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Backward Simulation Methods for Monte Carlo Statistical Inference

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Backward Simulation Methods for Monte Carlo Statistical Inference

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Abstract

Monte Carlo methods, in particular those based on Markov chains and on interacting particle systems, are by now tools that are routinely used in machine learning. These methods have had a profound impact on statistical inference in a wide range of application areas where probabilistic models are used. Moreover, there are many algorithms in machine learning which are based on the idea of processing the data sequentially, first in the forward direction and then in the backward direction. In this tutorial, we will review a branch of Monte Carlo methods based on the forward–backward idea, referred to as backward simulators. These methods are useful for learning and inference in probabilistic models containing latent stochastic processes. The theory and practice of backward simulation algorithms have undergone a significant development in recent years and the algorithms keep finding new applications. The foundation for these methods is sequential Monte Carlo (SMC). SMC-based backward simulators are capable of addressing smoothing problems in sequential latent variable models, such as

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general, nonlinear/non-Gaussian state-space models (SSMs). However, we will also clearly show that the underlying backward simulation idea is by no means restricted to SSMs. Furthermore, backward simulation plays an important role in recent developments of Markov chain Monte Carlo (MCMC) methods. Particle MCMC is a systematic way of using SMC within MCMC. In this framework, backward simulation gives us a way to significantly improve the performance of the samplers. We review and discuss several related backward-simulation-based methods for state inference as well as learning of static parameters, both using a frequentistic and a Bayesian approach.

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1

Introduction

A basic strategy to address many inferential problems in machine learning is to process data sequentially, first in the forward direction and then in the backward direction. Examples of this approach are the well-known forward–backward algorithm for hidden Markov models (HMMs) and the Rauch–Tung–Striebel smoother [119] for linear Gaussian state-space models. Moreover, two decades of research on sequential Monte Carlo and Markov chain Monte Carlo have enabled inference in increasingly more challenging models. Many developments have been made in order to make use of the forward–backward idea together with these Monte Carlo methods, providing inferential techniques collectively referred to as backward simulation. This tutorial provides a unifying view of these methods. In this introductory section we review some relevant background materials and also derive a first backward simulator for the special case of linear Gaussian state-space models.

1.1 Background and Motivation

For over half a century, Monte Carlo methods have been recognized as potent tools for statistical inference in complex probabilistic

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models; see [103] for an early discussion. A continuous development and refinement of these methods have enabled inference in increasingly more challenging models. A key milestone in this development was the introduction of Markov chain Monte Carlo (MCMC) methods through the inventions of the Metropolis–Hastings algorithm [71, 102] and the Gibbs sampler [58]. Parallel to this, sequential importance sampling [70] and sampling/importance resampling [122] laid the foundation of sequential Monte Carlo (SMC). In its modern form, SMC was first introduced in [64, 129]. During the 1990s, several independent developments were made by, among others, [77, 83]. Recently, SMC and MCMC have been combined in a systematic manner through the developments of pseudo-marginal methods [6, 11] and particle MCMC [3].

Backward simulation is a strategy which is useful as a Monte Carlo method for learning of probabilistic models containing latent stochastic processes. In particular, we will consider inference in dynamical systems, i.e., systems that evolve over time. Dynamical systems play a central role in a wide range of scientific fields, such as signal processing, automatic control, epidemiology and econometrics, to mention a few.

One of the most widely used models of a dynamical system is the state-space model (SSM), reviewed in more detail in Sections 1.4–1.6. The structure of an SSM can be seen as influenced by the notion of a physical system. At each time t, the system is assumed to be in a certain state x_t. The state contains all relevant information about the system, i.e., if we would know the state of the system we would have full insight into its internal condition. However, the state is typically not known. Instead, we measure some quantity y_t which depend on the state in some way. Given a sequence of observations $y_{1:T} \triangleq (y_1, \ldots, y_T)$, we seek to draw inference about the latent state process $x_{1:T}$ (state inference), as well as about unknown static parameters of the model (parameter inference).

The class of SSMs will play a central role in this tutorial. Indeed, many of the inferential methods that we will review have been developed explicitly for SSMs. However, as will become apparent in Sections 4 and 5, most of the methods are more general and can be used for learning interesting models outside the class of SSMs.

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Backward simulation is based on the forward–backward idea. That is, the data is processed first in the forward direction and then in the backward direction. In the backward pass, the state process is simulated backward in time, i.e., by first simulating x_T, then x_{T-1} etc., until a complete state trajectory $x_{1:T}$ is generated. This procedure gives us a tool to address the state smoothing problem in models for which no closed form solution is available. This is done by simulating multiple backward trajectories from the smoothing distribution, i.e., conditionally on the observations $y_{1:T}$, which can then be used for Monte Carlo integration. State smoothing is of key relevance, e.g., to obtain refined state estimates in offline settings. Furthermore, it lies at the core of many parameter inference methods (see Section 1.5) and it can be used to address problems in optimal control (see Section 4.1).

Backward simulation is also useful in MCMC, as a way of grouping variables to improve the mixing of the sampler. A common way to construct an MCMC sampler for an SSM is to sample the state variables x_t, for different t, one at a time (referred to as single-state sampling). However, since the states are often strongly dependent across time, this can lead to poor performance. Backward simulation provides a mean of grouping the state variables and sampling the entire trajectory $x_{1:T}$ as one entity. As we will illustrate in Section 1.3, this can lead to a considerable improvement upon the single-state sampler.

In Section 1.7 we will derive a first backward simulator for the class of linear Gaussian state-space (LGSS) models. Apart from LGSS models, exact backward simulation is tractable, basically only for finite state-space HMMs (see also Section 4.1.1). The main focus in this tutorial will be on models outside these restricted classes, for which exact backward simulation is not possible. Instead, we will make use of SMC (and MCMC) to enable backward simulation in challenging probabilistic models, such as nonlinear/non-Gaussian SSMs, as well as more general non-Markovian latent variable models.

1.2 Notation and Definitions

For any sequence $\{x_k\}_{k\in\mathbb{N}}$ and integers $m \leq n$ we write $x_{m:n} \triangleq (x_m, \ldots, x_n)$. We let $\wedge$ be the minimum operator, i.e., $a \wedge b \triangleq \min(a, b)$.

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For a matrix A, the matrix transpose is written as A^{T}. For two probability distributions μ_1 and μ_2, the total variation distance is given by $\|\mu_1 - \mu_2\|_{\mathrm{TV}} \triangleq \sup_A |\mu_1(A) - \mu_2(A)|$. A Dirac point-mass located at some point x' is denoted as $\delta_{x'}(dx)$. We write $X \sim \mu$ to mean that the random variable X is either distributed according to μ, or sampled from μ. The uniform probability distribution on the interval $[a, b]$ is written as $\mathcal{U}([a, b])$. $\mathrm{Cat}(\{p_i\}_{i=1}^n)$, with $\sum_{i=1}^n p_i = 1$, is the categorical (i.e., discrete) probability distribution on the set $\{1, \ldots, n\}$, with probabilities $\{p_i\}_{i=1}^n$. Finally, $\mathcal{N}(m, \Sigma)$ and $\mathcal{N}(x; m, \Sigma)$ are the Gaussian (i.e., normal) probability distribution and density function, respectively, with mean vector m, covariance matrix Σ and argument x.

1.3 A Preview Example

Before we continue with this section on background theory, we consider an example to illustrate the potential benefit of using backward simulation. A simple stochastic volatility SSM is given by,

$$x_{t+1} = a x_t + v_t, \qquad v_t \sim \mathcal{N}(0, q), \tag{1.1a}$$

$$y_t = e_t \exp\left(\tfrac{1}{2} x_t\right), \qquad e_t \sim \mathcal{N}(0, 1), \tag{1.1b}$$

where the state process $\{x_t\}_{t \geq 1}$ is latent and observations are made only via the measurement process $\{y_t\}_{t \geq 1}$. Similar models have been used to generalize the Black–Scholes option pricing equation to allow for the variance to change over time [27, 101]. The same model was used by [30] to illustrate the poor mixing of a single-state Gibbs sampler; an example which is replicated here.

For simplicity, we assume that the parameters $a = 0.99$ and $q = 0.01$ are known. We seek the density $p(x_{1:T} \mid y_{1:T})$, i.e., the conditional density of the state process $x_{1:T}$ given a sequence of observations $y_{1:T}$ for some fixed final time point T. This conditional density is referred to as the joint smoothing density (JSD). For the model under study, the JSD is not available in closed form due to the nonlinear measurement Equation (1.1b). To remedy this, we construct an MCMC method to approximately sample from it. MCMC will be reviewed in more detail in Section 2.2. However, the basic idea is to simulate a Markov chain which is constructed in such a way that it admits the target

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distribution as limiting distribution. The sample path from the Markov chain can then be used to draw inference about the target density $p(x_{1:T} \mid y_{1:T})$.

As an initial attempt, we try a single-state Gibbs sampler. That is, we sample each state x_t conditionally on $\{x_{1:t-1}, x_{t+1:T}\}$ (and the observations $y_{1:T}$). At each iteration of the Gibbs sampler we thus simulate according to,

$$\begin{aligned} x_1' &\sim p(x_1 \mid x_{2:T}, y_{1:T}); \\ &\vdots \\ x_t' &\sim p(x_t \mid x_{1:t-1}', x_{t+1:T}, y_{1:T}); \\ &\vdots \\ x_T' &\sim p(x_T \mid x_{1:T-1}', y_{1:T}). \end{aligned}$$

This procedure will leave $p(x_{1:T} \mid y_{1:T})$ invariant (see Section 2.2 for more on Gibbs sampling) and it results in a valid MCMC sampler. The conditional densities $p(x_t \mid x_{1:t-1}, x_{t+1:T}, y_{1:T})$ are not available in closed form. However, for this model (Equation (1.1)), they are log-concave and we can employ the efficient rejection sampling strategy by [145] to sample exactly from these distributions.

The single-state Gibbs sampler will indeed converge to samples from $p(x_{1:T} \mid y_{1:T})$. However, it is well recognized that single-state samplers can suffer from poor mixing, due to the often strong dependencies between consecutive state variables. That is, the convergence can be slow in the sense that we need to iterate the above sampling scheme a large number of times to get reliable samples.

To analyze this, we generate $T = 100$ samples from the model (Equation (1.1)) and run the Gibbs sampler for 100 000 iterations (in each iteration, we loop over all the state variables for $t = 1, \ldots, T$). The first 10 000 iterations are discarded, to avoid transient effects. We then compute the empirical autocorrelation function (ACF) of the state x_{50}, which is given in Figure 1.1. As can be seen, the ACF decreases very slowly, indicating a poorly mixing Gibbs kernel. This simply reflects the fact that, when the state variables are highly correlated, the single-state sampler will be inefficient at exploring the state-space. This is a

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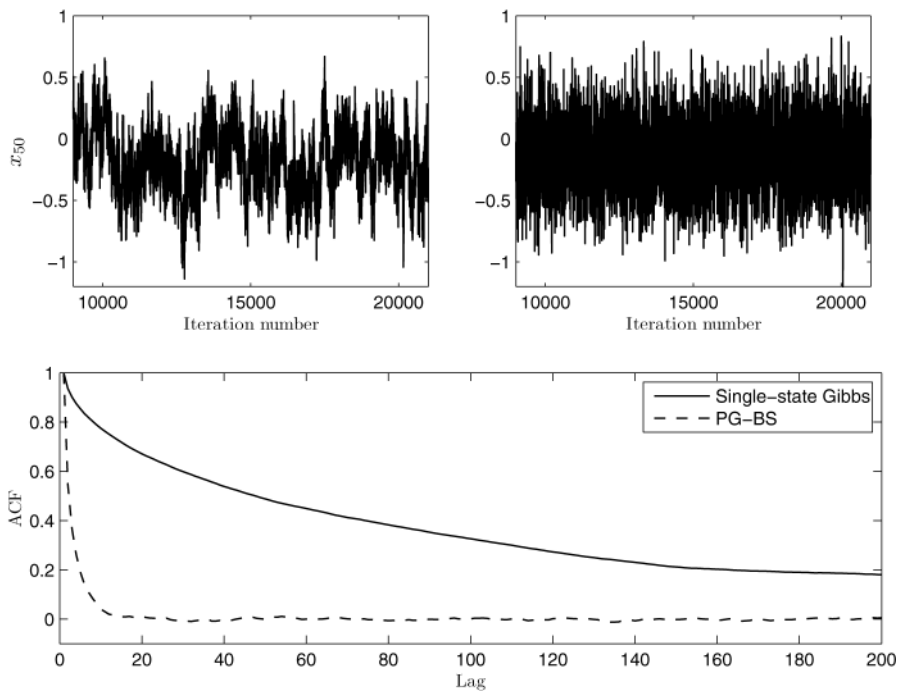

Fig. 1.1 (Top left) Part of sample path for the single-state Gibbs sampler; (Top right) Part of sample path for PGBS; (Bottom) Empirical ACF for x_{50} for the single-state Gibbs sampler and for PGBS using $N = 15$ particles.

common and well-recognized problem when addressing the state inference problem for SSMs.

One way to remedy this is to group the variables and sample a full state trajectory $x_{1:T}$ jointly. This is what a backward simulator aims to accomplish. Grouping variables in a Gibbs sampler will in general improve upon the mixing of the single-state sampler [97, Section 6.7], and in practice the improvement can be quite considerable.

To illustrate this, we have included the ACF for a backward-simulation-based method in Figure 1.1. Since the model (Equation (1.1)) is nonlinear, exact backward simulation is not possible. Instead, the results reported here are from a backward simulator based on SMC, using (only) $N = 15$ particles. The specific method that we have used is denoted as particle Gibbs with backward simulation (PGBS), and it will be discussed in detail in Section 5.4. For the PGBS,

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the ACF drops off much more rapidly, indicating a more efficient sampler. Furthermore, a key property of PGBS is that, despite the fact that it relies on a crude SMC approximation, it does not alter the stationary distribution of the Gibbs sampler, nor does it introduce any additional bias. That is, PGBS will, just as the single-state Gibbs sampler, target the exact JSD $p(x_{1:T} \mid y_{1:T})$. This property is known as *exact approximation*, a concept that we will return to in Section 5.

1.4 State-Space Models

State-space models (SSMs) are commonly used to model time series and dynamical systems. Additionally, many models that are not sequential "by nature" can also be written on state-space form. It is a comprehensive and important class of models, and it serves as a good starting point for introducing the concepts that will be discussed throughout this tutorial.

We consider here discrete-time SSMs on a general state-space X. The system state is a Markov process $\{x_t\}_{t\geq 1}$ on X, evolving according to a Markov transition kernel $F(dx_{t+1} \mid x_t)$ and with initial distribution $\nu(dx_1)$. The state x_t is assumed to summarize all relevant information about the system at time t. However, the state process is latent and it is observed only implicitly through the observations $\{y_t\}_{t\geq 1}$, taking values in some set Y. Given x_t, the measurement y_t is conditionally independent of past and future states and observations, and it is distributed according to a kernel $G(dy_t \mid x_t)$. A graphical model, illustrating the conditional dependencies in an SSM, is given in Figure 1.2.

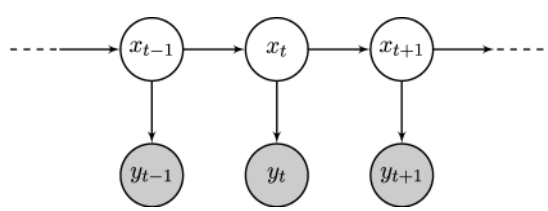

Fig. 1.2 Graphical model of an SSM. The white nodes represent latent variables and the gray nodes represent observed variables.

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We shall assume that the observation kernel G admits a probability density g w.r.t. some dominating measure, which we simply denote dy. Such models are referred to as partially dominated. If, in addition, the transition kernel F admits a density f and the initial distribution ν admits a density μ, both w.r.t. some dominating measure dx, the model is called fully dominated. In summary, a fully dominated SSM can be expressed as,

$$x_{t+1} \sim f(x_{t+1} \mid x_t), \tag{1.2a}$$

$$y_t \sim g(y_t \mid x_t), \tag{1.2b}$$

and $x_1 \sim \mu(x_1)$. Two examples of SSMs follow below.

Example 1.1 (Finite state-space hidden Markov model). A finite state-space HMM, or simply HMM, is an SSM with $\mathsf{X} = \{1, \ldots, K\}$ for some finite K. The transition density (w.r.t. counting measure) can be summarized in a $K \times K$ transition matrix Π, where the (i,j)th entry is given by,

$$\Pi_{i,j} = P(x_{t+1} = j \mid x_t = i) = f(j \mid i).$$

Hence, $f(j \mid i)$ denotes the probability of moving from state i at time t, to state j at time $t+1$.

Example 1.2 (Additive noise model). In engineering applications, SSMs are often expressed on functional form with additive noise,

$$x_{t+1} = a(x_t) + v_t,$$
$$y_t = c(x_t) + e_t,$$

for some functions a and c. Here, the noises v_t and e_t are commonly referred to as process noise and measurement noise, respectively. If the noise distributions admit densities w.r.t. dominating measures, then the model is fully dominated. The transition density is then given by $f(x_{t+1} \mid x_t) = p_{v_t}(x_{t+1} - a(x_t))$ and similarly for the observation density.

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Throughout this tutorial, we will mostly be concerned with fully dominated SSMs and therefore do most of our derivations in terms of probability densities. There are, however, several examples of interesting models that are *degenerate*, i.e., that are not fully dominated. We will return to this in the sequel and discuss how it affects the methods presented in here.

1.5 Parameter Learning in SSMs

The basic inference problem for SSMs is typically that of state inference, i.e., to infer the latent states given measurements from the system. In fact, even when the actual task is to learn a model of the system dynamics, state inference tends to play a crucial role as an intermediate step of the learning algorithm. To illustrate this, assume that the SSM (Equation (1.2)) is parameterized by some unknown parameter $\theta \in \Theta$,

$$x_{t+1} \sim f_\theta(x_{t+1} \mid x_t), \tag{1.3a}$$

$$y_t \sim g_\theta(y_t \mid x_t), \tag{1.3b}$$

and $x_1 \sim \mu_\theta(x_1)$. Given a batch of measurements $y_{1:T}$, we wish to draw inference about θ. In the Bayesian setting, a prior distribution $\pi(\theta)$ is assigned to the parameter and the learning problem amounts to computing the posterior distribution $p(\theta \mid y_{1:T})$.

A complicating factor is that the likelihood $p(y_{1:T} \mid \theta)$ in general cannot be computed in closed form. To address this difficulty, it is common to make use of *data augmentation* [136, 132]. That is, we target the joint state and parameter posterior $p(\theta, x_{1:T} \mid y_{1:T})$, rather than the marginal posterior $p(\theta \mid y_{1:T})$. The latent states are thus viewed as auxiliary variables. This opens up for using Gibbs sampling (see Section 2.2), for instance by initializing $\theta[0] \in \Theta$ and iterating;

(i) Draw $x_{1:T}[r] \sim p(x_{1:T} \mid \theta[r-1], y_{1:T})$;
(ii) Draw $\theta[r] \sim p(\theta \mid x_{1:T}[r], y_{1:T})$.

Under weak assumptions, this procedure will generate a Markov chain $\{\theta[r], x_{1:T}[r]\}_{r\geq 1}$ with stationary distribution $p(\theta, x_{1:T} \mid y_{1:T})$. Consequently, the stationary distribution of the subchain $\{\theta[r]\}_{r\geq 1}$ will be the

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marginal parameter posterior distribution $p(\theta \mid y_{1:T})$. Note that Step (i) of the above sampling scheme requires the computation of the JSD, for a fixed value of the parameter θ. That is, we need to address an intermediate smoothing problem in order to implement this Gibbs sampler.

Data augmentation is commonly used also in the frequentistic setting. Assume that we, instead of the posterior distribution, seek the maximum likelihood estimator (MLE),

$$\widehat{\theta}_{\mathrm{ML}} = \arg\max_{\theta \in \Theta} \log p_\theta(y_{1:T}), \tag{1.4}$$

where $p_\theta(y_{1:T})$ is the likelihood of the observed data for a given value of the system parameter θ. Again, since the log-likelihood $\log p_\theta(y_{1:T})$ is not available in closed form, direct maximization in Equation (1.4) is problematic. Instead, we can make use of the expectation maximization (EM) algorithm [33] (see also [100]). The EM algorithm is an iterative method, which maximizes $p_\theta(y_{1:T})$ by iteratively maximizing an auxiliary quantity,

$$Q(\theta, \theta') = \int \log p_\theta(x_{1:T}, y_{1:T}) p_{\theta'}(x_{1:T} \mid y_{1:T})\, dx_{1:T}. \tag{1.5}$$

The EM algorithm is useful when maximization of $\theta \mapsto Q(\theta, \theta')$, for fixed θ', is simpler than direct maximization of the log-likelihood, $\theta \mapsto \log p_\theta(y_{1:T})$. The procedure is initialized at some $\theta[0] \in \Theta$ and then iterates between two steps, expectation (E) and maximization (M);

(E) Compute $Q(\theta, \theta[r-1])$;
(M) Compute $\theta[r] = \arg\max_{\theta \in \Theta} Q(\theta, \theta[r-1])$.

The resulting sequence $\{\theta[r]\}_{r \geq 0}$ will, under weak assumptions, converge to a stationary point of the likelihood $p_\theta(y_{1:T})$ [148].

Using the conditional independence properties of an SSM, we can write the complete data log-likelihood as

$$\begin{aligned} &\log p_\theta(x_{1:T}, y_{1:T}) \\ &\quad = \log \mu_\theta(x_1) + \sum_{t=1}^{T} \log g_\theta(y_t \mid x_t) + \sum_{t=1}^{T-1} \log f_\theta(x_{t+1} \mid x_t). \end{aligned} \tag{1.6}$$

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From Equation (1.5), we note that the auxiliary quantity is defined as the expectation of expression (1.6) under the JSD. Hence, to carry out the E-step of the EM algorithm, we again need to address an intermediate smoothing problem for fixed values of the system parameters.

1.6 Smoothing Recursions

As noted above, the JSD is a quantity of central interest for learning and inference problems in SSMs. It summarizes all the information about the latent states which is available in the observations. Many densities that arise in various state inference problems are given as marginals of the JSD. There are a few that are of particular interest, which we summarize in Table 1.1. To avoid a cluttered notation, we now drop the (possible) dependence on an unknown parameter θ from the notation and write the JSD as $p(x_{1:T} \mid y_{1:T})$.

As in Equation (1.6), the conditional independence properties of an SSM implies that the complete data likelihood can be written as,

$$p(x_{1:T}, y_{1:T}) = \mu(x_1) \prod_{t=1}^{T} g(y_t \mid x_t) \prod_{t=1}^{T-1} f(x_{t+1} \mid x_t). \tag{1.7}$$

The JSD is related to the above expression by Bayes' rule,

$$p(x_{1:T} \mid y_{1:T}) = \frac{p(x_{1:T}, y_{1:T})}{\int p(x_{1:T}, y_{1:T})\, dx_{1:T}}. \tag{1.8}$$

Despite the simplicity of this expression, it is of limited use in practice due to the high-dimensional integration needed to compute the normalization factor in the denominator. Instead, most practical methods

Table 1.1 Filtering and smoothing densities of particular interest.

	Density
Filtering[a]	$p(x_t \mid y_{1:t})$
Joint smoothing	$p(x_{1:T} \mid y_{1:T})$
Marginal smoothing ($t \leq T$)	$p(x_t \mid y_{1:T})$
Fixed-interval smoothing ($s < t \leq T$)	$p(x_{s:t} \mid y_{1:T})$
Fixed-lag smoothing (ℓ fixed)[a]	$p(x_{t-\ell+1:t} \mid y_{1:t})$

[a] The filtering and fixed-lag smoothing densities are marginals of the JSD at time t, $p(x_{1:t} \mid y_{1:t})$.

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(and in particular the ones discussed in this tutorial) are based on a recursive evaluation of the JSD.

Again by using Bayes' rule, we get the following two-step procedure,

$$p(x_{1:t} \mid y_{1:t}) = \frac{g(y_t \mid x_t)p(x_{1:t} \mid y_{1:t-1})}{p(y_t \mid y_{1:t-1})}, \tag{1.9a}$$

$$p(x_{1:t+1} \mid y_{1:t}) = f(x_{t+1} \mid x_t)p(x_{1:t} \mid y_{1:t}). \tag{1.9b}$$

The above equations will be denoted as the forward recursion for the JSD, since they evolve forward in time. Step (1.9a) is often referred to as the measurement update, since the current measurement y_t is taken into account. Step (1.9b) is known as the time update, moving the density forward in time, from t to $t+1$.

An interesting fact about SSMs is that, conditioned on $y_{1:T}$, the state process $\{x_t\}_{t=1}^T$ is an inhomogeneous Markov process. Under weak assumptions (see [23, Section 3.3.2] for details), the same holds true for the time-reversed chain, starting at time T and evolving backward in time according to the so-called backward kernel,

$$B_t(A \mid x_{t+1}) \triangleq P(x_t \in A \mid x_{t+1}, y_{1:T}). \tag{1.10}$$

Note that the backward kernel is time inhomogeneous. In the general case, it is not possible to give an explicit expression for the backward kernel. However, for a fully dominated model, this can always be done, and its density is given by

$$p(x_t \mid x_{t+1}, y_{1:T}) = \frac{f(x_{t+1} \mid x_t)p(x_t \mid y_{1:t})}{\int f(x_{t+1} \mid x_t)p(x_t \mid y_{1:t})\,dx_t}. \tag{1.11}$$

From the conditional independence properties of an SSM, it also holds that $p(x_t \mid x_{t+1}, y_{1:T}) = p(x_t \mid x_{t+1}, y_{1:t})$.

Using the backward kernel, we get an alternative recursion for the JSD, evolving backward in time,

$$p(x_{t:T} \mid y_{1:T}) = p(x_t \mid x_{t+1}, y_{1:t})p(x_{t+1:T} \mid y_{1:T}), \tag{1.12}$$

starting with the filtering density at time T, $p(x_T \mid y_{1:T})$. This is known as the backward recursion. At time $t = 1$, the JSD for the time interval $1, \ldots, T$ is obtained.

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The backward kernel density at time t depends only on the transition density $f(x_{t+1} \mid x_t)$ and on the filtering density $p(x_t \mid y_{1:t})$, a property which is of key relevance. Hence, to utilise the backward recursion (Equation (1.12)) for computing the JSD, the filtering densities must first be computed for $t = 1, \ldots, T$. Consequently, this procedure is generally called forward filtering/backward smoothing.

1.7 Backward Simulation in Linear Gaussian SSMs

An important special case of Equation (1.2) is the class of linear Gaussian state-space models. A functional representation of an LGSS model is given by,

$$x_{t+1} = Ax_t + v_t, \qquad v_t \sim \mathcal{N}(0, Q), \tag{1.13a}$$

$$y_t = Cx_t + e_t, \qquad e_t \sim \mathcal{N}(0, R). \tag{1.13b}$$

Here, y_t is an n_y-dimensional vector of observations, x_t is an n_x-dimensional state vector and the system matrices A and C are of appropriate dimensions. The process and measurement noises are multivariate Gaussian with zero means and covariances Q and R, respectively.

Example 1.3 (Partially or fully dominated SSM). Assume that the measurement noise covariance R in Equation (1.13b) is full rank. Then, the observation kernel is Gaussian and dominated by Lebesgue measure. Hence, the model is partially dominated. If, in addition, the process noise covariance Q in Equation (1.13a) is full rank, then the transition kernel is also Gaussian and dominated by Lebesgue measure. In this case, the model is fully dominated.

However, for singular Q the model is degenerate (i.e., not fully dominated). Rank deficient process noise covariances arise in many applications, for instance if there is a physical connection between some of the states (such as between position and velocity).

A fully dominated LGSS model can equivalently be expressed as in Equation (1.2) with,

$$f(x_{t+1} \mid x_t) = \mathcal{N}(x_{t+1}; Ax_t, Q), \tag{1.14a}$$

$$g(y_t \mid x_t) = \mathcal{N}(y_t; Cx_t, R). \tag{1.14b}$$

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LGSS models are without doubt one of the most important and well-studied classes of SSMs. There are basically two reasons for this. First, LGSS models provide sufficiently accurate descriptions of many interesting dynamical systems. Second, LGSS models are one of the few model classes, simple enough to allow for a fully analytical treatment.

When addressing inferential problems for SSMs, we are often asked to generate samples from the JSD, typically as part of an MCMC sampler used to learn a model of the system dynamics, as discussed above. For an LGSS model, the JSD is Gaussian and it can be computed using Kalman filtering and smoothing techniques (see e.g., [80]). Hence, we can make use of standard results for Gaussian distributions to generate a sample from $p(x_{1:T} \mid y_{1:T})$. This is possible for small T, but for increasing T it soon becomes infeasible due to the large matrix inversions involved.

To address this issue, it was recognized by [24, 56] that we can instead use the backward recursion (Equation (1.12)). It follows that the JSD can be factorized as,

$$p(x_{1:T} \mid y_{1:T}) = \left(\prod_{t=1}^{T-1} p(x_t \mid x_{t+1}, y_{1:t}) \right) p(x_T \mid y_{1:T}). \tag{1.15}$$

Initially, we generate a sample from the filtering density at time T,

$$\widetilde{x}_T \sim p(x_T \mid y_{1:T}). \tag{1.16a}$$

We then, successively, augment this *backward trajectory* by generating samples from the backward kernel,

$$\widetilde{x}_t \sim p(x_t \mid \widetilde{x}_{t+1}, y_{1:t}), \tag{1.16b}$$

for $t = T-1, \ldots, 1$. After a complete backward sweep, the backward trajectory $\widetilde{x}_{1:T}$ is (by construction) a realization from the JSD (Equation (1.15)).

To compute the backward kernel, we first run a forward filter to find the filtering densities $p(x_t \mid y_{1:t})$ for $t = 1, \ldots, T$. For an LGSS model, this is done by a standard Kalman filter [81]. It follows that the filtering densities are Gaussian according to,

$$p(x_t \mid y_{1:t}) = \mathcal{N}(x_t; \hat{x}_{t|t}, P_{t|t}), \tag{1.17}$$

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for some tractable sequences of mean vectors $\{\hat{x}_{t|t}\}_{t\geq 1}$ and covariance matrices $\{P_{t|t}\}_{t\geq 1}$, respectively. From Equation (1.14a), we note that the transition density function is Gaussian and affine in x_t. Using Equations (1.11) and (1.17) and standard results on affine transformations of Gaussian variables, it then follows that

$$p(x_t \mid x_{t+1}, y_{1:t}) = \mathcal{N}(x_t; \mu_t, M_t), \tag{1.18a}$$

with

$$\mu_t = \hat{x}_{t|t} + P_{t|t}A^{\mathsf{T}}(Q + AP_{t|t}A^{\mathsf{T}})^{-1}(x_{t+1} - A\hat{x}_{t|t}), \tag{1.18b}$$

$$M_t = P_{t|t} - P_{t|t}A^{\mathsf{T}}(Q + AP_{t|t}A^{\mathsf{T}})^{-1}AP_{t|t}. \tag{1.18c}$$

Note that, if more than one sample is desired, multiple backward trajectories can be generated independently, without having to rerun the forward Kalman filter. We illustrate the backward simulator in the example below.

Example 1.4. To illustrate the possibility of generating samples from the JSD using backward simulation, we consider a first-order LGSS model,

$$x_{t+1} = 0.9x_t + v_t, \qquad v_t \sim \mathcal{N}(0, 0.1),$$
$$y_t = x_t + e_t, \qquad e_t \sim \mathcal{N}(0, 1),$$

and $x_1 \sim \mathcal{N}(x_1; 0, 10)$. We simulate $T = 50$ samples $y_{1:T}$ from the model. Since the model is linear Gaussian, the marginal smoothing densities $p(x_t \mid y_{1:T})$ can be computed by running a Kalman filter followed by a Rauch–Tung–Striebel smoother [119]. However, we can also generate samples from the JSD $p(x_{1:T} \mid y_{1:T})$ by running a backward simulator. We simulate $M = 5\,000$ independent trajectories $\{\widetilde{x}^j_{1:T}\}_{j=1}^M$, by first running a Kalman filter and then repeating the backward simulation procedure given by Equations (1.16) and (1.18) M times. Histograms over the simulated states at three specific time points, $t = 1$, $t = 25$ and $t = 50$, are given in Figure 1.3. As expected, the histograms are in close agreement with the true marginal smoothing distributions.

The strategy given by Equation (1.16), i.e., to sequentially sample (either exactly or approximately) from the backward kernel to generate a realization from the JSD, is what we collectively refer to as

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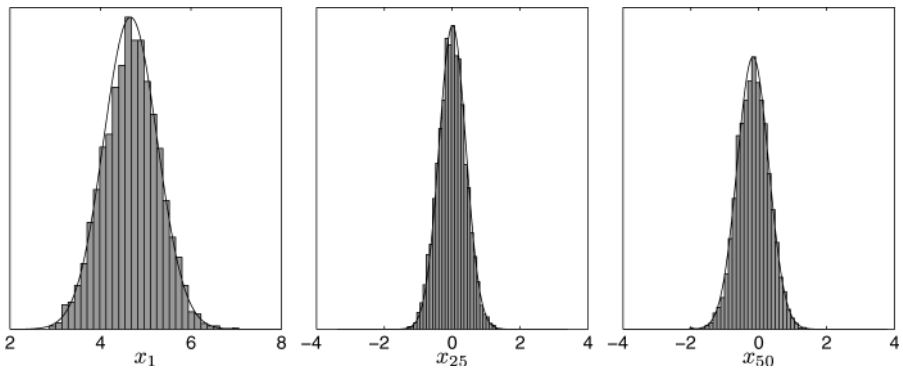

Fig. 1.3 Histograms of $\{\widetilde{x}_t^j\}_{j=1}^M$ for $t = 1$, $t = 25$ and $t = 50$ (from left to right). The true marginal smoothing densities $p(x_t \mid y_{1:T})$ are shown as black lines.

backward simulation. We will now leave the world of LGSS models. In the remainder of this tutorial we address backward simulation for general nonlinear/non-Gaussian models. In these cases, the backward kernels will in general not be available in closed form. Instead, we will rely on SMC approximations of the kernels to carry out the backward simulation.

Before we leave this section, it should be noted that the backward simulator for LGSS models derived here is provided primarily to illustrate the concept. For LGSS models, more efficient samplers exist, e.g., based on disturbance simulation. See [30, 47, 146] for further details and extensions.

1.8 Outline

The rest of this tutorial is organized as follows. Section 2 reviews the two main Monte Carlo methods that are used throughout SMC and MCMC. The section is self-contained, but for obvious reasons it does not provide an in-depth coverage of these methods. Several references which may be useful for readers with no background in this area are given in Section 2.

Section 3 addresses SMC-based backward simulation for SSMs. The focus in this section is on smoothing in general nonlinear/non-Gaussian SSMs. More precisely, we discuss algorithms for generating

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state trajectories, approximately distributed according to the joint smoothing distribution. These algorithms can be categorized as *particle smoothers*. Hence, readers with particular interest in smoothing problems may want to focus their attention on this section. However, smoothing is also addressed in Section 5 (see in particular Section 5.7), and the methods presented there can be useful alternatives to the particle smoothers discussed in Section 3.

Section 4 generalizes the backward simulation idea to latent variable models outside the class of SSMs. A general backward simulator is introduced and we discuss its properties and the type of models for which it is applicable. As a special case of the general backward simulator, we derive a Rao–Blackwellized particle smoother for conditionally linear Gaussian SSMs.

In Section 5, we discuss backward simulation in the context of so-called particle MCMC (PMCMC) methods. The focus in this section is on parameter inference, primarily in the Bayesian setting, but we also discuss PMCMC for maximum-likelihood-based inference. As mentioned above, the smoothing problem is also addressed. Finally, in Section 6 we conclude with a discussion about the various methods reviewed throughout this tutorial and outline possible directions for future work.

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