Sequential Monte Carlo Methods for System Identification*

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Abstract: One of the key challenges in identifying nonlinear and possibly non-Gaussian state space models (SSMs) is the intractability of estimating the system state. Sequential Monte Carlo (SMC) methods, such as the particle filter (introduced more than two decades ago), provide numerical solutions to the nonlinear state estimation problems arising in SSMs. When combined with additional identification techniques, these algorithms provide solid solutions to the nonlinear system identification problem. We describe two general strategies for creating such combinations and discuss why SMC is a natural tool for implementing these strategies.

Keywords: Nonlinear system identification, nonlinear state space model, particle filter, particle smoother, sequential Monte Carlo, MCMC.

1. INTRODUCTION

This paper is concerned with system identification of nonlinear state space models (SSMs) in discrete time. The general model that we consider is given by,

\[ x_{t+1} | x_t, u_t \sim f(x_{t+1} | x_t, u_t), \quad (1a) \]
\[ y_t | x_t \sim g(y_t | x_t, u_t), \quad \theta \sim \pi(\theta), \quad (1b) \]
\[ E \in R^n, \quad u_t \in U \subseteq R^m \quad \text{and} \quad y_t \in Y \subseteq R^n, \quad \text{respectively.} \]

where the states, the known inputs and the observed measurements are denoted by \( x_t \in X \subseteq \mathbb{R}^n \), \( u_t \in U \subseteq \mathbb{R}^m \) and \( y_t \in Y \subseteq \mathbb{R}^n \), respectively. The dynamics and the measurements are modeled by the probability density functions (PDFs) \( f_0(\cdot) \) and \( g_0(\cdot) \), respectively, parameterised by the unknown vector \( \theta \in \Theta \subseteq \mathbb{R}^d \). The initial state \( x_1 \) is distributed according to some distribution \( \mu_0(x_1) \). For notational simplicity, we will from hereon (without loss of generality) drop the known input \( u_t \) from the notation. When considering Bayesian identification, meaning that \( \theta \) is modelled as an unobserved random variable, we also place a prior \( \pi(\theta) \) on \( \theta \). We are concerned with off-line identification, i.e. we wish to find the unknown parameters \( \theta \) in (1) based on a batch of \( T \) measurements.

The key challenge that will drive the development throughout this paper is how to deal with the difficulty that the states \( x_{1:T} \) in (1) are unknown. We will distinguish between two different strategies for handling this:

1. Marginalisation amounts to marginalising (integrating out) the states from the problem and viewing \( \theta \) as the only unknown quantity of interest. In the frequentistic problem formulation, the prediction error method (Ljung, 1999) and direct maximisation of the likelihood belong to this strategy. In the Bayesian formulation, the Metropolis Hastings algorithm (Metropolis et al., 1953; Hastings, 1970) can be used to approximate the posterior distribution of the parameters conditionally on the data.

2. Data augmentation treats the states as auxiliary variables that are estimated together with the parameters. The expectation maximisation (EM) algorithm of Dempster et al. (1977) solves the maximum likelihood formulation in this way and the Gibbs sampler of Geman and Geman (1984) solves the Bayesian problem by this strategy.

In the special case when the model (1) is linear and Gaussian, there are closed form expressions available from the Kalman filter and the associated smoother. The primary focus of this paper, however, is the more challenging nonlinear and/or non-Gaussian case. More than two decades ago (e.g., Gordon et al., 1993; Kitagawa, 1993) sequential Monte Carlo (SMC) methods started to emerge with the introduction of the particle filter. These methods have since then undergone a rapid development and today they constitute a standard solution to the problem of computing the latent (i.e. unobserved/unknown/hidden) states in nonlinear/non-Gaussian SSMs.

The aim of this paper is to show how SMC can be used in solving the nonlinear system identification problems that arise in finding the unknown parameters in (1). We do not aim to cover all different methods that are available, but instead we aim to clearly describe exactly where and how the need for SMC arises and focus on the key principles. Complementary overview paper are provided by Kantas et al. (2015) and by Andrieu et al. (2004).

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We consider the Bayesian and the maximum likelihood formulations, as defined in Section 2. The rest of the paper is divided into three parts. In the first part (Sections 3 and 4) we describe the marginalisation and data augmentation strategies and show where the need for SMC arise. The second part (Section 5) provides a rather self-contained derivation of the particle filter and outlines some of its properties. Finally, in the third part (Section 6–8) we show how these particle methods can be used to implement the identification strategies described in the first part, resulting in several state-of-the-art algorithms for nonlinear system identification. Loosely speaking, the SMC-part of the various algorithms that we introduce is essentially a way of systematically exploring the state space $X^T$ in a nonlinear SSM (1) in order to address the key challenge of dealing with the latent state sequence $x_{1:T}$.

2. PROBLEM FORMULATION

There are different ways in which the system identification problem can be formulated. Two common formalisms are grounded in frequentistic and Bayesian statistics, respectively. We will treat both of these formalizations in this paper, without making any individual ranking among them. First, we consider the frequentistic, or maximum likelihood (ML), formulation. This amounts to finding the point estimate of the unknown parameters in (4) for which the observed data is as likely as possible. This is done by maximizing the data likelihood function according to

$$\theta_{ML} = \arg \max_{\theta \in \Theta} p_{\theta}(y_{1:T}) = \arg \max_{\theta \in \Theta} \log p_{\theta}(y_{1:T}). \tag{2}$$

For a thorough treatment of the use of ML for system identification, see e.g., Ljung (1999); Söderström and Stoica (1989).

Secondly, in the Bayesian formulation, the unknown parameters in (4) are modeled as a random variable (or random vector) according to (1c). The system identification problem thus amounts to computing the posterior distribution of $\theta$ given the observed data. According to Bayes’ theorem, the posterior distribution is given by,

$$p(\theta | y_{1:T}) = \frac{p_{\theta}(y_{1:T})p(\theta)}{p(y_{1:T})}. \tag{3}$$

Note that the likelihood function should now be interpreted as the conditional PDF of the observations given the parameters $\theta$, i.e. $p_{\theta}(y_{1:T}) = p(y_{1:T} | \theta)$. However, to be able to discuss the different identification criteria in a common setting, we will, with a slight abuse of notation, denote the likelihood by $p(y_{1:T})$ also in the Bayesian formulation. An early account of Bayesian system identification is provided by Peterka (1981) and a more recent description is available in Ninness and Henrikson (2010).

The central object in both formulations above is the observed data likelihood $p_{\theta}(y_{1:T})$, or its constituents $p_{\theta}(y_{1:t-1})$ as,

$$p_{\theta}(y_{1:T}) = \prod_{t=1}^{T} p_{\theta}(y_{t} | y_{1:t-1}). \tag{4}$$

where we have used the convention $y_{t}|0 \triangleq \emptyset$. For the nonlinear SSM (1), the likelihood (4) is not available in closed form. This is a result of the fact that the latent state sequence $x_{1:T}$, i.e. $p(x_{1:T} | y_{1:T})$, is unknown. Indeed, a relationship between the likelihood and the latent states can be obtained via marginalization of the joint density $p_{\theta}(x_{1:T}, y_{1:T})$ w.r.t. $x_{1:T}$ according to,

$$p_{\theta}(y_{1:T}) = \int p_{\theta}(x_{1:T}, y_{1:T})dx_{1:T}. \tag{5}$$

where the model provides a closed form expression for the integrand according to,

$$p(x_{1:T}, y_{1:T}) = \mu_{\theta}(x_{1}) \prod_{t=1}^{T} g_{\theta}(y_{t} | x_{t}) \prod_{t=1}^{T} f_{\theta}(x_{t+1} | x_{t}). \tag{6}$$

This expression does not involve any marginalisation, whereas the observed data likelihood $p_{\theta}(y_{1:T})$ is found by averaging the joint distribution $p_{\theta}(x_{1:T}, y_{1:T})$ over all possible state sequences according to (5). Equivalently, we can express $p_{\theta}(y_{1:T})$ as in (4) where the one-step predictive likelihood can be written (using marginalisation) as,

$$p_{\theta}(y_{t} | y_{1:t-1}) = \int g_{\theta}(y_{t} | x_{t})p_{\theta}(x_{t} | y_{1:t-1})dx_{t}. \tag{7}$$

These expressions highlight the tight relationship between the system identification problem and the state inference problem. A key challenge that will drive the developments in this work is how to deal with the latent states. For nonlinear system identification, the need for computational methods, such as SMC, is tightly coupled to the intractability of the integrals in (5) and (7).

To illustrate the strategies and algorithms introduced we will use them to solve two concrete problems, which are formulated below.

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**Example 1: Linear Gaussian model**

Our first illustrative example is a simple linear Gaussian space (LGSS) model, given by

$$x_{t+1} = 0.7x_{t} + v_{t}, \quad v_{t} \sim \mathcal{N}(0, \theta^{-1}), \tag{8a}$$

$$y_{t} = x_{t} + e_{t}, \quad e_{t} \sim \mathcal{N}(0, 0.1), \tag{8b}$$

$$(\theta \sim \mathcal{G}(0.01, 0.01)), \tag{8c}$$

where the unknown parameter $\theta$ corresponds to the precision (inverse variance) of the process noise $v_{t}$. Note that the prior for the Bayesian model is chosen as the Gamma ($\mathcal{G}$) distribution with known parameters, for reasons of simplicity, since this is the conjugate prior for this model. The initial distribution $p_{\theta}(x_{1})$ is chosen as the stationary distribution of the state process. Identification of $\theta$ is based on a simulated data set consisting of $T = 100$ samples $y_{1:100}$ with true parameter $\theta_{0} = 1$.

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**Example 2: Nonlinear non-Gaussian model**

Our second example, involving real data, is related to a problem in paleoclimatology. Shumway and Stoffer (2011) considered the problem of modeling the thickness of ice varves (layers of sediments that are deposited from melting glaciers). The silt and sand that is deposited over melting glaciers). The silt and sand that is deposited over ice varves formed at a location in Massachusetts between years 9883 and 9250 BC. We make use of a nonlinear and non-Gaussian SSM proposed by Langrock (2011) to model this data:

$$x_{t+1} | x_{t} \sim \mathcal{N}(x_{t+1}; \phi x_{t}, \tau^{-1}), \tag{9a}$$

$$y_{t} | x_{t} \sim \mathcal{G}(y_{t}; 0.25, 0.256 \exp(-x_{t})), \tag{9b}$$

with parameters $\theta = \{\phi, \tau\}$. The initial distribution $p_{\theta}(x_{1})$ is chosen as the stationary distribution of the state process. The data set and a more complete description of the problem is provided by Shumway and Stoffer (2011).
Full details concerning the examples and the numerical experiments that we provide throughout the paper are available in the appendix of the arXiv-version of this paper. The code used to generate the results is available from the first authors web-site.

3. IDENTIFICATION STRATEGY – MARGINALISATION

The marginalisation strategy amounts to solving the identification problem—either (2) or (3)—by computing the integral appearing in (7) (or, equivalently, (5)). That is, we marginalize (integrate out) the latent states \( x_{1:T} \) and view \( \theta \) as the only unknown quantity of interest.

In some special cases the marginalisation can be done exactly. In particular, for LGSS models the one-step predictive density in (7) is Gaussian and computable by running a Kalman filter. For the general case, however, some numerical approximation of the integral in (7) is needed. We will elaborate on this in Section 6, where we investigate the possibility of using SMC to perform the marginalisation. For now, however, to illustrate the general marginalisation strategy, we will assume that the integral in (7) can be solved exactly.

3.1 ML identification via direct optimisation

Consider first the ML formulation (2). Direct optimisation (DO) amounts to working directly on the problem

\[
\hat{\theta}_{ML} = \arg \max_{\theta \in \Theta} \sum_{t=1}^{T} \log p(y_t | x_t) p_0(x_t | y_{1:t-1}) dx_t,
\]

where we have rewritten the data log-likelihood using (4) and (7). Even though we momentarily neglect the difficulty in computing the integral above it is typically not possible to solve the optimisation problem (10) in closed form. Instead, we have to resort to numerical optimisation methods, see e.g. Nocedal and Wright (2006). These methods typically find a maximiser of the log-likelihood function \( \log p(y_{1:T}) \) by iteratively refining an estimate \( \hat{\theta}_k \) of the maximiser \( \theta_{ML} \) according to

\[
\hat{\theta}_{k+1} = \hat{\theta}_k + \alpha_k s_k.
\]

Here, \( s_k \) denotes the search direction which is computed based on information about the cost function available from previous iterations. The step size \( \alpha_k \), tells us how far we should go in the search direction. The search direction is typically computed according to

\[
s_k = H_k^{-1} g_k, \quad g_k = \nabla_{\theta} \log p(y_{1:T}) |_{\theta = \hat{\theta}_k},
\]

where \( H_k \) denotes a positive definite matrix (for example the Hessian \( \nabla_{\theta}^2 \log p(y_{1:T}) \) or approximations thereof) adjusting the gradient \( g_k \).

--- Example 3: DO applied to the LGSS model ---

To apply the update in (10) for estimating \( \theta \) in (8), we need to determine the search direction \( s_k \) and the step length \( \alpha_k \). Here, we select the search direction as the gradient of the log-likelihood, i.e. \( H_k \) is the identity matrix. The log-likelihood for (8) can be expressed as

\[
\log p_0(y_{1:T}) = \sum_{t=1}^{T} \log \mathcal{N}(y_t; 0.5 \hat{x}_t|t-1, P_t|t-1 + 0.1),
\]

where \( \hat{x}_t|t-1 \) and \( P_t|t-1 \) denotes the predicted state estimate and its covariance obtained from a Kalman filter. The gradient \( g_k \) in (12) of the log-likelihood (13) can therefore be obtained by calculating \( \nabla_{\theta} \hat{x}_t|t-1 \) and \( \nabla_{\theta} P_t|t-1 \), which can be obtained from the Kalman filter, using the so-called sensitivity derivatives introduced by Aström (1980). In the upper part of Figure 1, we present the log-likelihood (blue) computed using the Kalman filter together with the estimate \( \hat{\theta}_{ML} \) (orange) obtained by the DO algorithm.

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With DO the use of SMC arise in evaluation of the cost function in (10) and its derivatives to compute the search directions \( s_k \) in (12).

3.2 Bayesian identification via Metropolis Hastings

Let us now turn to the Bayesian formulation (3). As above, to illustrate the idea we consider first the simple case in which the marginalisation in (7) can be done exactly. Still, in most nontrivial cases the posterior PDF in (3) cannot be computed in closed form. The difficulty comes from the factor \( p(y_{1:T}) \), known as the marginal likelihood, which ensures that the posterior PDF is properly normalised (i.e., that it integrates to one). The marginal likelihood can be expressed as

\[
p(y_{1:T}) = \int p_0(y_{1:T}) \pi(\theta) d\theta.
\]

Even if the likelihood \( p_0(y_{1:T}) \) is analytically tractable, we see that we need to carry out an integration w.r.t. \( \theta \). Furthermore, computing a point estimate, say the posterior mean of \( \theta \), also amounts to solving an integral

\[
E[\theta | y_{1:T}] = \int \theta p(\theta | y_{1:T}) d\theta,
\]

which may also be intractable.
A generic way of approximating such intractable integrals, in particular those related to Bayesian posterior distributions, is to use a Monte Carlo method. In Section 5 we will discuss, in detail, how SMC can be used to approximately integrate over the latents states of the system. The sequential nature of SMC makes it particularly well suited for integrating over latent stochastic processes, such as the states in an SSM. However, to tackle the present problem of integrating over the latent parameters we shall consider a different class of methods denoted as Markov chain Monte Carlo (MCMC).

The idea behind MCMC is to simulate a Markov chain \( \{ \theta[m] \}_{m=1}^{\infty} \). The chain is constructed in such a way that its stationary distribution coincides with the so-called target distribution of interest, here \( p(\theta | y_{1:T}) \). If, in addition, the chain is ergodic—essentially meaning that spatial averages coincide with “time” averages—the sample path from the chain can be used to approximate expectations w.r.t. to the target distribution:

\[
\frac{1}{M-k+1} \sum_{m=k}^{M} \varphi(\theta[m]) \xrightarrow{k \to \infty} \int \varphi(\theta)p(\theta | y_{1:T})d\theta, \quad (16)
\]

as \( M \to \infty \), for some test function \( \varphi \). Here \( \xrightarrow{a.s.} \) denotes almost sure convergence. Note that the first \( k \) samples have been neglected in the estimator (16), to avoid the transient phase of the chain. This is commonly referred to as the burn-in of the Markov chain.

Clearly, for this strategy to be useful we need a systematic way of constructing the Markov chain with the desired properties. One such way is to use the Metropolis Hastings (MH) algorithm. At iteration \( m+1 \), we propose a new sample \( \theta' \) according to,

\[
\theta' \sim q(\cdot | \theta[m]),
\]

where \( q(\cdot) \) denotes a proposal distribution designed by the user and \( \theta[m] \) denotes the sample from the previous iteration \( m \). The newly proposed sample \( \theta' \) will then be added to the sequence (i.e. \( \theta[m+1] = \theta' \)) with probability

\[
\alpha = 1 \wedge \frac{p(\theta' | y_{1:T})q(\theta[m] | \theta')}{p(\theta[m] | y_{1:T})q(\theta' | \theta[m])}, \quad (18a)
\]

\[
= 1 \wedge \frac{p(\theta' | y_{1:T})\pi(\theta')}{p(\theta[m] | y_{1:T})\pi(\theta[m])} \frac{q(\theta' | \theta[m])}{q(\theta | \theta[m])}, \quad (18b)
\]

where \( \wedge \) denotes to use min \((a,b)\) and \( \alpha \) is referred to as the acceptance probability. Hence, with probability \( 1-\alpha \) the newly proposed sample is not added to the sequence (i.e. rejected) and in that case the previous sample is once more added to the sequence \( \theta[m+1] = \theta[m] \).

There exists a well established theory for the MH algorithm, which for example establish that it is ergodic and converges to the correct stationary distribution. This has been developed since the algorithm was first introduced by Metropolis et al. (1953) and Hastings (1970). Ninness and Henriksen (2010) provides a nice account on the use of the MH algorithm for Bayesian system identification.

### Example 4: MH applied to the LGSS model

To apply the MH algorithm for parameter inference in the LGSS model, we require a proposal distribution \( q(\cdot) \) in (17) and to calculate the acceptance probability \( \alpha \) in (18b). A standard choice for \( q(\cdot) \) is a Gaussian random walk

\[
q(\theta' | \theta[m]) = \mathcal{N}(\theta'; \theta[m], \sigma_r^2),
\]

where \( \sigma_r^2 \) denotes the variance of the random walk. For this choice of proposal, the acceptance probability is

\[
\alpha = 1 \wedge \frac{p(\theta' | y_{1:T})\pi(\theta')}{p(\theta[m] | y_{1:T})\pi(\theta[m])},
\]

where \( q \) cancels since it is symmetric in \( \theta \). Note that the likelihood can be computed using the Kalman filter in analogue with (13) for the LGSS model. In the lower left part of Figure 1, we present the resulting posterior estimate obtained from running the algorithm \( M = 20000 \) iterations (discarding the first 10000 as burn-in).

### 4. IDENTIFICATION STRATEGY – DATA AUGMENTATION

An alternative strategy to marginalisation is to make use of data augmentation. Intuitively, we can think of this strategy as a systematic way of separating one hard problem into two new and closely linked sub-problems, each of which is hopefully easier to solve than the original problem. For the SSM (1) these two problems amounts to

1. (finding information about the state sequence \( x_{1:T} \))
2. (finding information about the parameters \( \theta \)).

The state sequence \( x_{1:T} \) is thus treated as an auxiliary variable that is estimated together with the parameters \( \theta \). Using the data augmentation terminology (Tanner and Wong, 1987; van Dyk and Meng, 2001), the state sequence \( x_{1:T} \) is referred to as the missing data, as opposed to the observed data \( y_{1:T} \). By augmenting the latter with the former, we obtain the complete data \( \{x_{1:T}, y_{1:T}\} \).

Naturally, if the complete data were known, then identifi-

cation of \( \theta \) would have been much simpler. In particular, we can directly write down the complete data likelihood \( p(x_{1:T}, y_{1:T}) \) according to (6), which contrary to the observed data likelihood \( p(x_{1:T}, y_{1:T}) \), does not involve any marginalisation. The two likelihoods are related via (5), suggesting that the complete data likelihood can indeed be used for identifying the unknown parameters.

#### 4.1 Expectation Maximisation (EM)

Analogously with the marginalisation strategy, we can make use of data augmentation to address both the frequen-

tistic and the Bayesian identification problems. For the former identification criteria, (2), the result is the ex-
pectation maximisation (EM) algorithm (Dempster et al., 1977). EM provides an iterative procedure to compute ML estimates of unknown parameters \( \theta \) in probabilistic models involving latent variables, like the SSM in (1).

As a direct result of the conditional probability identity

\[
p(\theta | x_{1:T}, y_{1:T}) = \int p(\theta, x_{1:T} | y_{1:T})d\theta,
\]

we can relate the observed and complete data log-likelihoods as

\[
\log p(\theta | y_{1:T}) = \log p(\theta | x_{1:T}, y_{1:T}) - \log p(\theta | x_{1:T} | y_{1:T}).
\]

The EM algorithm operates by iteratively maximising the intermediate quantity

\[
Q(\theta, \theta') = \int \log p(\theta | x_{1:T}, y_{1:T})p(\theta | x_{1:T}, y_{1:T})d\theta \quad (21a)
\]

\[
= \mathbb{E}_\theta[\log p(\theta | x_{1:T}, y_{1:T}) | y_{1:T}],
\]

as

\[
\text{arg max}_{\theta \in \Theta} Q(\theta, 0) \quad (21b)
\]

according to:

\[
(E) Q(\theta, \theta[k]) = \mathbb{E}_{\theta[k]}[\log p(\theta | x_{1:T}, y_{1:T}) | y_{1:T}],
\]

\[
(M) \theta[k+1] = \arg \max_{\theta \in \Theta} Q(\theta, \theta[k]).
\]
We can show that iterating the above Expectation (E) and Maximisation (M) steps implies
\[ Q(\theta, \theta') \ge Q(\theta', \theta') \implies p_\theta(y_{1:T}) \ge p_{\theta'}(y_{1:T}). \]  
(22)

Hence, the sequence \{\theta[k]\}_{k \ge 1} will by construction result in a monotonic increase in likelihood values. Hence, the complete data log-likelihood \( \log p_\theta(x_{1:T}, y_{1:T}) \) can, via the intermediate quantity \( Q \) in (21), be used as a surrogate for the original observed data likelihood \( p_\theta(y_{1:T}) \) in solving the ML problem (2). We are still required to compute the integral (21) and an important observation is now that we can approximate this integral (and its derivatives w.r.t. \( \theta \)) using SMC.

### Example 5: EM applied to the LGSS model

We need to compute the intermediate quantity to apply the EM algorithm for estimating the parameter in the LGSS model. For this model, we can write
\[ Q(\theta, \theta') = \text{const.} + \sum_{t=2}^{T} \log N(x_t; 0.7x_{t-1}, \theta^{-1}) | y_{1:T} \]

Note, that this expression results from that the parameter only is present in the latent state process.

We can directly maximise the intermediate quantity for \( \theta \) since the system is linear in the parameters. By taking the gradient of \( Q(\theta, \theta') \), we obtain terms proportional to \( \sum_{t=2}^{T} \log N(x_t; 0.7x_{t-1}, \theta^{-1}) | y_{1:T} \), where \( \tilde{x}_t \) is a smoothed state estimate and \( \tilde{x}_{1:T} \) is its corresponding covariance. These are typically obtained using a Kalman smoother and we refer the reader to Gibson and Ninness (2005) for the explicit expressions for implementing this. In the upper part of Figure 1, we present the parameter estimate \( \hat{\theta}_{ML} \) (blue) obtained by the EM algorithm. We note that the parameter estimates obtained by the DO and EM algorithms are identical and overlapping. However, they differ from the true parameter due to the finite value of \( T \).

#### 4.2 Gibbs sampler

The Gibbs sampler is an MCMC method that produce samples from the joint distribution by alternatively sampling from its conditionals. Let us consider the Bayesian formulation, with the aim of computing (3). Inspired by the data augmentation strategy, start by assuming that the complete data \( \{x_{1:T}, y_{1:T}\} \) is available. Bayes’ theorem then results in
\[ p(\theta | x_{1:T}, y_{1:T}) = \frac{p_\theta(x_{1:T}, y_{1:T})p(\theta)}{p(x_{1:T}, y_{1:T})}. \]  
(23)

Intuitively, if the states \( x_{1:T} \) were known, then the identification problem would be much simpler and, indeed, computing the posterior in (23) is typically easier than in (3). Firstly, the complete data likelihood is provided in (6), whereas the likelihood \( p_\theta(y_{1:T}) \) is intractable in the general case. Secondly, in many cases of interest it is possible to identify a prior for \( \theta \) that is conjugate to the complete data likelihood, in which case the posterior (23) is available in closed form.

The problem with (23) is of course that it hinges upon the state sequence being known. However, assume that we can simulate a sample of the state trajectory \( x_{1:T} \) from its conditional distribution given the observed data \( y_{1:T} \) and the system parameters \( \theta \), i.e. from the joint smoothing distribution. Furthermore, assume that it is possible to sample from the distribution in (23). We can then implement the following algorithm: Initialise \( \theta[0] \in \Theta \) arbitrarily and, for \( m \ge 0 \),
\[ \text{Sample } x_{1:T}[m] \sim p_\theta[m](x_{1:T} | y_{1:T}). \]  
(24a)
\[ \text{Sample } \theta[m+1] \sim p(\theta | x_{1:T}[m], y_{1:T}). \]  
(24b)
This results in the generation of the following sequence of random variables
\[ \theta[0], x_{1:T}[0], \ldots, \theta[1], x_{1:T}[1], \ldots, \theta[2], x_{1:T}[2], \ldots, \]  
(25)
which forms a mutual Markov chain in the parameters \( \theta \) and the states \( x_{1:T} \). The joint smoothing distribution in (24) represents a valid MCMC method. More specifically, it is a particular instance of the so-called Gibbs sampler. The simulated Markov chain admits the joint distribution \( p(\theta, x_{1:T} | y_{1:T}) \) as a stationary distribution. Furthermore, under weak conditions it can be shown to be ergodic. That is, the Markov chain generated by the procedure (24) can be used to estimate posterior expectations, and the estimators are consistent in the sense of (16). Note that, if we are only interested in the marginal distribution \( p(\theta | y_{1:T}) \), then it is sufficient to store the sub-sequence constituted by \( \{\theta[m]\}_{m \ge 1} \), obtained by simply discarding the samples \( \{x_{1:T}[m]\}_{m \ge 1} \) from (25).

It is worth pointing out that it is possible to combine Gibbs sampling with other MCMC methods. For instance, if it is not possible to sample from posterior distribution (23) exactly, then a valid approach is to replace step (24b) of the Gibbs sampler with, e.g., an MH step with target distribution \( p(\theta | x_{1:T}, y_{1:T}) \).

#### Example 6: Gibbs applied to the LGSS model

To implement the Gibbs sampler for parameter inference in the LGSS model, we need to sample from the conditional distributions in (24). To generate samples of state trajectories given \( \theta \) and \( y_{1:T} \), we can make use of the factorisation
\[ p_\theta(x_{1:T} | y_{1:T}) = \prod_{t=1}^{T-1} p_\theta(x_t | x_{t+1}, \theta) p_\theta(x_t | y_{1:T}). \]  
(26)

of the joint smoothing distribution. Consequently, we can sample \( x_{1:T}[m] \) using the following backward simulation strategy: Sample \( \tilde{x}_T \sim p_\theta(x_T | y_{1:T}) \) and, for \( t = T - 1, \ldots, 1 \), sample
\[ \tilde{x}_t \sim p_\theta(x_t | \tilde{x}_{t+1}, y_{1:t}) \propto p_\theta(\tilde{x}_{t+1} | x_t)p_\theta(x_t | y_{1:t}). \]  
(27)
We see that the backward simulation relies on the filtering distributions \( p_\theta(x_t | y_{1:t}) \) and, indeed, for the LGSS model we can obtain closed form expressions for all the involved densities by running a Kalman filter.

In the second step, (24b), we sample the parameters \( \theta \) by
\[ \theta \sim p(\theta | \tilde{x}_{1:T}, y_{1:T}) \equiv \mathbb{G}(\theta | \alpha, \beta), \]  
(28a)
\[ \alpha = 0.01 + \frac{T}{2}, \]  
(28b)
\[ \beta = 0.01 + \frac{1}{2} \left( 0.51\tilde{x}_t^2 + \sum_{t=1}^{T-1}(\tilde{x}_{t+1} - 0.5\tilde{x}_t)^2 \right), \]  
(28c)
which is the result of a standard prior-posterior update with a Gamma prior and Gaussian likelihood. The closed-
form expression for \( p(\theta | x_{1:T}, y_{1:T}) \) is an effect of using a prior which is conjugate to the complete data likelihood.

In the lower right part of Figure 1, we present the resulting posterior estimate obtained from the Gibbs sampler with the same settings as for the MH algorithm. We note that the posterior estimates are almost identical for the two methods, which corresponds well to the established theory.

The data augmentation strategy (here implemented via the Gibbs sampler) enabled us to approximate the posterior distribution \( p(\theta | y_{1:T}) \) by separating the problem into two connected sub-problems (24).

5. SEQUENTIAL MONTE CARLO

Sequential Monte Carlo (SMC) methods offer numerical approximations to the state estimation problem associated with the nonlinear/non-Gaussian SSM (1). The particle filter (PF) approximates the filtering PDF \( p(y_{1:t} | y_{1:T}) \) and the particle smoother (PS) approximates the joint smoothing PDF \( p(y_{1:t} | y_{1:T}) \), or some of its marginals. The PF can intuitively be thought of as the equivalent of the Kalman filter for nonlinear/non-Gaussian SSMs.

The SMC approximation is an empirical distribution of the form

\[
\hat{p}_N(x_t | y_{1:t}) = \sum_{i=1}^{N} w_t^i \delta_{x_t^i} (x_t). \tag{29}
\]

The samples \( \{x_t^i\}_{i=1}^{N} \) are often referred to as particles—they are point-masses “spread out” in the state space, each particle representing one hypothesis about the state of the system. We can think of each particle \( x_t^i \) as one possible system state and the corresponding weight \( w_t^i \) contains information about how probable that particular state is.

To make the connection to the marginalisation and data augmentation strategies introduced in the two previous sections clear, we remind ourselves where the need for SMC arise in implementing these strategies to identify \( \theta \) in (1). The PF is used to compute the cost function (10) and its derivatives in order to find the search directions (12). To set up an MH sampler, we can make use of a likelihood estimate provided by the PF in order to compute the acceptance probabilities in (18). When it comes to data augmentation strategies, the PS is used to approximate the intermediate quantity in (21) and in order to set up the Gibbs sampler, particle methods are used to draw a realisation from the joint smoothing distribution in (24a).

5.1 Particle filter

A principled solution to the nonlinear filtering problem is provided by the following two recursive equations:

\[
p_0(x_1 | y_{1:T}) = \frac{g_0(y_1 | x_1)p_0(x_1 | y_{1:y_1})}{p_0(y_1 | y_{1:T})}, \tag{30a}
\]

\[
p_0(x_{t-1} | y_{1:t-1}) = \int f_0(x_t | x_{t-1})p_0(x_{t-1} | y_{1:y_{t-1}})dx_{t-1}, \tag{30b}
\]

These equations can only be solved in closed form for very specific special cases, e.g., the LGSS model which results in a general approximation of (30) for general nonlinear/non-Gaussian SSMs.

The particle filter—at least in its most basic form—can be interpreted as a sequential application of importance sampling. At each time step \( t \) we use importance sampling to approximate the filtering PDF \( p_0(x_t | y_{1:t}) \). This is made possible by using the expressions in (30) and by exploiting the already generated importance sampling approximation of \( p_0(x_{t-1} | y_{1:y_{t-1}}) \). At time \( t \) we can find an empirical distribution (29) by approximating \( p_0(x_t | y_{1:t}) \propto g_0(y_t | x_t)p_0(x_t) \) using importance sampling in the normal sense. We sample independently the particles \( \{x_t^i\}_{i=1}^{N} \) from some proposal distribution \( r_0(x_t) \). To account for the discrepancy between the proposal distribution and the target distribution, the particles are assigned importance weights, given by the ratio between the target and the proposal (up to proportionality), i.e., \( w_t^i \propto \frac{g_0(y_t | x_t^i)p_0(x_t^i)}{r_0(x_t^i)} \), where the weights are normalised to sum to one.

We proceed in an inductive fashion and assume that we have an empirical approximation of the filtering distribution at time \( t-1 \) according to

\[
\hat{p}_N(x_{t-1} | y_{1:t-1}) = \sum_{i=1}^{N} w_{t-1}^i \delta_{x_{t-1}^i} (x_{t-1}). \tag{31}
\]

Inserting this into (30b) results in

\[
\hat{p}_N(x_t | y_{1:t-1}) = \int f_0(x_t | x_{t-1}) \sum_{i=1}^{N} w_{t-1}^i \delta_{x_{t-1}^i} (x_{t-1})dx_{t-1} = \sum_{i=1}^{N} w_{t-1}^i f_0(x_t | x_{t-1}^i). \tag{32}
\]

That is, we obtain a mixture distribution approximating \( p_0(x_t | y_{1:t-1}) \), where we have one mixture component for each of the \( N \) particles at time \( t-1 \). Furthermore, inserting (32) into (30a) results in the following approximation of the filtering PDF

\[
p_0(x_t | y_{1:y_t}) \approx \frac{g_0(y_t | x_t)}{p_0(y_t | y_{1:y_{t-1}})} \sum_{i=1}^{N} w_{t-1}^i f_0(x_t | x_{t-1}^i). \tag{33}
\]

The task is now to approximate (33) using importance sampling. Inspired by the structure of (33) we choose a proposal density (again denoted by \( r_0 \)) of the same form, namely as a mixture distribution,

\[
r_0(x_t | y_{1:y_t}) \Delta \sum_{i=1}^{N} \nu_{t-1}^i r_0(x_t | x_{t-1}^i, y_t), \tag{34}
\]

where both the mixture components \( r_0(x_t | x_{t-1}^i, y_t) \) and the mixture weights \( \nu_{t-1}^i \) are design choices constituting parts of the proposal distribution.

To generate a sample from the mixture distribution (34) the following two-step procedure is used: first we randomly select one of the components, and then we generate a sample from that particular component. Note that we will sample \( N \) particles from the proposal distribution (34). Let us use \( a_t^i \) to denote the index of the mixture component selected for the \( i \)th particle at time \( t \). Now, since the probability of selecting component \( r_0(x_t | x_{t-1}^i, y_t) \) is encoded by its weight \( \nu_{t-1}^i \), we have that

\[
P(a_t^i = j) = \nu_{t-1}^i, \quad j = 1, \ldots, N. \tag{35}
\]

Subsequently, we can generate a sample from the selected component \( a_t^j \) according to \( x_t^i \sim r_0(x_t | x_{t-1}^i, y_t) \), where \( x_{t-1}^i \triangleq x_{t-1}^j \). By construction \( x_t^i \) is now a sample from the proposal density (34). The particle \( x_{t-1}^i \) is referred
to as the ancestor particle of \(x_i^t\), since \(x_i^t\) is generated conditionally on \(x_i^{t-1}\). This also explains why the index \(a_i^t\) is commonly referred to as the *ancestor index*, since it indexes the ancestor of particle \(x_i^t\) at time \(t-1\).

In practice we sample the \(N\) ancestor indices \(\{a_i^t\}_{i=1}^N\) according to (35) in one go. This results in a new set of particles \(\{\tilde{x}_i^t\}_{i=1}^N\) that are subsequently used to propagate the particles to time \(t\). This procedure, which (randomly) generates \(\{\tilde{x}_i^{t-1}\}_{i=1}^N\) by selection (sampling with replacement) from among \(\{x_i^{t-1}\}_{i=1}^N\) according to some weights, is commonly referred to as *resampling*.

The next step is to assign importance weights to the new particles accounting for the discrepancy between the target distribution \(p_\theta(x_t \mid y_{1:t})\) and the proposal distribution \(r_\phi(x_t \mid y_{1:t})\). As before, the weights are computed as the ratio (the unnormalised) target PDF and the proposal PDF. Direct use of (33) and (34) results in

\[
\hat{w}_i^t = \frac{\hat{p}_\theta(y_t \mid x_i^t)}{\hat{r}_\phi(x_i^t \mid x_i^{t-1}, y_t)}.
\]

By evaluating \(\hat{w}_i^t\) for \(i = 1, \ldots, N\) and normalising the weights, we obtain a new set of weighted particles \(\{x_i^t, \hat{w}_i^t\}_{i=1}^N\), constituting an empirical approximation of \(p_\theta(x_t \mid y_{1:t})\). This completes the algorithm, since these weighted particles in turn can be used to approximate the filtering PDF at time \(t+1\), then at time \(t+2\) and so on.

A problem with the algorithm presented above is that the weight calculation in (36) has a computational complexity of \(O(N)\) for each particle, rendering an overall computational complexity of \(O(N^2)\), since the weights need to be computed for all \(N\) particles. A pragmatic solution to this problem is to use the freedom available in the proposal density and select it according to \(r_\phi(x_t \mid y_{1:t}) = \sum_{j=1}^N \hat{w}_i^{t-1} f_\phi(x_t \mid x_j^{t-1}, y_t)\). That is, we select ancestor particles with probabilities given by their importance weights and sample new particles by simulating the system dynamics from time \(t-1\) to \(t\). Inserting this into (36) results in the expression \(\hat{w}_i^t = \hat{g}_\theta(y_t \mid x_i^t)\), which brings the overall computational complexity down to \(O(N)\). The resulting algorithm is referred to as the *bootstrap particle filter* and it is summarised in Algorithm 1.

**Algorithm 1 Bootstrap particle filter (all operations are for \(i = 1, \ldots, N\))**

1. **Initialisation** (\(t = 1\)):
   1. Sample \(x_1^t \sim \mu_0(x_1)\).
2. 
3. Compute \(\hat{w}_i^t = \hat{g}_\theta(y_1 \mid x_i^t)\), normalise, \(w_i^t = \hat{w}_i^t / \sum_{j=1}^N \hat{w}_j^t\).
4. 
5. **Resampling**: Sample \(a_i^t\) with \(\mathbb{P}(a_i^t = j) = w_i^t\).
6. 
7. **Propagation**: Sample \(x_i^t \sim f_\phi(x_t \mid x_i^{t-1})\).
8. 
9. **Weighting**: Compute \(\tilde{w}_i^t = \hat{g}_\theta(y_t \mid x_i^t)\) and normalise, \(w_i^t = \tilde{w}_i^t / \sum_{j=1}^N \tilde{w}_j^t\).

The bootstrap PF was the first working particle filter, an early and influential derivation is provided by Gordon et al. (1993). It is arguably the simplest possible implementation of SMC, but nevertheless, it incorporates the essential methodological ideas that underpin the general SMC framework. *Importance sampling* (i.e. propagation and weighting in Algorithm 1 above) and *resampling* are used to sequentially approximate a sequence of probability distributions of interest; here \(\{p_\theta(x_t \mid y_{1:t})\}_{t>1}\).

Selecting the dynamics as proposal distribution, as in the bootstrap particle filter, is appealing due to the simplicity of the resulting algorithm. However, this choice is unfortunately also suboptimal, since the current measurement \(y_t\) is not taken into account when simulating the particles \(\{x_i^t\}_{i=1}^N\) from the proposal distribution. A better strategy of reducing the computational complexity of the weight computation from \(O(N^2)\) to \(O(N)\) is to target the joint distribution of \((x_t, \theta)\) with an importance sampler, instead of directly targeting the marginal distribution of \(x_t\) as was done above. Indeed, by explicitly introducing the ancestor indices as auxiliary variables in the importance sampler, we obtain the weight expression

\[
\tilde{w}_i^t = \frac{w_{i,t-1} g_\theta(y_t \mid x_i^t) f_\phi(x_i^t \mid x_i^{t-1})}{\sum_{i=1}^N w_{i,t-1} r_\phi(x_i^t \mid x_i^{t-1}, y_t)},
\]

as a more practical alternative to (36). With this approach we have the possibility of freely selecting the mixture weights \(\pi_i\) and mixture components \(r_\phi(x_t \mid x_i^{t-1}, y_t)\) of the proposal, while still enjoying an overall linear computational complexity. The resulting algorithm is referred to as the *auxiliary particle filter* (APF). Rather than providing the details of the derivation we simply refer to the original paper by Pitt and Shephard (1999) or our complete derivation in Schönb etc. (2015).

### 5.2 Some useful properties of the PF

As any Monte Carlo algorithm, the PF can be interpreted as a *random number generator*. Indeed, the particles and the ancestor indices used within the algorithm are random variables, and executing the algorithm corresponds to simulating a realisation of these variables. It can be useful, both for understanding the properties of the PF and for developing more advanced algorithms around SMC, to make this more explicit. Let

\[
x_t \triangleq \{x_1^t, \ldots, x_N^t\}, \quad \text{and} \quad a_t \triangleq \{a_1^t, \ldots, a_N^t\},
\]

(38) refer to all the particles and ancestor indices, respectively, generated by the PF at time \(t\). The PF in Algorithm 1 then generates a *single realisation* of a collection of random variables \(\{x_1^t, a_2^t\} \in \mathbb{X}^{N \times T} \times \{1, \ldots, N\}^N\). Furthermore, since we know how these variables are generated, we can directly write down their joint PDF\(^1\) as,

\[
\psi_\theta(x_1^T, a_2^T \mid y_1^T) \triangleq \prod_{i=1}^N \mu_0(x_1^t) \prod_{t=2}^T \prod_{i=1}^N \pi_{i} f_\phi(x_i^t \mid x_i^{t-1})
\]

(39). Naturally, any estimator derived from the PF will also be a random variable. From (39) we note that the distribution of this random variable will depend on the number of particles \(N\), and *convergence* of the algorithm can be identified with convergence in some sense, of this random variable. Specifically, let \(\varphi : \mathbb{X} \mapsto \mathbb{R}\) be some *test function* of interest. The posterior expectation \(\mathbb{E}_\theta[\varphi(x_t) \mid y_{1:t} = 1 \varphi(x_t) p_\theta(x_t | y_{1:t}) \mathrm{d}x_t\) can be estimated by the PF by computing (cf., (16)),

\[
\hat{\mathbb{E}}_\theta^N \triangleq \sum_{i=1}^N w_i^t \varphi(x_i^t).
\]

There is a solid theoretical foundation for SMC, e.g., investigating the convergence of (40) to the true expectation as

\[\text{w.r.t. a natural product of Lebesgue and counting measure.}\]
asymptotic estimator variance is convergent at a rate \( N \to \infty \) and establishing non-asymptotic bounds on the approximation error. The (types of) existing theoretical results are too numerous to be mentioned here, and we refer to the book by Del Moral (2004) for a comprehensive treatment. However, to give a flavour of the type of results that can be obtained we state a central limit theorem (CLT) for the estimator (40). Under weak regularity assumptions it holds that (Del Moral and Miclo, 2000; Del Moral, 2004; Chopin, 2004),

\[
\sqrt{N} \left( \hat{\varphi}_t - \mathbb{E}_0 [\varphi(x_t) \mid y_{1:t}] \right) \xrightarrow{d} \mathcal{N}(0, \sigma^2(\varphi)), \tag{41}
\]

as \( N \to \infty \) where \( \xrightarrow{d} \) denotes convergence in distribution. The asymptotic estimator variance \( \sigma^2(\varphi) \) depends on the test function \( \varphi \), the specific PF implementation that is used and, importantly, the properties of the state space model (an explicit expression for \( \sigma^2(\varphi) \) is given by Doucet and Johansen (2011)).

The CLT in (41) is reassuring since it reveals that the one-step predictive likelihood, by (7), can be understood by considering the factorisation (4) and noting that the one-step predictive likelihood, by (7), can be approximated without (directly) suffering from path degeneracy, this opens up for a solution to the path degeneracy problem. An important step in this direction was provided by Godsill et al. (2004), who made use of backward simulation to simulate complete state trajectories \( \tilde{x}_{1:T} \), approximately distributed according to the joint smoothing distribution \( p_\theta(x_{1:T} \mid y_{1:T}) \). The idea has since then been refined, see e.g. Douc et al. (2011); Bunch and Godsill (2013). Algorithms based on the combination of MCMC and SMC introduced by Andrieu et al. (2010), resulting in the particle MCMC (PMCMC) method, also offer promising solutions to the nonlinear state smoothing problem. For a self-contained introduction to particle smoothers, see Lindsten and Sch"on (2013).

6. MARGINALISATION IN THE NONLINEAR SSM

Now that we have seen how SMC can be used to approximate the filtering distribution, as well as the predictive and
Consider the maximum likelihood problem in (2). The objective function, i.e., the log-likelihood, can be approximated by SMC by using (42). However, many standard optimisation methods require not only evaluation of the cost function, but also the gradient and possibly the Hessian, in solving (2). SMC can be used to compute the gradient via the use of Fisher’s identity, in solving (2). SMC can be used to compute the gradient of the log-likelihood, i.e. the log-likelihood, can be approximated by a particle smoother, as discussed in Section 3.3; see e.g., Poyiadjis et al. (2011) for further details. The Hessian can also be approximated using, for example, Louis’ identity (e.g., Cappé et al., 2005).

Note that the gradient computed in this way will be stochastic, since it is approximated by an SMC method. It is therefore common to choose a diminishing step-size sequence of the gradient ascent method according to standard stochastic approximation rules; see e.g., Kushner and Yin (1997); Benveniste et al. (1990). However, it should be noted that the approximation of the gradient of the log-likelihood will be biased for a finite number of particles N, and the identification method therefore relies on asymptotics in N for convergence to a maximiser of (2).

6.2 Using unbiased likelihoods within MH

We can make use of the likelihood estimator (42) also for Bayesian identification of nonlinear SSMs via the MH algorithm. Indeed, an intuitive idea is to simply replace the intractable likelihood in the acceptance probability (18) by the (unbiased) estimate \( \hat{p}(y_1:T) \). What is maybe less intuitive is that this simple idea does in fact result in a valid (in the sense that it has \( p(\theta | y_1:T) \) as its stationary distribution) MH algorithm, for any number of particles \( N \geq 1 \). Let us now sketch why this is the case.

We start by introducing a (high-dimensional) auxiliary variable \( u \) constituted by all the random quantities generated by the PF, i.e. \( u \in \{ x_1:T, \phi_1:T, \phi_2:T \} \) distributed according to \( \psi_0(u | y_1:T) \) defined in (39). Note that the joint distribution of the parameters \( \theta \) and the auxiliary variables \( u \),

\[
p(\theta, u | y_1:T) = \psi_0(u | y_1:T)p(\theta | y_1:T) \quad (48a)
\]

\[
= \frac{p(y_1:T)\psi_0(u | y_1:T)p(\theta)}{p(y_1:T)}, \quad (48b)
\]

has the original target distribution \( p(\theta | y_1:T) \) as one of its marginals. Inspired by (48b), consider the following extended target distribution

\[
\phi(\theta, u | y_1:T) = \hat{p}(\theta, u | y_1:T)\psi_0(u | y_1:T)p(\theta), \quad (49)
\]

where we have made use of the unbiased likelihood estimate \( \hat{p}(\theta, u | y_1:T) \) from the PF (and indicate explicitly the dependence on \( u \) in the notation for clarity). We can now set up a standard MH algorithm that operates in the (huge) extended target distribution \( \Theta \times \times N^{NT} \times \{ 1, \ldots, N \}^{N(T-1)} \) approximating the extended target distribution (49). The resulting algorithm will generate samples asymptotically from \( p(\theta | y_1:T) \) despite the fact that we employ an approximate likelihood in (49)!

To understand why this is the case, let us marginalise (49) w.r.t. the auxiliary variable \( u \):

\[
\int \phi(\theta, u | y_1:T)du = \pi(\theta)/\hat{p}(\theta, y_1:T)\int \hat{p}(\theta, u | y_1:T)\psi_0(u | y_1:T)du. \quad (50)
\]

The fact that the likelihood estimate \( \hat{p}(\theta, u | y_1:T) \) produced by the PF is unbiased means that

\[
\hat{E}_{\theta}| \hat{p}(\theta, u | y_1:T)) = \int \hat{p}(\theta, u | y_1:T)\psi_0(u | y_1:T)du = p(\theta | y_1:T). \quad (51)
\]

The marginalisation in (50) can now be finalised, resulting in

\[
\int \phi(\theta, u | y_1:T)du = \pi(\theta)/\hat{p}(\theta, y_1:T), \quad \text{proving that } \pi(\theta | y_1:T) \text{ is recovered exactly as the marginal of the extended target distribution (49),}
\]

despite the fact that we employed a PF approximation of the likelihood using a finite number of particles \( N \). This explains why it is sometimes referred to as an exact approximation. An interpretation is that using the likelihood estimate from the PF does change the marginal distribution w.r.t. \( u \) in (48), but it does not change the marginal w.r.t. \( \theta \).

Based on the current sample \( (\theta[m], u[m]) \) a new sample \( (\theta', u') \) is proposed according to

\[
\theta' \sim q(\cdot | \theta[m]), \quad u' \sim \psi_0(\cdot | y_1:T). \quad (52)
\]

We emphasise that simulation of \( u' \) corresponds to running a PF with the model parameterised by \( \theta' \). The probability of accepting the sample proposed in (52) as the next sample \( (\theta[m+1], u[m+1]) \) is given by

\[
\alpha = 1 \land \frac{\hat{p}(\theta, u | y_1:T)p(\theta)}{\hat{p}(\theta[m], u[m])p(\theta[m])} \pi(\theta[m])\pi(\theta) \quad (53)
\]

which was obtained by inserting (49) and (52) into (18).

In practice it is sufficient to keep track of the likelihood estimates \( \{ \hat{p}(\theta[m], u[m]) \}_{m=1}^{\infty} \), and we do not need to store the complete auxiliary variable \( u[m] \) according to (42).

The above development is summarised in Algorithm 2. It can be further improved by incorporating gradient and Hessian information about the posterior into the proposal (52), resulting in more efficient use of the generated particles (Dahlin et al., 2015).

Algorithm 2: Particle Metropolis Hastings (PMH) for Bayesian system identification of nonlinear SSMs

1: Run a PF (Algorithm 1) targeting \( p(x_{1:T} | \theta[1]) \) to obtain \( u' \sim \psi_0(u | y_1:T) \) and \( \theta'[u'] \sim \psi_0(u | y_1:T) \) according to (42).
2: for \( m = 1 \to M \) do
3: Sample \( \theta' \sim q(\cdot | \theta[m]) \).
4: Run a PF (Algorithm 1) targeting \( p(x_{1:T} | \theta') \) to obtain \( u' \sim \psi_0(u | y_1:T) \) and \( \theta'[u'] \sim \psi_0(u | y_1:T) \) according to (42).
5: Sample \( d_m \sim \mathcal{U}(0, 1) \).
6: Compute the acceptance probability \( \alpha \) by (53).
7: if \( d_m < \alpha \) then
8: \( \theta'[m+1] \leftarrow \theta' \) and \( \hat{p}(\theta[m+1], y_1:T) \leftarrow \hat{p}(\theta'[u'], y_1:T) \).
9: else
10: \( \theta'[m+1] \leftarrow \theta[m] \) and \( \hat{p}(\theta[m+1], y_1:T) \leftarrow \hat{p}(\theta[m], y_1:T) \).
11: end if
12: end for

The particle Metropolis Hastings algorithm constitutes one member of the particle MCMC (PMCMC) family of
algorithms introduced in the seminal paper by Andrieu et al. (2010). The derivation above is along the lines of the pseudo-marginal approach due to Andrieu and Roberts (2009). The extended target construction \( \phi \), however, is the core of all PMCMC methods and they differ in that different (more or less standard) MCMC samplers are used for this (non-standard) target distribution. They also have in common that SMC is used as a proposal mechanism on the space of state trajectories \( X^T \).

---

**Example 7: PMH applied to the NL-SSM**

We make use of Algorithm 2 to estimate the parameters in (9) together with a simple Gaussian random walk, 
\[
\theta' \sim q(\cdot | \theta[m]) = \mathcal{N}(\theta[m], 2.562^2 \Sigma/2),
\]

where \( \Sigma \) denotes an estimate of the posterior covariance matrix. This choice is optimal for some target distributions as is discussed by Sherlock et al. (2013). The posterior covariance estimate is obtained as
\[
\Sigma = 10^{-5} \begin{bmatrix} 22.51 & -4.53 \\ -4.53 & 2.57 \end{bmatrix}
\]

using a pilot run of the algorithm. In the upper part of Figure 2, we present the resulting marginal posterior estimates. The posterior means \( \theta_{\text{PMH}} = \{0.95, 51.05\} \) are indicated by dotted lines.

7. DATA AUGMENTATION IN NONLINEAR SSM

Algorithms implementing the data augmentation strategy treats the states as auxiliary variables that are estimated along with the parameters, rather than integrating them out. Intuitively this results in algorithms that alternate between updating \( \theta \) and \( x_{1:T} \).

---

7.1 Expectation maximisation

The expectation maximisation algorithm introduced in Section 4.1 separates the maximum likelihood problem (2) into two closely linked problems, namely the computation of the intermediate quantity \( Q(\theta, \theta[k]) \) and its maximisation w.r.t. \( \theta \). As previously discussed, computing the intermediate quantity corresponds to solving a smoothing problem. Hence, for a nonlinear/non-Gaussian SSM, a natural idea is to use a particle smoother, as discussed in Section 5.3, to solve this subproblem. The details of the algorithm are provided by Cappé et al. (2005); Olsson et al. (2008); Schön et al. (2011), whereas the general idea of making use of Monte Carlo integration to approximate the E-step dates back to Wei and Tanner (1990).

By this approach, a completely new set of simulated particles has to be generated at each iteration of the algorithm, since we continuously update the value of \( \theta \). Once an approximation of \( Q(\theta, \theta[k]) \) has been computed, the current particles are discarded and an entirely new set has to be generated at the next iteration. While it does indeed result in a working algorithm it makes for an inefficient use of the particles. The PMCMC family of algorithms opens up for the construction of Markov kernels that can be used to generate samples of the state trajectory (to be used in the approximation of \( Q(\theta, \theta[k]) \)) in a computationally more efficient fashion, which serves as one (of several) motivation of the subsequent development.

7.2 Sampling state trajectories using Markov kernels

We now introduce another member of the PMCMC family of algorithms (recall PMH from Section 6.2) that can be used whenever we are faced with the problem of sampling from an intractable joint smoothing distribution \( p_\theta(x_{1:T} | y_{1:T}) \). In those situations an exact sample can be replaced with a draw from an MCMC kernel with stationary distribution \( p_\theta(x_{1:T} | y_{1:T}) \), without introducing any systematic error, and PMCMC opens up for using SMC to construct such MCMC kernels.

Here, we review a method denoted as particle Gibbs with ancestor sampling (PGAS), introduced by Lindsten et al. (2014). To construct the aforementioned Markov kernel, PGAS makes use of a procedure reminiscent of the PF in Algorithm 1. The only difference is that in PGAS we condition on the event that an \( a \text{ priori} \) specified state \( x'_{t} \) is always present in the particle system, for each time \( t \). Hence, the states \( \{x'_1, \ldots, x'_T\} \) must be retained throughout the sampling procedure. To accomplish this we sample \( x'_t \) according to the bootstrap PF only for \( i = 1, \ldots, N - 1 \). The remaining \( \mathcal{N}^{\text{th}} \) particle \( x'_N \) is set deterministically as \( x'_N = x'_{t} \). It is often the case that we are interested in complete particles trajectories; cf., (45). To generate a genealogical trajectory for \( x'_t \), it is possible to connect it to one of the particles at time \( t - 1 \), \( \{x'_{t-1}\}_{i=1}^{N} \) by sampling a value for the corresponding ancestor index \( a_i^N \) from its conditional distribution. This is referred to as ancestor sampling, see Algorithm 3.

Note that Algorithm 3 takes as input a state trajectory \( x_{1:T} = \{x'_1, \ldots, x'_T\} \) and returns another state trajectory \( x_{1:T} \), which is simulated randomly according to some distribution (which, however, cannot be written on closed form). Hence, we can view Algorithm 3 as sampling from a Markov kernel defined on the space of state trajectories \( X^T \). This Markov kernel is referred to as the PGAS kernel.
Algorithm 3 PGAS kernel (with a bootstrap PF)
1: **Initialisation** $(t = 1)$: Draw $x_{1,t}^{i} \sim \mu(x_{1})$ for $i = 1, \ldots, N - 1$ and set $x_{1,0}^{i} = x_{1}^{i}$. Compute $\bar{w}_{1}^{i} = g_{0}(y_{1} | x_{1}^{i})$ for $i = 1, \ldots, N$.
2: for $t = 2$ to $T$ do
3: Sample $a_{t}^{i} \sim P \left( a_{t}^{j} = j \right) = w_{t-1}^{i,j}$ for $i = 1, \ldots, N - 1$.
4: Sample $x_{1,t}^{i} \sim f_{0}(x_{t} | x_{t-1}^{i})$ for $i = 1, \ldots, N - 1$.
5: Set $x_{1,t}^{N} = x_{1}^{N}$.
6: Draw $a_{t}^{N}$ with $P \left( a_{t}^{N} = j \right) \propto w_{t-1}^{i,j} f_{0}(x_{t}^{j} | x_{t-1}^{j})$.
7: Set $x_{1,t}^{i} = \{x_{1,t-1}^{i}, x_{1,t}^{i}\}$ for $i = 1, \ldots, N$.
8: Compute $\bar{w}_{t}^{i} = g_{0}(y_{t} | x_{t}^{i})$ for $i = 1, \ldots, N$.
9: end for
10: Draw $k$ with $P \left( k = i \right) \propto \bar{w}_{t}^{i}$.
11: Return $x_{1,T}^{*} = x_{1,T}^{k}$.

The usefulness of the method comes from the fact that the PGAS kernel is a valid MCMC kernel for the joint smoothing distribution $p(x_{1:T} | y_{1:T})$ for any number of particles $N \geq 2$. A nonnull kernel in it is provided way Lindsten et al. (2014), who show that the PGAS kernel is ergodic and that it admits the joint smoothing distribution as its unique stationary distribution. This implies that the state trajectories generated by PGAS can be used as samples from the joint smoothing distribution. Hence, the method is indeed an interesting alternative to other particle smoothers. Moreover, the PGAS kernel can be used as a component in any (standard) MCMC method. In the subsequent section we will make explicit use of this, both for ML and Bayesian identification.

8. IDENTIFICATION USING MARKOV KERNELS

8.1 Expectation maximisation revisited

In Section 7.1 we made use of particle smoothers to approximate the intractable integral defining the intermediate quantity $Q(\theta, \theta[m])$. However, it is possible to make more efficient use of the simulated variables by using the PGAS Algorithm 3 and employing a stochastic approximation update of the intermediate quantity $Q_{k}(\theta, \theta[k])$.

$$\hat{Q}_{k}(\theta, \theta[k]) = (1 - \alpha_{k}) \hat{Q}_{k-1}(\theta, \theta[k-1]) + \alpha_{k} \sum_{i=1}^{N} w_{t}^{i}_{k} \log p(x_{1:T}, y_{1:T}), \quad (54)$$

where $\alpha_{k}$ is the step size and $\{w_{t}^{i_{k}}, x_{1:T}^{i_{k}}\}_{i_{k}=1}^{N}$ is generated by Algorithm 3. Stochastic approximation EM (SAEM) was introduced and analysed by Delyon et al. (1999) and it was later realised that it is possible to use MCMC kernels within SAEM (Andrieu et al., 2005) (see also Benveniste et al. (1990)). The aforementioned particle SAEM algorithm for nonlinear system identification was presented by Lindsten (2013) and it is summarised in Algorithm 4.

Algorithm 4 PGAS for ML sys. id. of nonlinear SSMs
1: **Initialisation**: Set $\theta[0]$ and $x_{1:T}[0]$ arbitrarily. Set $\hat{Q}_{0} = 0$.
2: for $k \geq 1$ do
3: Run Algorithm 3 with $x_{1:T}^{i} = x_{1:T}[k-1]$. Set $x_{1:T}[k] = x_{1:T}^{k}$.
4: Compute $\hat{Q}_{k}(\theta)$ according to (54).
5: Compute $\hat{\theta}[k] = \arg \max \hat{Q}_{k}(\theta)$.
6: if convergence criterion is met then return $\hat{\theta}[k]$ end if
7: end for

Note the important difference between the SMC-based EM algorithm outlined in Section 7.1 and Algorithm 4. In the former we generate a completely new set of particles at each iteration, whereas in particle SAEM all simulated particles contribute, but they are down-weighted using a forgetting factor given by the step size. This approach is more efficient in practice, since we can use much fewer particles at each iteration. In fact, the method can be shown to converge to a maximiser of (2) even when using a fixed number of particles $N \geq 2$ when executing Algorithm 4.

8.2 Bayesian identification

Gibbs sampling can be used to simulate from the posterior distribution (3) or more generally, the joint state and parameter posterior $p(\theta, x_{1:T} | y_{1:T})$. The PGAS kernel allows us to sample the complete state trajectory $x_{1:T}$ in one block. Due to the invariance and ergodicity properties of the PGAS kernel, the validity of the Gibbs sampler is not violated. We summarise the procedure in Algorithm 5.

Algorithm 5 PGAS for Bayesian sys. id. of nonlinear SSMs
1: **Initialisation**: Set $\theta[0]$ and $x_{1:T}[0]$ arbitrarily.
2: for $m = 1$ to $M$ do
3: Run Algorithm 3 conditionally on $(x_{1:T}[m-1], \theta[m-1])$ and set $x_{1:T}[m] = x_{1:T}^{*}$.
4: Draw $\theta[m] \sim p(\theta | x_{1:T}[m], y_{1:T})$.
5: end for

Example 8: PGAS applied to (9)

To make use of Algorithm 5 to estimate the parameters in (9), we need to sample from the conditional distribution $p(\theta | x_{1:T}[m], y_{1:T])$. This distribution is not available in closed form, however we can generate samples from it by using rejection sampling with the following instrumental distribution

$$q(\phi, \tau | x_{1:T}[m], y_{1:T}) = G \left( \tau; \phi, \tilde{\mu}, \tilde{\tau}^{-1} \right),$$

$$\alpha = 0.01 + \frac{T - 1}{2},$$

$$\beta = 0.01 + \frac{1}{2} \sum_{t=1}^{T} x_{t}[m]^{2} - \frac{1}{2} \sum_{t=1}^{T} x_{t}[m]^{2},$$

$$\tilde{\mu} = \sum_{t=1}^{T} x_{t}[m] x_{t}[m], \quad \tilde{\tau} = \tau \sum_{t=1}^{T} x_{t}[m]^{2}.$$ 

In the lower part of Figure 2, we present the resulting marginal posterior estimates. The posterior means $\hat{\theta}_{PG} = \{0.953, 44.37\}$ are indicated by dotted lines.

9. FUTURE CHALLENGES

We end this tutorial by pointing out directions for future research involving interesting challenges where we believe that SMC can open up for significant developments.

Over two decades ago the SMC development started by providing a solution to the intractable filtering problem inherent in the nonlinear SSM. We have since then seen that SMC is indeed much more widely applicable and we strongly believe that this development will continue, quite possibly at a higher pace. This opens up entirely new arenas where we can use SMC to solve hard inference problems. To give a few concrete examples of this we
have the Bayesian nonparametric models (such as the Dirichlet and the Beta processes) that are extensively used in machine learning. There are also the so-called spatio-temporal models, which do not only have structure in time, but also in a spatial dimension, imagine the weather forecasting problem. A known deficiency of the standard (bootstrap) particle filter is its inability to handle high-dimensional variables \( x_t \) (Bickel et al., 2008), which is usually the case in for example spatio-temporal models. However, recent work has shown promising directions to tackle high-dimensional models in a consistent way using SMC (Naesseth et al., 2014; Beskos et al., 2014; Naesseth et al., 2015).

There is a well-known (but underutilised) duality between the control problem and the system identification problem. Coupled with the various SMC based approximations this opens up for fundamentally new controllers to be learnt by formulating the policy optimisation in control problems as an inference problem. For some work along this direction, see e.g. (Doucet et al., 2010; Hoffman et al., 2009; Toussaint and Storkey, 2006).

The PPMC family of methods that has been discussed and used throughout this tutorial is a concrete example of another interesting trend, namely that of coupling various sampling methods into more powerful solutions. This is a trend that will continue to evolve. The online (Bayesian) inference problem is also a future challenge where we believe that SMC will play an important role.

REFERENCES


