( p_{\text{ERS}} \) is 4.73\% estimated using 500 samples.

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