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Resampling Strategy in Sequential Monte Carlo for Constrained Sampling Problems

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Abstract: Monte Carlo sample paths of a dynamic system are useful for studying the underlying system and making statistical inferences related to the system. In many applications the dynamic system under study involves various types of constraints or observable features that need to be incorporated. In this paper we investigate efficient methods for generating sample paths (with importance weights) of dynamic systems with rare and strong constraints, under a sequential Monte Carlo (SMC) framework. Specifically, we present a general formulation of the constrained sampling problem. Under such a formulation, we propose a flexible resampling strategy based on a potentially time-varying lookahead timescale and identify the corresponding optimal resampling priority scores based on an ensemble of forward or backward pilots. Several examples are used to illustrate the performance of the proposed methods.

Key words and phrases: Constrained sampling, Pilot, Priority score, Resampling, Sequential Monte Carlo

1. Introduction

Stochastic dynamic systems are used in a wide range of applications in physics, finance, engineering and other fields. One of the important tools of studying complex dynamic system is to obtain Monte Carlo sample paths of the underlying stochastic process. Such samples can be used for statistical inferences under the Monte Carlo framework, as well as for providing better understanding of the behavior of the system. The sequential Monte Carlo (SMC) method is a class of efficient sampling methods that utilize the sequential nature of the underlying dynamic process. It has been used in a wide range of applications (Gordon et al., 1993; Kong et al., 1994; Avitzour, 1995; Liu and Chen, 1995; Kitagawa, 1996; Kim et al., 1998; Pitt and Shephard, 1999; Chen et al., 2000; Godsill et al., 2004; Doucet and Johansen, 2011). Although SMC is often used to estimate the marginal distribution of the underlying state at each time point (either filtering or smoothing), it also naturally provides sample paths (with importance weights) of the joint distribution of the entire state sequence. In this paper we focus on the problem of efficiently generating such sample paths under the SMC framework.

In practice, a stochastic system often comes with external observable information, including direct/indirect measurements, constraints and others. For example, in many physics and financial applications, one is interested in the distribution of all possible paths of a diffusion process with fixed starting and ending points (a diffusion bridge) (Pedersen, 1995; Durham and Gallant, 2002; Lin et al., 2010). In RNA and protein structure studies, the properties of self-loops (a single strand of RNA or protein that forms a loop in space by an internal chemical bond) are often studied through samples from the distribution of self-avoiding walks on a lattice with the same starting and ending points (Zhang et al., 2009; Lin et al., 2008). In computing long-run marginal expected shortfall in financial risk management, sample paths of a bivariate GARCH process need to be generated, under a crisis constraint enforced on one of the processes (the one representing the market) to end below a threshold, say, 40% loss (Acharya et al., 2012).

In this article, we provide a general formulation that includes many constrained path simulation problems. The formulation allows the discussion of a general guidance for designing efficient SMC implementations for such problems. Since the standard SMC approach encounters difficulties in dealing with the constrained systems, we propose a flexible resampling strategy and identify the optimal resampling priority scores. Two efficient approaches for estimating the optimal priority scores are developed, using forward pilots and backward pilots correspondingly.

The rest of this paper is organized as follows. In Section 2, the constrained sampling problem is formally stated. A general framework of SMC with constraints (SMCc) method is proposed, with a flexible resampling strategy and optimal resampling priority scores. Section 3 presents two efficient pilot methods to estimate the optimal priority scores. Three examples with different types of constraints are used to demonstrate performance of the proposed methods in Section 4. Section 5 concludes.

2. SMC with Constraints

2.1 Stochastic Dynamic System with Constraints

The class of stochastic dynamic system we consider contains a sequence of latent random states variables $x_{0:T} = \{x_0, x_1, \cdots, x_T\}$ defined on a probability space $(\Omega, \mathcal{F}, \mathbb{P})$. The dynamics of the system are governed by an initial state distribution $p(x_0)$ and a known forward propagation distribution $p(x_t \,|\, x_{0:t-1})$, where $p(\cdot)$ denotes the density function/probability. In addition, there are external constraints imposed on the latent states. Here we consider the new constraints available at time t as an event I_t. Let $C_t = I_0 \cap I_1 \cap \cdots \cap I_t$ be the cumulative constraint event up to time t. Then, $C_0 \supset C_1 \supset \cdots \supset C_T$ forms a sequence of monotonically non-increasing events. When there is no additional constraint at time t, we have $I_t = \Omega$ and $C_t = C_{t-1}$.

We focus on effective SMC method under the importance sampling framework to obtain properly weighted samples of the entire path $x_{0:T}$ given the full constraint set C_T. The target posterior distribution of $x_{0:T}$ is

$$p(x_{0:T} \,|\, C_T) \propto p(x_{0:T}, C_T) = p(x_0, C_0) \prod_{t=1}^{T} p(x_t, C_t \,|\, x_{0:t-1}, C_{t-1}), \tag{2.1}$$

where $p(x_0, C_0)$ and $p(x_t, C_t \,|\, x_{0:t-1}, C_{t-1}) = p(x_t \,|\, x_{0:t-1}, C_{t-1}) p(C_t \,|\, x_{0:t}, C_{t-1})$, $t = 1, \cdots, T$, are often specified by the system.

Many dynamic systems can be reformulated as a constrained sampling problem, including state space models. We provide five examples in Appendix A, showing the setting includes several classical problems as well as several new classes of problems.

We can measure the *strength* of a constraint through the difference between the joint distributions of the latent states with and without such a constraint. Specifically, we define the strength of I_t, the constraint imposed at time t, as the following χ^2-divergence:

$$G(t) := \chi^2\Big(p(x_{0:t}\,|\,C_{t-1}) \parallel p(x_{0:t}\,|\,C_t)\Big) = \mathrm{Var}_{p(x_{0:t}\,|\,C_{t-1})}\left[\frac{p(x_{0:t}\,|\,C_t)}{p(x_{0:t}\,|\,C_{t-1})}\right]. \tag{2.2}$$

It is closely related to importance sampling, as it is the variance of the importance weight $w(x_{0:t}) = p(x_{0:t}\,|\,C_t)/p(x_{0:t}\,|\,C_{t-1})$ when one generates samples from the proposal distribution $p(x_{0:t}\,|\,C_{t-1})$ to make inference with respect to the target distribution $p(x_{0:t}\,|\,C_t)$. A "strong" constraint would alter the distribution of underlying states significantly.

2.2 Intermediate Distributions under Constraints

In this paper, we consider generating a *properly weighted* sample set $\{(x_{0:T}, w_T^{(i)})\}_{i=1,\cdots,n}$ with respect to $p(x_{0:T}\,|\,C_T)$ under a general SMC framework, which satisfies

$$\frac{\sum_{i=1}^n w_T^{(i)} h(x_{0:T}^{(i)})}{\sum_{i=1}^n w_T^{(i)}} \xrightarrow{a.s.} \mathbb{E}_{p(x_{0:T}\,|\,C_T)}\big[h(x_{0:T})\big], \tag{2.3}$$

as $n \to \infty$ for any function $h(\cdot)$ with finite expectation under $p(x_{0:T}\,|\,C_T)$.

The SMC method has been extensively studied in the literature, for example, Liu and Chen (1998); Doucet and Johansen (2011) and the references therein. We will use the following notations for clarity. Consider a sequence of forward intermediate target propagation distributions with densities $\pi_0(x_0)$, $\pi_1(x_{0:1})$, $\cdots$, $\pi_T(x_{0:T})$. The SMC approach proposes to generate samples $x_{0:T}^{(i)} = (x_0^{(i)}, x_1^{(i)}, \cdots, x_T^{(i)})$, $i = 1, \cdots, n$, sequentially from a series of proposal conditional distributions $q(x_t\,|\,x_{0:t-1})$, $t = 0, 1, \cdots$, and update the corresponding *importance weights* by

$$w_t^{(i)} = \frac{\pi_t(x_{0:t}^{(i)})}{q(x_0^{(i)})\prod_{s=1}^t q(x_s^{(i)}\,|\,x_{0:s-1}^{(i)})} = w_{t-1}^{(i)}\frac{\pi_t(x_{0:t}^{(i)})}{\pi_{t-1}(x_{0:t-1}^{(i)})q(x_t^{(i)}\,|\,x_{0:t-1}^{(i)})},$$

with $w_0^{(i)} = \pi_0(x_0^{(i)})/q(x_0^{(i)})$. The distribution $q(x_0)\prod_{s=1}^T q(x_s \mid x_{0:s-1})$, from which the samples $x_{0:T}^{(i)}$, $i = 1,\cdots,n$, are generated, is called the *sampling distribution* or *proposal distribution*. At each time t, if the intermediate target distribution $\pi_t(x_{0:t})$ is absolutely continuous with respect to the proposal distribution $q(x_0)\prod_{s=1}^t q(x_s\,|\,x_{0:s-1})$, the sample set $\{(x_{0:t}^{(i)}, w_t^{(i)})\}_{i=1,\cdots,n}$ is properly weighted with respect to $\pi_t(x_{0:t})$.

If we set $\pi_T(x_{0:T})$ to be the joint posterior distribution $p(x_{0:T}\,|\,C_T)$ in (2.1), then at the end, the weighted sample set $\{(x_{0:T}^{(i)}, w_T^{(i)})\}_{i=1,\cdots,n}$ can be used for statistical inferences of $p(x_{0:T}\,|\,C_T)$ as in (2.3). We consider the following three distributions as the potential intermediate target distributions $\pi_t(x_{0:t})$: for $t = 0,1,\ldots,T$,

$$\bar{p}_t(x_{0:t}) := p(x_{0:t}\,|\,C_T), \tag{2.4}$$

$$p_t^+(x_{0:t}) := p(x_{0:t}\,|\,C_{t_+}), \tag{2.5}$$

$$\tilde{p}_t(x_{0:t}) := p(x_{0:t}|C_t), \tag{2.6}$$

where $t_+ \geqslant t$ is the next time when a "strong" constraint is imposed after time t.

The marginal posterior distribution $\bar{p}_t(x_{0:t})$ in (2.4) is naturally induced by the joint posterior distribution $p(x_{0:T}\,|\,C_T)$, but it is usually infeasible to use as the intermediate target distribution $\pi_t(x_{0:t})$ since it involves the high dimensional integral

$$p(x_{0:t} \mid C_T) \propto \int\cdots\int \prod_{s=1}^T p(x_s, C_s\,|\,x_{0:s-1}, C_{s-1})\,dx_{t+1}\cdots dx_T. \tag{2.7}$$

Conventional SMC approaches (Gordon et al., 1993; Liu and Chen, 1998) use the forward propagation distributions $\tilde{p}_t(x_{0:t})$ in (2.6), using only the information up to time t. Most of the time it is not efficient, especially when future constraints have a strong impact on the distribution of the current state. To overcome this drawback, we propose to use $p_t^+(x_{0:t})$ in (2.5) as $\pi_t(x_{0:t})$. It uses part of the future events and constraints to correct the Monte Carlo samples proactively. Recall that $t_+ \geqslant t$ is the next time when a strong constraint is imposed after time t. This is essentially a partial lookahead scheme with a variable lookahead timescale.

The distribution $p_t^+(x_{0:t}) = p(x_{0:t} \,|\, C_{t_+})$ in (2.5) is a compromise between $\bar{p}_t(x_{0:t}) = p(x_{0:t} \,|\, C_T)$ in (2.4) and $\tilde{p}_t(x_{0:t}) = p(x_{0:t} \,|\, C_t)$ in (2.6), where the former considers the whole constraint set and the latter ignores all future constraints. At time t, the distribution $p_t^+(x_{0:t})$ seeks the next available strong constraint for guidance, but not the entire future constraint set as $\bar{p}_t(x_{0:t})$ would require. In most cases, the next available strong constraint plays an important role in shaping the path distribution. The compromised distribution $p_t^+(x_{0:t})$ balances the use of future constraints and the computational efficiency.

To use $p_t^+(x_{1:t})$ in (2.5) as the intermediate target distribution $\pi_t(x_{1:t})$, the "optimal" proposal distribution is $q(x_t \,|\, x_{0:t-1}) = p_t^+(x_t \,|\, x_{0:t-1}) = p(x_t \,|\, x_{0:t-1}, C_{t_+})$ that incorporate the cumulative constraints up to time t_+, as suggested by Kong et al. (1994) and Liu and Chen (1998). However, it is difficult in many cases, especially when t_+ is far away from t, since it involves a high dimensional integral similar to that in (2.7). On the other hand, $\tilde{p}_t(\cdot)$ in (2.6) is often easy to work with, using the proposal distributions equal or close to $\tilde{p}_t(x_t \mid x_{0:t-1}) = p(x_t \mid x_{0:t-1}, C_t)$. Specifically, we propose to generate samples under the distribution $\tilde{p}_t(\cdot)$, but use a resampling step so that the resulting samples (before weighting) follow $p_t^+(\cdot)$.

2.3 Optimal Resampling Scores under Constraints

An important component of SMC implementation is the resampling step, in which each sample $x_{0:t}^{(i)}$ is assigned with a priority score $\beta_t^{(i)} > 0$ that reflects the algorithm's preference on this sample, then a new set of samples $\{x_{0:t}^{*(i)}\}_{i=1,\cdots,n}$ are drawn from the current set of samples $\{x_{0:t}^{(i)}\}_{i=1,\cdots,n}$ with replacement, with probabilities proportional to the priority scores. The sample weights are then adjusted to $w_t^{*(i)} = w_t^{(i)}/\beta_t^{(i)}$. The resampling step tends to remove the samples with low priority scores and duplicate those with high priority scores. The resulting weighted sample set $\{(x_{0:t}^{*(i)}, w_t^{*(i)})\}_{i=1,\cdots,n}$ remains to be properly weighted with respect to $\pi_t(x_{0:t})$ (Douc et al. (2014) Chapter 10.3 and Tsay and Chen (2019), Lemma 8.7).

In conventional SMC approaches, the resampling priority scores are often chosen as the sample weights, *i.e.*, $\beta_t^{(i)} = w_t^{(i)}$, so that the samples will have equal weights after resampling and hence can be viewed as samples of the intermediate target distribution $\pi_t(x_{0:t})$ (Gordon et al., 1993; Kong et al., 1994; Liu and Chen, 1998). This is a natural choice for filtering problems. However, it is not necessarily a good choice if we focus on the final target distribution $\pi_T(x_{0:T})$. There is a great flexibility in the selection of the priority scores, as long as it does not assign a zero score to any of the samples. With a careful construction it may improve sampling efficiency significantly (Pitt and Shephard, 1999; Zhang et al., 2007). Its design is the key in developing efficient SMC for the constrained systems in this paper.

In the constraint problem with intermediate target distribution $p_t^+(x_{0:t})$, we notice that

$$p_t^+(x_{0:t}) \propto \tilde{p}_t(x_{0:t})p(C_{t_+}|x_{0:t}, C_t).$$

A convenient way to draw samples from the distribution $p_t^+(\cdot)$ utilizing this fact is to conduct a resampling step of the samples generated from $\tilde{p}_t(\cdot)$. Specifically, we propose to track the exact weight $w_t^{(i)}$ under the distribution $\tilde{p}_t(\cdot)$, but use a resampling step with the priority score

$$\beta_t^{(i)} := w_t^{(i)} \frac{p_t^+(x_{0:t}^{(i)})}{\tilde{p}_t(x_{0:t}^{(i)})} \propto w_t^{(i)} p(C_{t_+} \,|\, x_{0:t}^{(i)}, C_t) \tag{2.8}$$

so that the resulting samples $\{x_{0:t}^{*(i)}\}_{i=1,\cdots,n}$ follow $p_t^+(\cdot)$. We call $\beta_t^{(i)} = w_t^{(i)} p(C_{t_+} \,|\, x_{0:t}^{(i)}, C_t)$ as the *optimal priority score* with respect to the constraint set C_{t_+}.

We choose to use the resampling approach to incorporate information of future constraints since it is easy to conduct. We refer to this method as the sequential Monte Carlo with constraints (SMCc) method. The exact value of $p(C_{t_+}|x_{0:t}^{(i)}, C_t)$ is often difficult to obtain. We can use an approximated value, $\hat{p}(C_{t_+} \,|\, x_{0:t}^{(i)}, C_t)$, to construct $\beta_t^{(i)}$ in (2.8). The method is presented in Algorithm 1. We will discuss how to approximate $p(C_{t_+} \,|\, x_{0:t}^{(i)}, C_t)$ in Section 3.

We point out that, in the SMCc algorithm in Algorithm 1, the sample set $\{(x_{0:t}^{(i)}, w_t^{(i)})\}_{i=1,\cdots,n}$ obtained at each time $t < T$ is properly weighted with respect to $\tilde{p}_t(x_{0:t}) = p(x_{0:t} \,|\, C_t)$, not $p_t^+(x_{0:t})$. However, we are only interested in the entire sample path $x_{0:T}$, which follows the desired distribution $\tilde{p}_T(x_{0:T}) = p_t^+(x_{0:T}) = p(x_{0:T} \,|\, C_T)$ at time T.

The simple random sampling with replacement in Algorithm 1 is not the most efficient

Algorithm 1 : Sequential Monte Carlo with Constraints (SMCc)

- *At times* $t = 0, 1, \cdots, T$*:*
  - *Propagation: For* $i = 1, \cdots, n$*,*
    - *Draw* $x_t^{(i)}$ *from distribution* $q(x_t | x_{0:t-1}^{(i)})$ *and let* $x_{0:t}^{(i)} = (x_{0:t-1}^{(i)}, x_t^{(i)})$*.*
    - *Update weights by setting*

$$\begin{aligned} w_t^{(i)} &\leftarrow w_{t-1}^{(i)} \cdot \frac{p(x_{0:t}^{(i)}, \mid C_t)}{p(x_{0:t-1}^{(i)}, \mid C_{t-1}) q(x_t^{(i)} \mid x_{0:t-1}^{(i)})} \\ &\propto w_{t-1}^{(i)} \cdot \frac{p(x_t^{(i)}, C_t \mid x_{0:t-1}^{(i)}, C_{t-1})}{q(x_t^{(i)} \mid x_{0:t-1}^{(i)})}. \end{aligned}$$

  - *Set priority scores* $\beta_t^{(i)} = w_t^{(i)} \hat{p}(C_{t_+} \mid x_{0:t}^{(i)}, C_t)$*,* $i = 1, \cdots, n$*.*
  - *Resampling:*
    - *Draw samples* $\{J_1, \ldots, J_n\}$ *from the set* $\{1, \ldots, n\}$ *with replacement, with probabilities proportional to* $\{\beta_t^{(i)}\}_{i=1,\ldots,n}$*.*
    - *Let* $x_{0:t}^{*(i)} = x_{0:t}^{(J_i)}$ *and* $w_t^{*(i)} = w_t^{(J_i)} / \beta_t^{(J_i)}$ *for* $i = 1, \cdots, n$*.*
    - *Return the new set* $\{(x_{0:t}^{(i)}, w_t^{(i)})\}_{i=1,\ldots,n} \leftarrow \{(x_{0:t}^{*(i)}, w_t^{*(i)})\}_{i=1,\ldots,n}$*.*
- *Return the weighted sample set* $\{(x_{0:T}^{(i)}, w_T^{(i)})\}_{i=1,\ldots,n}$*.*

method for resampling. Some improved resampling schemes, such as the residual resampling method (Liu and Chen, 1998) and the systematic resampling method (Carpenter et al., 1999), are developed to reduce variation introduced by the resampling step.

2.4 Some Discussions

Determination of t_+: In practice, the selection of t_+ depends on specific problems and can be user-defined. For example, in the rare and strong constraint cases such as the one in the diffusion bridge sampling problem (Lin et al., 2010), one may use $t_+ = T$, the end constraint. In frequent and weak constraints case such as in the state space model where the observation y_t serves as a weak constraint, we may use $t_+ = \min\{t+d, T\}$, taking into account the information of the next d observations $y_{t+1}, \ldots, y_{t+d}$ as in Lin et al. (2013). This is a fixed lookahead approach. We can also use the constraint strength measure $G(t)$ defined in (2.2) as a general guidance to determine t_+. For example, we may set $t_+ = \min_{s>t}\{G(s) > c\}$ for some threshold value c. In practice, the exact value of $G(t)$ may not be easy to compute, but can be estimated using a trial run of SMC with a small sample size, since $G(t)$ can be estimated by the variance of the importance weights of the target distribution $p(x_{0:t} \mid C_t)$ to the proposal distribution $p(x_{0:t} \mid C_{t-1})$. Specifically, using $q(x_t \mid x_{0:t-1}^{(i)}) = p(x_t \mid x_{0:t-1}^{(i)}, C_{t-1})$ as the proposal distribution and resampling with the importance weights as the priority score at every step, $G(t)$ can be estimated by $\widehat{G}(t) = \widehat{\text{var}}(w_t)/\overline{w}_t^2$, where $\overline{w}_t$ and $\widehat{\text{var}}(w_t)$ are the sample mean and sample variance of the weights $\{w_t^{(i)}\}_{i=1,\cdots,n}$, respectively. Then the time t is identified as a time point with a strong constraint when $\widehat{G}(t)$ exceeds a certain threshold value, or equivalently, when the effective sample size, which is defined as $n/\big[1+\widehat{G}(t)\big]$ in the SMC literature (Kong et al., 1994), is less than a certain value. The procedure only needs to be carried out once to identify all strong constraints.

Relation to other particle filters: The idea of using future constraints to estimate the current state under the framework of SMC has been studied in Pitt and Shephard (1999); Doucet et al. (2006); Lin et al. (2013); Whiteley and Lee (2014) and others. The auxiliary particle filter (Pitt and Shephard, 1999) suggests first conducting resampling according to the priority score $\beta_t = w_t p(C_{t+\Delta} \mid x_{0:t}, C_t)$ for a certain number of lookahead steps $\Delta > 0$ at time t (usually $\Delta = 1$), then drawing samples of x_{t+1} from $q(x_{t+1} \mid x_{0:t}) = p(x_{t+1} \mid x_{0:t}, C_{t+\Delta})$. The twisted particle filter in Whiteley and Lee (2014) introduces a special sample to incorporate information of future constraints in SMC implementation. Whiteley and Lee (2014) showed the theoretical properties of using such a procedure. The block sampling method in Doucet et al. (2006) also proposes to use future constraints to update x_t. All these methods involve evaluation of $p(C_{t+\Delta} \mid x_{0:t}, C_t)$. When $p(C_{t+\Delta} \mid x_{0:t}, C_t)$ does not have a closed form, the extended Kalman filter is often used to find an approximation (Jazwinski, 1970). This approximation often requires high computational costs and can be poor when Δ is large. In Section 3, we focus on developing computationally efficient methods to approximate $p(C_{t_+} \mid x_{0:t}, C_t)$ in the optimal priority score $\beta_t = w_t p(C_{t_+} \mid x_{0:t}, C_t)$.

3. Approximation of the Optimal Priority Score Using Pilots

We consider the evaluation of the term $p(C_{t_+} \mid x_{0:t}, C_t)$ in the optimal priority score (2.8), which is

$$p(C_{t_+}|x_{0:t}, C_t) = \int \cdots \int \prod_{s=t+1}^{t_+} p(x_s, C_s \mid x_{0:s-1}, C_{s-1}) dx_{t+1} \cdots dx_{t_+}. \tag{3.9}$$

The integrand is often well-defined by the system, but the integral does not have a closed-form solution in most cases.

In some cases one may assume a parametric form for $p(C_{t_+}|x_{0:t}, C_t)$, based on some prior knowledge. Zhang et al. (2007) and Lin et al. (2008) used the SMCc approach with $t_+ = T$ to generate protein conformation samples satisfying certain distance constraints between molecules of the conformation. The parametric functions they used to approximate $p(C_T|x_{0:t}, C_t)$ are based on distance of the current location x_t and the final destination x_T. The particle efficient importance sampling (PEIS) method of Scharth and Kohn (2016) uses $t_+ = T$ and approximates the optimal conditional proposal distributions $p(x_t \mid x_{0:t-1}, C_T)$ and resampling priority scores $\beta_t = w_t\, p(C_T|x_{0:t}, C_t)$ within some parametric families. The method tunes the parameters in the functions by an iterative local optimization routine. However, the performance of these parametric approximation methods greatly depends on the choice of the parametric family.

Here we propose two *ensemble* pilot approaches to estimate $p(C_{t_+} \mid x_{0:t}^{(j)}, C_t)$ nonparametrically. Compared with the "individual" pilot approaches in the existing literature (Wang et al., 2002; Zhang and Liu, 2002; Lin et al., 2013), the proposed "ensemble" pilot approaches pool all pilot samples together and use nonparametric smoothing technique to improve estimation accuracy and reduce computational costs.

For ease of presentation, we consider the case of approximating $p(C_{t_+} \mid x_{0:t}^{(j)}, C_t)$ for all t between two predetermined time points $t_1 < t_2$, both with strong constraints. Under this setting, we have $t_+ = t_2$ for every $t_1 < t \le t_2$.

3.1 Approximation based on Forward Pilots

Suppose there exists a low dimensional statistic $S(x_{0:t})$ that summarizes $x_{0:t}$ such that

$$p(x_{t+1:t+d}, C_{t+d} \,|\, x_{0:t}, C_t) = p(x_{t+1:t+d}, C_{t+d} \,|\, S(x_{0:t}), C_t) \tag{3.10}$$

for all t and $d = 0, 1, \cdots$. Under this assumption, $p(C_{t_+} \,|\, x_{0:t}, C_t) = p(C_{t_+} \,|\, S(x_{0:t}), C_t)$ is a function of $S(x_{0:t})$. We further assume that there exists a function $\phi(\cdot)$ such that $S(x_{0:t+1}) = \phi\big(S(x_{0:t}), x_{t+1}\big)$. When the system is Markovian, then $S(x_{0:t}) = x_t$.

In the forward pilot approach, we apply SMC to generate pilot samples sequentially from time t_1 to t_2 using a proposal distribution that encourages the pilot samples to satisfy the constraints C_{t_2}. The pilots and their corresponding weights would bear the information of C_{t_2} and can be used to estimate $p(C_{t_+} \mid x_{0:t}^{(j)}, C_t)$ for $t_1 < t < t_2 = t_+$. The detailed implementation is presented in Algorithm 2. Note that for $U_t^{(j)} = \prod_{s=t+1}^{t_2} \widetilde{u}_s^{(j)}$ defined in Algorithm 2, we have

$$\mathbb{E}(U_t^{(j)} \,|\, S_t^{(j)} = S) = p(C_{t_+} | S(x_{0:t}) = S, C_t)$$

for all $t_1 < t < t_2$. Therefore, we can use $\big\{(U_t^{(j)}, S_t^{(j)})\big\}_{j=1,\cdots,m}$ to estimate $p\big(C_{t_+} | S(x_{0:t}), C_t\big)$ by the nonparametric histogram function (3.11) in Algorithm 2. We choose not to use the kernel smoothing method here in order to control the computational cost, because $\widehat{p}(C_{t_+} | S(x_{0:t}), C_t)$ needs to be evaluated for all $x_{0:t}^{(j)}, j = 1, \ldots, n$, and at each time t.

The pilot sample idea has been proposed by Wang et al. (2002) and Zhang and Liu (2002), and is used for delayed estimation in Lin et al. (2013). They considered individual pilot algorithm in the sense that the pilot samples are generated for each sample path $x_{0:t}^{(i)}$ in Algorithm 1, and are only used for computing $\beta_t^{(i)}$ of that particular sample path. The computational cost of such an individual pilot algorithm is very high since it requires the generation of pilot samples for every $x_{0:t}^{(i)}$, $i = 1, \cdots, n$, at each time t.

Instead, in the ensemble pilot approaches, we use all pilot samples $\widetilde{x}_{0:t}^{(j)}$, $j = 1, \cdots, m$, with $\widetilde{S}_t^{(j)} = S(\widetilde{x}_{0:t}^{(j)})$ close to $S(x_{0:t}^{(i)})$ for estimating $p(C_{t_+}|x_{0:t}^{(i)}, C_t)$. Since this is a global operation, we can afford to use a large number of pilots hence can obtain accurate estimates of $\widehat{p}(C_{t_+} \,|\, x_{0:t}^{(i)}, C_t) = \widehat{p}\big(C_{t_+} \,|\, S(x_{0:t}^{(i)}), C_t\big)$. Additionally, this algorithm only needs to be conducted once to obtain $\widehat{p}\big(C_{t_+} \,|\, S(x_{0:t}), C_t\big)$ for all $t_1 < t < t_2$, with significant reduction of computational cost.

The accuracy of $\widehat{p}\big(C_{t_+} \,|\, S(x_{0:t}), C_t\big)$ depends on the choice of the proposal distribution $\varphi(x_s \,|\, S(x_{0:s-1}^{(i)})$ in Algorithm 2 to generate the pilots. Since there is a strong constraint I_{t_2} at time t_2, it is important to incorporate I_{t_2} in the proposal distribution $\varphi(\cdot)$ when generating pilot samples from t_1 to t_2. This ensures that the pilot samples will have a reasonable large probability to satisfy the constraint at time t_+.

3.2 Approximation Based on Backward Pilots

Assume that the stochastic dynamic system is Markovian, that is,

$$p(x_t, I_t \,|\, x_{0:t-1}, C_{t-1}) = p(x_t, I_t \,|\, x_{t-1})$$

Algorithm 2 : Forward Pilot Algorithm

- *Initialization: For* $j = 1, \cdots, m$*, draw samples* $\widetilde{S}_{t_1}^{(j)}$ *from a proposal distribution* $\varphi(S)$ *that covers the support of* $S(x_{0:t_1})$*.*

- *For* $t = t_1 + 1, \cdots, t_2$*, draw pilot samples forwardly as follows.*

  - *Generate samples* $\widetilde{x}_t^{(j)}$ *from a proposal distribution* $\varphi(\widetilde{x}_t \mid \widetilde{S}_{t-1}^{(j)})$*, and calculate* $\widetilde{S}_t^{(j)} = \phi(\widetilde{S}_{t-1}^{(j)}, \widetilde{x}_t^{(j)})$ *for* $j = 1, \cdots, m$*.*

  - *Calculate the incremental weights*

$$\widetilde{u}_t^{(j)} = \frac{p(\widetilde{x}_t^{(j)}, C_t \mid S(\widetilde{x}_{0:t-1}^{(j)}) = \widetilde{S}_{t-1}^{(j)}, C_{t-1})}{\varphi(\widetilde{x}_t^{(j)} \mid \widetilde{S}_{t-1}^{(j)})}, \quad j = 1, \cdots, m.$$

- *For* $t = t_2 - 1, t_2 - 2, \cdots, t_1 + 1$*:*

  - *Compute* $U_t^{(j)} = \prod_{s=t+1}^{t_2} \widetilde{u}_s^{(j)}$ *for* $j = 1, \cdots, m$*.*

  - *Let* $\mathcal{S}_1 \cup \cdots \cup \mathcal{S}_D$ *be a partition of the support of* $S(x_{0:t})$*. Estimate* $p(C_{t_+} \mid x_{0:t}, C_t) = p(C_{t_+} | S(x_{0:t}), C_t)$ *by*

$$f_t(S(x_{0:t})) = \sum_{d=1}^{D} \gamma_{t,d} \mathbb{I}\big(S(x_{0:t}) \in \mathcal{S}_d\big) \tag{3.11}$$

  with $\gamma_{t,d} = \frac{\sum_{j=1}^m U_t^{(j)} \mathbb{I}\left(\widetilde{S}_t^{(j)} \in \mathcal{S}_d\right)}{\sum_{j=1}^m \mathbb{I}\left(\widetilde{S}_t^{(j)} \in \mathcal{S}_d\right)}$*. where* $\mathbb{I}(\cdot)$ *is the indicator function.*

- *Return the estimated functions* $\left\{\widehat{p}(C_{t_+} \mid x_{0:t}, C_t) = f_t(S(x_{0:t}))\right\}_{t=t_1+1,\cdots,t_2-1}$ *to compute the priority scores to be used in Algorithm 1.*

for all t. Then, $p(C_{t_+} \,|\, x_{0:t}, C_t) = p(I_{t+1:t_+} \,|\, x_t)$ is a function of x_t and does not depend on the past constraints before time t. Here $I_{t+1:t_+}$ denotes the cumulative constraints imposed between time $t+1$ and t_+ (inclusive). For such a Markovian system, we can extend the backward pilot sampling method proposed in Lin et al. (2010) to a more general SMCc setting. In this approach, the pilot samples are generated in the reverse time direction, starting from $t = t_+$, the time point with a strong constraint, and propagating backward. The method is presented in Algorithm 3.

In Algorithm 3, the weight for the backward pilot $\widetilde{x}_{t:t_+}$ is

$$\widetilde{w}_t = \frac{p(\widetilde{x}_{t+1:t_+}, I_{t+1:t_+} \,|\, \widetilde{x}_t)}{r(\widetilde{x}_{t:t_+})},$$

where $r(\widetilde{x}_{t:t_+})$ is the proposal distribution to generate the backward pilots. Taking expectation conditional on $\widetilde{x}_t$, we have

$$\begin{aligned}
\mathbb{E}(\widetilde{w}_t \,|\, \widetilde{x}_t) &= \int \cdots \int \frac{p(\widetilde{x}_{t+1:t_+}, I_{t+1:t_+} \,|\, \widetilde{x}_t)}{r(\widetilde{x}_t, \widetilde{x}_{t+1:t_+})} \, r(\widetilde{x}_{t+1:t_+} \,|\, \widetilde{x}_t) \, d\widetilde{x}_{t+1:t_+} \\
&= p(I_{t+1:t+}|\widetilde{x}_t)/r(\widetilde{x}_t),
\end{aligned}$$

where $r(\widetilde{x}_{t+1:t_+} \,|\, \widetilde{x}_t)$ and $r(\widetilde{x}_t)$ are the conditional distribution and the marginal distribution induced from $r(\widetilde{x}_{t:t_+})$, respectively. Therefore,

$$p(C_{t_+} \,|\, \widetilde{x}_{0:t}, C_t) = p(I_{t+1:t+}|\widetilde{x}_t) = r(\widetilde{x}_t)\mathbb{E}(\widetilde{w}_t \,|\, \widetilde{x}_t).$$

Again, we use the pilot samples $\big\{(\widetilde{x}_t^{(j)}, \widetilde{w}_t^{(j)})\big\}_{j=1,\cdots,m}$ to estimate $r(\widetilde{x}_t)$ and $\mathbb{E}(\widetilde{w}_t \,|\, \widetilde{x}_t)$ by nonparametric smoothing. A histogram estimator is

$$\begin{aligned}
\widehat{p}(I_{t+1:t+}|x_t) &= \widehat{r}(x_t)\widehat{\mathbb{E}}(\widetilde{w}_t \,|\, x_t) \\
&= \sum_{d=1}^{D} \frac{\sum_{j=1}^{m} \mathbb{I}\big(\widetilde{x}_t^{(j)} \in \mathcal{X}_d\big)}{m|\mathcal{X}_d|} \mathbb{I}\big(x_t \in \mathcal{X}_d\big) \cdot \sum_{d=1}^{D} \frac{\sum_{j=1}^{m} \widetilde{w}_t^{(j)} \mathbb{I}\big(\widetilde{x}_t^{(j)} \in \mathcal{X}_d\big)}{\sum_{j=1}^{m} \mathbb{I}\big(\widetilde{x}_t^{(j)} \in \mathcal{X}_d\big)} \mathbb{I}\big(x_t \in \mathcal{X}_d\big) \\
&= \sum_{d=1}^{D} \frac{\sum_{j=1}^{m} \widetilde{w}_t^{(j)} \mathbb{I}\big(\widetilde{x}_t^{(j)} \in \mathcal{X}_d\big)}{m|\mathcal{X}_d|} \mathbb{I}\big(x_t \in \mathcal{X}_d\big),
\end{aligned}$$

where $\mathbb{I}(\cdot)$ is the indicator function, $\mathcal{X}_1 \cup \mathcal{X}_2 \cup \cdots \cup \mathcal{X}_D$ is a partition of the support of x_t and $|\mathcal{X}_d|$ denotes the volume of $\mathcal{X}_d$.

Compared with the forward pilot method in Algorithm 2, the backward pilots here are generated backward, starting from the constrained time point t_+. The strong constraint I_{t_+} is automatically incorporated in the proposal distribution to generate $\widetilde{x}_{t_+}$ at the beginning. Hence it is often expected to have a more accurate estimate of $p(C_{t_+} \,|\, x_{0:t}, C_t) = p(I_{t+1:t_+} \,|\, x_t)$. However, it requires the system to be Markovian to apply this method.

This algorithm extends the backward pilot algorithm in Lin et al. (2010) for generating samples of diffusion bridges. This extension allows for more general constraint problems, including the cases that frequent (but weak) constraints exist between two rare and strong constraints. It also allows for more flexible constraints, instead of only the fixed point constraints considered in Lin et al. (2010).

Algorithm 3 : Backward Pilot Algorithm

- *Initialization: For* $j = 1, \cdots, m$, *draw samples* $\widetilde{x}_{t_2}^{(j)}$ *from a proposal distribution* $r(x_{t_2})$ *approximately proportional to* $p(I_{t_2} \mid x_{t_2})$ *and set* $\widetilde{w}_{t_2}^{(j)} = 1/r(\widetilde{x}_{t_2}^{(j)})$.

- *For* $t = t_2 - 1, \cdots, t_1 + 1$, *draw pilot samples backward as follows.*

  - *Generate samples* $\widetilde{x}_t^{(j)}$, $j = 1, \cdots, m$, *from a proposal distribution* $r(\widetilde{x}_t \mid \widetilde{x}_{t+1}^{(j)})$.

  - *Update weights by*

$$\widetilde{w}_t^{(j)} = \widetilde{w}_{t+1}^{(j)} \frac{p(\widetilde{x}_{t+1}^{(j)}, I_{t+1} \mid \widetilde{x}_t^{(j)})}{r(\widetilde{x}_t^{(j)} \mid \widetilde{x}_{t+1}^{(j)})}, \quad j = 1, \cdots, m.$$

  - *Let* $\mathcal{X}_1 \cup \cdots \cup \mathcal{X}_D$ *be a partition of the support of* x_t. *Estimate* $p(C_{t_+} \mid x_{0:t}, C_t) = p(\mathcal{I}_{t+1:t_+} \mid x_t)$ *by*

$$f_t(x_t) = \sum_{d=1}^{D} \eta_{t,d} \mathbb{I}\big(x_t \in \mathcal{X}_d\big), \tag{3.12}$$

    where $\eta_{t,d} = \frac{1}{m|\mathcal{X}_d|} \sum_{j=1}^{m} \widetilde{w}_t^{(j)} \mathbb{I}(\widetilde{x}_t^{(j)} \in \mathcal{X}_d)$, *and* $|\mathcal{X}_d|$ *denotes the volume of the subset* $\mathcal{X}_d$.

- *Return the estimated functions* $\Big\{\widehat{p}(C_{t_+} \mid x_{0:t}, C_t) = f_t(x_t)\Big\}_{t=t_1+1,\cdots,t_2-1}$ *to compute the priority scores to be used in Algorithm 1.*

4. Examples

In this section, we apply SMCc to several problems with different types of constraints in Appendix A. The first example (expected shortfall) belongs to the rare and strong constraint case with a strong constraint at the end; the second example (discretized diffusion process) belongs to the intermediate constraint case; and the last example (robotic control) is a stopping time problem.

For each problem, we compare feasible SMCc approaches with other SMC algorithms without using the proposed special design of priority scores. The acceptance-rejection sampling is abbreviated as Rejection. Conventional SMC algorithm with a manipulated drift is denoted as SMC-drift. We also abbreviate the SMCc approach using parametric function, the forward pilots or the backward pilots to approximate $p(C_{t_+}|x_{0:t}, C_t)$ by SMCc-PA, SMCc-FP or SMCc-BP, correspondingly. The system in the first example is not Markovian hence only SMCc-FP is used. For the other examples, it is more convenient to use SMCc-BP, since it is difficult to construct an effective proposal distribution for generating forward pilots to meet the end-point constraints, while the backward pilot generation is relatively easy to do. We will provide the details of specific implementations which may differ in different examples.

4.1 Long-Run Marginal Expected Shortfall

Measuring the systemic risk of a firm is important for risk management. Acharya et al. (2012) proposed to use the long-run marginal expected shortfall (LRMES) as a systemic risk index, which is defined as the expected capital shortfall of a firm during a financial crisis. Particularly, a financial crisis is defined when the market index falls by 40% in the next six months (126 trading days). Let $x_{m,t}$ and $x_{f,t}$ be the daily logarithmic prices of the market and the firm at time t, respectively. The LRMES of the firm is defined as (with $T = 126$)

$$\text{LRMES} = \mathbb{E}\big(1 - e^{x_{f,T} - x_{f,0}} \,|\, e^{x_{m,T} - x_{m,0}} < 60\%\big)$$

Following Brownlees and Engle (2012) and Duan and Zhang (2016), we assume that the bivariate process $(x_{m,t}, x_{f,t})$ follows a GJR-GARCH model as in Glosten et al. (1993). Particularly, the $(x_{m,t}, x_{f,t})$ process follows

$$\begin{bmatrix} x_{m,t} \\ x_{f,t} \end{bmatrix} = \begin{bmatrix} x_{m,t-1} \\ x_{f,t-1} \end{bmatrix} + \begin{bmatrix} \sigma^2_{m,t} & \rho_t \sigma_{m,t} \sigma_{f,t} \\ \rho_t \sigma_{m,t} \sigma_{f,t} & \sigma^2_{f,t} \end{bmatrix}^{1/2} \begin{bmatrix} \varepsilon_{m,t} \\ \varepsilon_{f,t} \end{bmatrix}, \tag{4.13}$$

where $[\cdot]^{1/2}$ stands for matrix square root, $\varepsilon_{m,t}$ and $\varepsilon_{f,t}$ are independent $N(0,1)$ innovations. The evolution law of the time varying covariance matrix in (4.13) is given in detail in Appendix B, along with the coefficient used in the simulation.

Without loss of generality, we set $x_{m,0} = x_{f,0} = 0$. In the following, we will use $p(\cdot)$ to denote the distribution law under model (4.13) with the parameters outlined in Appendix B. If we draw the sample paths $\{(x^{(i)}_{m,0:T}, x^{(i)}_{f,0:T}, w^{(i)}_T)\}_{i=1,\cdots,n}$ properly weighted with respect to the distribution $p(x_{m,1:T}, x_{f,1:T} \,|\, x_{m,0} = 0, x_{f,0} = 0, x_{m,T} < c)$ with $c = \log 0.6$, then the

LRMES can be estimated by $\sum_{i=1}^{n} w_T^{(i)}(1-e^{x_{f,T}^{(i)}})/\sum_{i=1}^{n} w_T^{(i)}$. Notice that

$$\begin{aligned} & p(x_{m,1:T}, x_{f,1:T} \,|\, x_{m,0}, x_{f,0}, x_{m,T} < c) \\ \propto\ & \mathbb{I}(x_{m,T} < c) p(x_{m,1:T}, x_{f,1:T} \,|\, x_{m,0}, x_{f,0}) \\ =\ & \mathbb{I}(x_{m,T} < c) \prod_{t=1}^{T} p(x_{m,t} \,|\, x_{m,0:t-1}) \prod_{t=1}^{T} p(x_{f,t} \,|\, x_{m,0:t}, x_{f,0:t-1}). \end{aligned}$$

Once we obtain a set of sample paths $\{(x_{m,0:T}^{(i)}, w_T^{(i)})\}_{i=1,\cdots,n}$ properly weighted with respect to the distribution $p(x_{m,1:T}, \,|\, x_{m,0}, x_{m,T} < c) \propto \mathbb{I}(x_{m,T} < c) \prod_{t=1}^{T} p(x_{m,t} \,|\, x_{m,0:t-1})$, the sample paths $\{x_{f,1:T}^{(i)}\}_{i=1,\ldots,n}$ can be easily drawn from $p(x_{f,1:T} \,|\, x_{m,0}, x_{m,1:T}^{(i)}, x_{f,0}) = \prod_{t=1}^{T} p(x_{f,t} \,|\, x_{m,0:t}, x_{f,0:t-1})$ using (4.13). Hence, here we focus on sampling $x_{m,0:T}$. We use Rejection, SMC-drift, SMCc-PA, and SMCc-FP to generate samples from the distribution $p(x_{m,1:T}, x_{f,1:T} \,|\, x_{m,0}, x_{m,T} < c)$. Their performances in estimating LRMES are compared. The implementation details are listed in Appendix B.

For fair comparison, the numbers of Monte Carlo samples in different methods are adjusted so that each method takes approximately the same CPU time. More specifically, we set the accepted sample sizes to $n = 5$ for the Rejection method, as the acceptance rate is about 0.0001. We use $n = 15,000, 12,000$ and $10,000$ for SMC-drift, SMCc-PA and SMCc-FP, respectively. SMCc-FP uses $m = 1,000$ forward pilots. In SMCc-PA and SMCc-FP, we perform resampling every 5 steps. Once $\{(x_{m,0:T}^{(i)}, w_T^{(i)})\}_{i=1,\cdots,n}$ is obtained, $x_{f,1:T}^{(i)}$ is sampled accordingly and the corresponding LRMES is estimated. The boxplots of 100 independent estimates of LRMES using different methods are reported in Figure 1. The horizontal line is the "true" LRMES estimated using 100,000 accepted samples generated by the rejection method. It shows that SMCc-FP performs the best under a fixed computational cost. Figure 2 plots 50 sample paths of $x_{m,0:T}$ generated using different methods (without weight adjustment). Note that the sample paths generated by Rejection exactly follow the true target distribution. The figures show that SMCc-FP can generate samples close to the true target distribution, with much less computational cost. The samples generated by SMC-drift and SMC-PA tend to have less diversity and move more aggressively towards the constraint region.

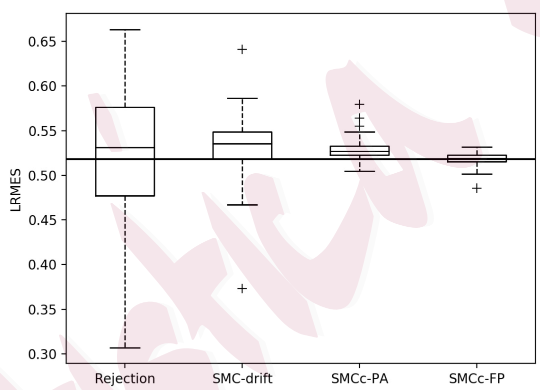

Figure 1: Boxplots of 100 independent estimates of LRMES using different methods. The horizontal line is the "true" LRMES estimated using 100,000 accepted samples generated by the rejection method.

4.2 A Diffusion System with Intermediate Noisy Observations

In this section, we conduct a simulation study with a system with periodic and intermediate constraints, corresponding to Case 3 in Appendix A. Consider a discretized diffusion process

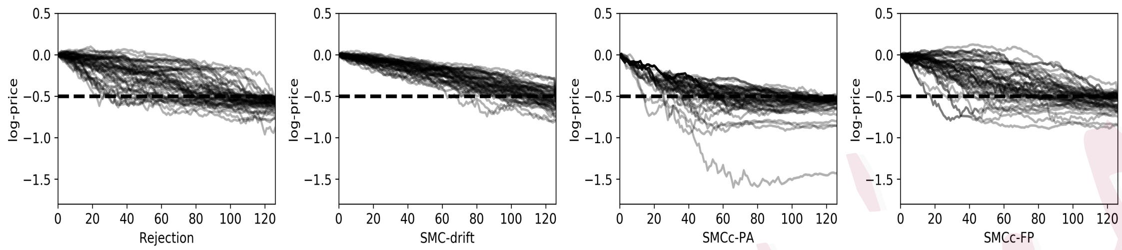

Figure 2: Sample paths of $X_{m,0:T}$ generated by different methods before weight adjustment. The horizontal line denotes a 40% price drop.

x_t governed by

$$x_t = x_{t-1} + \delta \sin(x_{t-1} - \pi) + \varepsilon_t, \tag{4.14}$$

where $\varepsilon_t \sim N(0, \delta)$, used in Beskos et al. (2006). It is a discretized version of the diffusion process $dX_\lambda = \sin(X_\lambda - \pi)d\lambda + dW_\lambda$, where W_λ is a standard Brownian motion, with step size δ. We take $\delta = 0.1$ in this example.

In this simulation study, two noisy observations of x_t are made at real times $T = 30$ and $T = 60$ (indices for x_t are $t = 30/\delta = 300$ and $60/\delta = 600$, respectively) with

$$Y_{30} \sim N(x_{30/\delta}, \sigma^2) \quad \text{and} \quad Y_{60} \sim N(x_{60/\delta}, \sigma^2).$$

We also fix the two endpoints at $x_0 = a$ and $x_{90/\delta} = b$. The discretized time points $T_0 = 0$, $T_1 = 30$, $T_2 = 60$ and $T_3 = 90$ are considered to be strong constraints. The SMCc-BP method is applied to generate sample paths of $x_{0:T}$ conditional on the constraints $(x_0, Y_{30}, Y_{60}, x_{90/\delta})$. We take equation (4.14) as the proposal distribution in generating forward paths. The backward pilots are generated from the proposal distribution

$r(\widetilde{x}_t \mid \widetilde{x}_{t+1}) \sim N\big(\widetilde{x}_{t+1} - \delta \sin(\widetilde{x}_{t+1} - \pi), \delta\big)$.

Note that this process shows a jump behavior among the stable levels at $x = 2k\pi$, $k = 0, \pm 1, \pm 2, \ldots$ (Lin et al., 2010). In this experiment, we set $x_0 = 0$, $Y_{30} = 6.49$, $Y_{60} = -5.91$ and $x_{90/\delta} = -1.17$, corresponding to the stable levels 0, 2π, -2π and 0, respectively. Since Y_{30} and Y_{60} differ by a gap of two stable levels, this is a very rare event.

Three levels of measurement errors for the observations Y_{30} and Y_{60} are investigated: $\sigma = 0.01$ for very accurate observations, $\sigma = 1.0$ for moderate accurate observations and $\sigma = 2.0$ for noisy observations. Note that in this experiment we fix the observations Y_{30} and Y_{60} but change the underlying assumption of their distributions to reflect strength of the constraints imposed by Y_{30} and Y_{60}. In each setting, a total of $5,000$ sample paths are generated, with 300 backward pilots to estimate the resampling priority scores. Figure 3 plots the generated sample paths before weight adjustment for each level of error. Figure 4 shows the histogram of the marginal samples of $x_{60/\delta}$ before weight adjustment, which is obtained from the generated sample set $\{x_{0:T}^{(i)}\}_{i=1,\cdots,n}$ without considering the weights. It can be seen that when the observations are accurate ($\sigma = 0.01$), the two observations act like fixed-point constraints that force all sample paths to pass through the observations. When the observation error is large ($\sigma = 2$), a high proportion of sample paths remains at the original stable level while only a small proportion of paths is drawn towards the observations. The marginal distributions of $x_{60/\delta}$ show clear differences in the above three cases. Samples from all three levels of error retain the jumping nature of underlying process and the SMCc-BP approach is capable of dealing with different levels of observational errors.

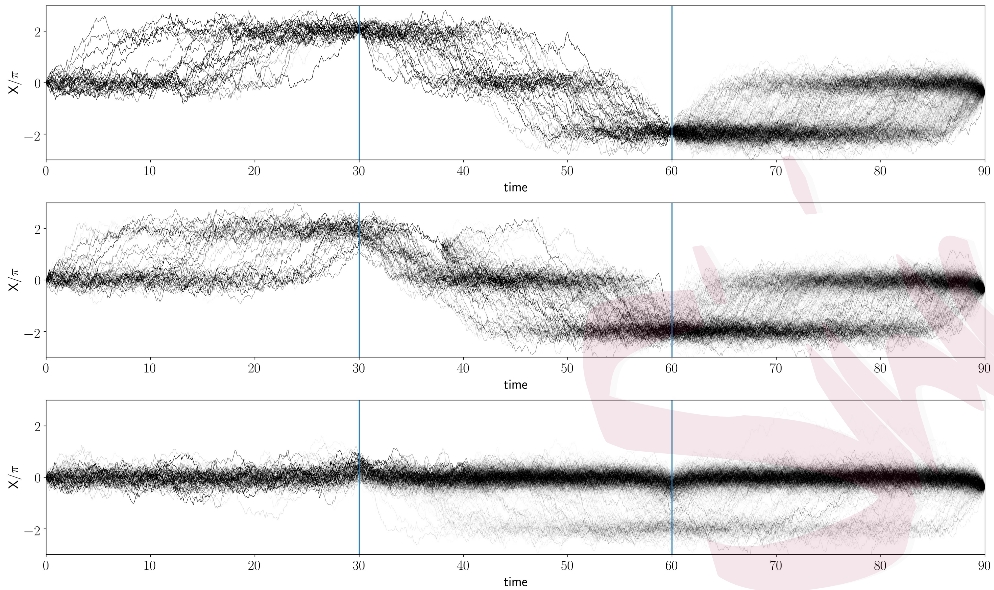

Figure 3: Sampled paths before weight adjustment for $\sigma = 0.01$ (top panel), $\sigma = 1.0$ (middle panel) and $\sigma = 2.0$ (bottom panel) when $x_0 = 0$, $Y_{30} = 6.49$, $Y_{60} = -5.91$ and $x_{90/\delta} = -1.17$.

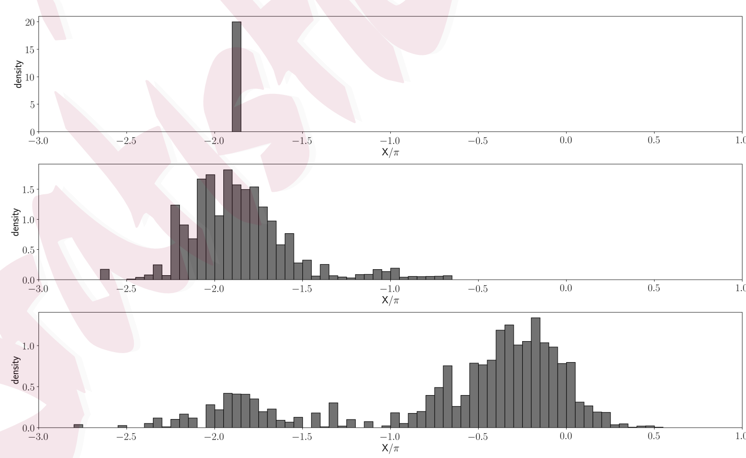

Figure 4: Histogram of the marginal samples of $x_{60/\delta}$ before weight adjustment for $\sigma = 0.01$ (top panel), $\sigma = 1.0$ (middle panel) and $\sigma = 2.0$ (bottom panel) when $x_0 = 0$, $Y_{30} = 6.49$, $Y_{60} = -5.91$ and $x_{90/\delta} = -1.17$.

4.3 Robotic Control

In this example, we consider a robotic control problem in a well-known mechanical system named "Acrobot" (Murray and Hauser, 1991), which consists of two arms of identical inertia and mass as demonstrated in the left panel of Figure 5. The two arms are only allowed to move in the vertical plane and its state is determined by a four dimensional vector $\boldsymbol{\theta} = (\theta_1, \theta_2, \dot{\theta}_1, \dot{\theta}_2)$, where θ_1 and θ_2 are the two angle positions as marked in Figure 5, and $\dot{\theta}_1, \dot{\theta}_2$ are their velocities, correspondingly. The system is controlled only through κ, the torque of an actuator at the joint of the two arms.

A common control task in robotics is to find a control sequence $\kappa_0, \kappa_1, \cdots$, following which a system starting at state $\boldsymbol{\theta}_0$ will reach the desired target state $\boldsymbol{\theta}_*$ as fast as possible (Spong, 1995; Perez et al., 2012; Duan et al., 2016). In our experiment, we set the starting state $\boldsymbol{\theta}_0 = (0, \pi/2, 0, 0)$ and the target state $\boldsymbol{\theta}_* = (0, -\pi/2, 0, 0)$, as shown in the middle panel and right panel of Figure 5, respectively.

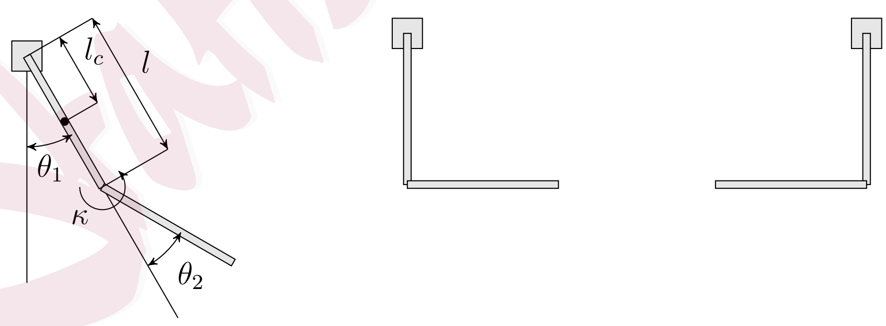

Figure 5: Acrobot with two arms (left panel), starting position $\boldsymbol{\theta}_0$ at $(0, \pi/2, 0, 0)$ (middle panel), and target position $\boldsymbol{\theta}_*$ at $(0, -\pi/2, 0, 0)$ (right panel) .

The detailed four-dimensional system of the Acrobot and its discretization to differential equations with a fixed time interval ($\delta = 0.02$ seconds) are shown in Appendix C. If we treat the control sequence κ_t as random innovations, then the problem of finding a sequence of controls to move the system from an initial state $\boldsymbol{\theta}_0$ to a fixed ending state θ_* becomes finding paths of a dynamic system with the end-point constraints. Here we assume that κ_t is independent over time and follows a uniform$[-5, 5]$ distribution. Note that κ_t can only provide a one-dimensional nonlinear control and takes values in a limited range. It is often a challenging problem to find the sequence of controls to reach the target state as the system is nonlinear, especially when the target position has zero velocity.

Let $x_0 = \boldsymbol{\theta}_0$ and define the target region be $\Gamma = \{x : \|x - \boldsymbol{\theta}_*\|_\infty \leq 0.01\}$, where $\|\cdot\|_\infty$ denotes the sup norm of a vector. The problem of finding a control sequence $\kappa_0, \kappa_1, \ldots$ that moves the system from $\boldsymbol{\theta}_0$ to $\boldsymbol{\theta}_*$ can be formulated to a constrained sampling problem as outlined in Case 5 of Appendix A.

We propose to use the (modified) SMCc-BP method outlined in Appendix D, where (C.19) is used for forward propagation and a resampling step is done with the priority scores $\beta_t^{(i)}$ in (D.22), which is estimated using backward pilots. The backward pilots $\{\widetilde{x}_{1:T}^{(j)}\}_{j=1}^m$ are generated backward from $\widetilde{x}_T^{(j)} = \boldsymbol{\theta}_*$, using

$$\widetilde{x}_{t-1}^{(j)} = \widetilde{x}_t^{(j)} - \widetilde{v}(\widetilde{x}_t^{(j)}, \widetilde{\kappa}_t)\delta,$$

where $\widetilde{\kappa}_t$ is drawn from a uniform$[-5, 5]$ distribution, and the function $\widetilde{v}(\cdot)$ is similar to $v(\cdot)$ in (C.20), but with δ replaced by $-\delta$.

In the simulation, we use $n = 10,000$ forward samples and $m = 5,000$ backward pilots for the SMCc-BP method, with $a = 0.1\delta$ in (D.21) and the maximum duration $T = 100$. The results are compared with the random search method using $n = 15,000$ samples. The sample trajectories from SMCc-BP and the random search method are plotted in Figure 6. The SMCc-BP found an "optimal" path that reaches the target state $\boldsymbol{\theta}_*$ at $t = 68$, corresponding to a total time of 1.36 seconds, shown by the black line in the left panel. On the other hand, the random search method was not able to find any paths close to $\boldsymbol{\theta}_*$ before time $T = 100$. Note that at $t = 50$, the "optimal" trajectory has a large velocity $\dot{\theta}_2 \approx -2\pi$ (the black line in the bottom figure in the left panel) to swing the second arm up to the target position. This state is quite far away from the target position, but was found and guided by the backward pilots. On the other hand, the simple random search does not have such information to use.

Figure 7 plots the minimum distance $\|x_t^{(j)} - \boldsymbol{\theta}_*\|_\infty$ of all the generated samples to the target state against time, under the SMCc-BP method and the simple random search method, respectively. We observed that the minimum distance at $t = 50$ obtained by the SMCc-BP method is much larger than that of the random search method. However, it seems to be necessary to allow the arms to gain velocity for θ_2 to move to the target quickly. Guided by the backward pilots, the SMCc-BP was able to find such a path. Then at $t = 68$, some of the SMCc-BP samples reach the target state.

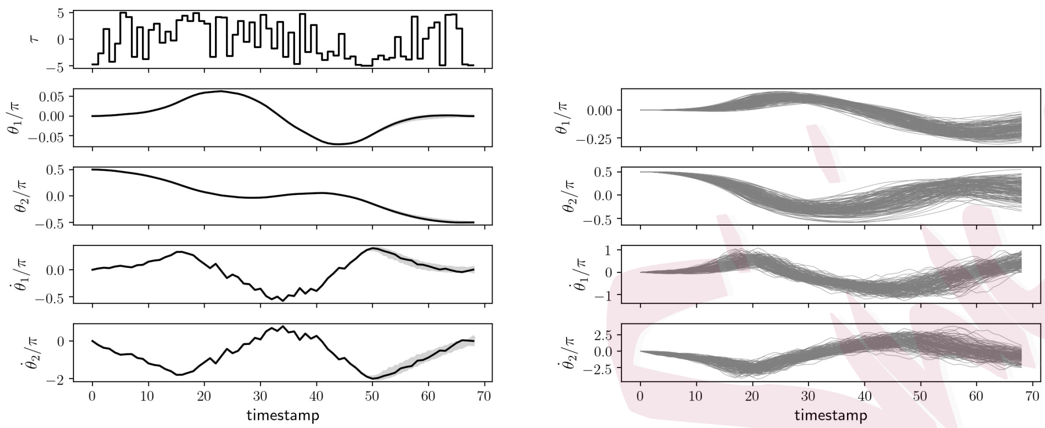

Figure 6: Left panel: Sample paths generated by the SMCc-BP method (in gray), with the "optimal" path (in black) that reaches the target state $\boldsymbol{\theta}_*$ at $t = 68$. The control sequence for the "optimal" path is on the top panel. Right panel: Sample paths generated by the random search method for $t = 0, 1, \cdots, 68$.

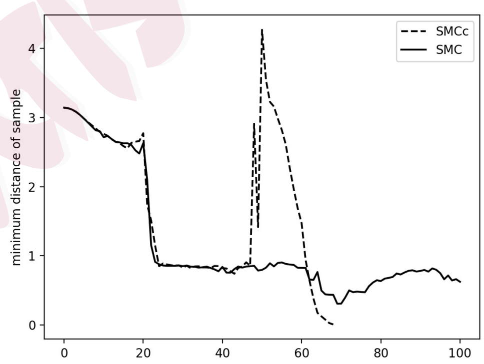

Figure 7: The minimum distance of the samples generated by the SMCc-BP method or the random search method (SMC) to the target state against time.

5. Summary

In this article we focus on the problem of generating (weighted) sample paths of a dynamic system with rare and strong constraints, under a SMC framework. There is a vast literature on SMC implementations on various problems and some algorithms and approaches can be used for constrained systems, though mostly on frequent and weak constraints such as the delayed approaches and fixed-lag smoothing algorithms in state space models, including the auxiliary particle filter (APF) of Pitt and Shephard (1999). We focus on generating the entire sample path from the joint distribution $x_{0:T}$, different from the typical filtering and smoothing problems that often mainly concern the marginal distributions. We also consider the problem that the objective is to reach a fixed target (constraint region) with a variable time duration – the stopping time problem. A systematic formulation of the problem is proposed by introducing a sequence of constraint events and their constraint strength measures. Under the guidance of three closely related distributions (the target, the compromised, and the propagation) induced under the system and a variable lookahead timescale, we introduce a resampling operation with optimal priority scores (resampling probabilities) for efficient operations. Two efficient approaches for approximating the needed optimal priority scores are developed, based on nonparametric smoothing technique using ensemble of forward pilots or backward pilots. The framework is general to encompass the earlier studies, and lays the foundation of further development of more efficient implementations of SMC in dealing with constrained dynamic systems. We show the effectiveness of the approach with several examples.

We note that our approach can be viewed as an extension of APF proposed in Pitt and Shephard (1999), the lookahead strategy of Chen et al. (2000) and Lin et al. (2013) and the iterated APF of Guarniero et al. (2016). These special SMC algorithms seek higher efficiency by incorporating future events and constraints in generating samples. For example, APF conducts resampling according to the priority score $\beta_t^{(i)} = w_t^{(i)} p(y_{t+1} \,|\, x_t^{(i)})$ (or its approximation). It corresponds to using $t_+ = t+1$ under SMCc framework for state space models, utilizing the observation y_{t+1}. In this paper we focus on sampling problems with rare and strong constraints.

The primary goal of the paper is on generating the entire sample path. It is essentially a smoothing problem. Because of the sequential nature of SMC, the inherited degeneracy problem cannot be avoided completely, especially as we rely on resampling scheme to deal with the constraints. The procedures of approximating the optimal priority scores at the very beginning of the sequential process help in improving the sample quality at the early stage, since these samples are designed to follow an approximation of the target smoothing distribution, instead of the filtering distribution. Experiments show that the SMCc approaches developed alleviate the degeneracy problem much better than simple implementations of SMC smoother.

The notation of conditional probability throughout the paper can be significantly simplified if the underlying dynamic system is Markovian such that $p(x_t, C_t \mid x_{0:t-1}, C_{t-1}) = p(x_t, C_t \mid x_{t-1}, C_{t-1})$. The proposed method in Section 3.1 also becomes simpler as the statistic $S(x_{0:t})$ can simply be chosen as $S(x_{0:t}) = x_t$.

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Appendix A. Some examples of the constrained problems

Case 1: Frequent constraints: In this case new constraints are imposed frequently on the system. For example, consider a state space model with state equation $x_t = f(x_{t-1}, \varepsilon_t)$ and observation equation $y_t = g(x_t, \epsilon_t)$, where ε_t and ϵ_t are random noises with known distributions. The observations y_t can be viewed as constraints imposed on the system. In this case we have a constraint at each time t, in the form $I_t = \{g(x_t, \epsilon_t) = y_t\}$ and the cumulative constraints $C_t = \{g(x_s, \epsilon_s) = y_s, s = 0, \cdots, t\}$. Using SMC to study state space models has been extensively studied with a vast literature, including the cases with small observation noises (ϵ_t with small variance), such as using the full information proposal distribution (Liu and Chen, 1998), the auxiliary particle filter (Pitt and Shephard, 1999), the independent particle filter (Lin et al., 2005) or certain short-range lookahead method (Lin et al., 2013). In this paper we do not focus on this frequent constraints case.

Case 2: Rare and strong constraints: In this case the constraints occur rarely, but with strong effect. For example, in the problem of generating diffusion bridge paths that connect two fixed endpoints $x_0 = a$ and $x_T = b$, the cumulative constraint events are $C_0 = \cdots = C_{T-1} = \{x_0 = a\}$ and $C_T = \{x_0 = a, x_T = b\}$. Then $p(x_{0:T} \mid C_{T-1}) = p(x_{0:T} \mid x_0 = a)$ and $p(x_{0:T} \mid C_T) = \delta_D(x_T - b)p(x_{0:T} \mid x_0 = a)/p(x_T = b \mid x_0 = a)$, where $\delta_D(\cdot)$ is the Dirac delta function. Hence $G(T) = \infty$, which indicates that $I_T = \{x_T = b\}$ is a strong constraint. If the constraint at T is not a fixed point, but a noisy measurement of x_T, then the strength of the constraint would depend on T and variance of the measurement error.

Case 3: Periodic and intermediate constraints: In certain systems we have noisy measurements of the unobservable states $x_{0:T}$ periodically. For example, let y_k be a sequence of noisy measurements at time $t_1, \ldots, t_K$. The intermediate observations split the whole path into K segments as shown in Figure 8. Again, the constraints strength depend on how frequent one observes the intermediate observations and how strong (or accurate) y_k's are.

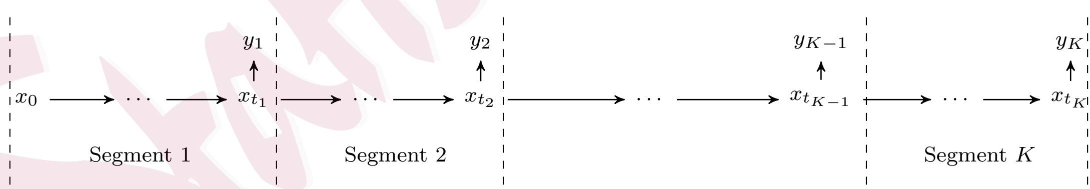

Figure 8: Segmentation of a stochastic process with intermediate observations.

Case 4. Multilevel Constraints: In some applications, there may exist multiple levels of constraints, including those with a hierarchical structure, such as one level of weak but frequent constraints and another level of strong but rare constraints. A special case is a standard state space model with two fixed endpoint constraints. Specifically, suppose a state space model is governed by the state dynamics $x_t = f(x_{t-1}, \varepsilon_t)$ and the observation equation $y_t = g(x_t, \epsilon_t)$. In addition, two fixed endpoint constraints are imposed on $x_{0:T}$ with $x_0 = a$ and $x_T = b$. The routine observations $y_1, \cdots, y_{T-1}$ can be viewed as a layer of weak constraints and the fixed point constraints are viewed as a layer of rare and strong constraints. Although $G(T)$ is still infinity here, this case is "easier" than that without the observations $y_1, \ldots, y_{T-1}$, if the observation sequence is "faithful" in the sense that it is based on one realization of the bridge $x_0 = a, x_1, \ldots, x_{T-1}, x_T = b$ (e.g. $y_t = x_t + \epsilon_t$). The observations $y_1, \ldots, y_{T-1}$ provide general guidance for the system to meet the endpoint constraint $x_T = b$.

Case 5. Constraints in stopping time problems: In the stopping time problems, we are often interested in generating sample paths that eventually reach a constrained set within a maximum duration T. Let

$$\tau = \min\left\{t \geq 0 : x_t \in \Gamma\right\} \tag{A.15}$$

be a stopping time, which is the first time that the process $\{x_0, x_1, \cdots\}$ reaches the constrained set Γ. The constraint of such problems is in the form of $C = \{x_{0:\infty} : \tau \leq T\}$. Note that C is a "global" constraint, which is different from the local constraints imposed on specific times as we discussed before. In the optimal stopping time problems, one would be interested in finding the "optimal path" that satisfies the constraint with the smallest stopping time τ. We show such an application in Section 4.3.

Appendix B. Detailed Information for the LRMES example in Section 4.1

The evolution of the covariance matrix in (4.13) follows two processes, one for the volatilities $(\sigma^2_{m,t}, \sigma^2_{f,t})$, and a different one for the correlation ρ_t. Specifically, given the initial values of $(\sigma_{m,1}, \sigma_{f,1}, \rho_1)$, and a realization of the innovation process $\{(\varepsilon_{m,t}, \varepsilon_{f,t})\}_{t=1,\ldots,T}$, the volatility process $(\sigma^2_{m,t}, \sigma^2_{f,t})$ used in (4.13) iteratively follows

$$\begin{aligned}
\sigma^2_{m,t} &= \omega_m + \left[\alpha_m + \gamma_m \mathbb{I}(\varepsilon_{m,t-1} < 0)\right](\sigma_{m,t-1}\varepsilon_{m,t-1})^2 + \beta_m \sigma^2_{m,t-1}, \\
\sigma^2_{f,t} &= \omega_f + \left[\alpha_f + \gamma_f \mathbb{I}(\varepsilon_{f,t-1} < 0)\right](\sigma_{f,t-1}\varepsilon_{f,t-1})^2 + \beta_f \sigma^2_{f,t-1},
\end{aligned} \tag{B.16}$$

for $t = 2, \ldots, T$. This is an asymmetric GARCH process taking into the account of the difference in positive or negative innovations (or shocks).

The time-varying correlation coefficient series $\{\rho_t\}$ follows a separate dynamic conditional correlation (DCC) model. Specifically, let

$$Q_t = \begin{bmatrix} \sigma^{*2}_{m,t} & \rho_t \sigma^*_{m,t}\sigma^*_{f,t} \\ \rho_t \sigma^*_{m,t}\sigma^*_{f,t} & \sigma^{*2}_{f,t} \end{bmatrix}$$

be a sequence of 2×2 covariance matrices. Using the same initial values of $\sigma_{m,1}, \sigma_{f,1}, \rho_1$, and the same realization of the innovation process $\{(\varepsilon_{m,t}, \varepsilon_{f,t})\}_{t=1,\ldots,T}$ as above, we let

$$Q_1 = \begin{bmatrix} \sigma^2_{m,1} & \rho_1 \sigma_{m,t}\sigma_{f,1} \\ \rho_1 \sigma_{m,1}\sigma_{f,1} & \sigma^2_{f,1} \end{bmatrix}$$

and

$$Q_t = (1 - \alpha_C - \beta_C)Q_1 + \alpha_C \begin{bmatrix} \sigma^*_{m,t-1}\varepsilon_{m,t-1} \\ \sigma^*_{f,t-1}\varepsilon_{f,t-1} \end{bmatrix} \begin{bmatrix} \sigma^*_{m,t-1}\varepsilon_{m,t-1} \\ \sigma^*_{f,t-1}\varepsilon_{f,t-1} \end{bmatrix}' + \beta_C Q_{t-1},$$

for $t = 2, \cdots, T$. Then we extract ρ_t from Q_t and use it in (4.13). We note that $\sigma^*_{m,t}$ and $\sigma^*_{f,t}$ in Q_t are different from $\sigma_{m,t}$ and $\sigma_{f,t}$ in (B.16) for $t > 1$. The simulation of the process (4.13) starts with setting the initial values and a realization of the innovations, then construct the covariance process and the $(x_{m.t}, x_{f,t})$ process.

To set parameters in (4.13) for our simulation, we apply the model to S&P500 index and the stock prices of Citigroup from January 2, 2012 to December 31, 2017. The maximum likelihood estimates of the parameters are $\omega_m = 3.35 \times 10^{-6}$, $\alpha_m = 3.35 \times 10^{-6}$, $\gamma_m = 0.152$, $\beta_m = 0.858$, $\omega_f = 4.22 \times 10^{-6}$, $\alpha_f = 0.0148$, $\gamma_f = 0.0542$, $\beta_f = 0.935$, $\alpha_C = 0.0755$, $\beta_C = 0.862$, $\sigma_{m,1} = 0.0113$, $\sigma_{f,1} = 0.03$, and $\rho_1 = 0.705$.

The detailed implementations of the Monte Carlo methods compared in this example are as follows:

[Rejection]: Samples are generated forward, following the distribution $p(x_{m,1:T} \mid x_{m,0})$ without considering the constraint. At the end, a sample is accepted if $x_{m,T} < c$.

[SMC-drift]: Samples are generated with a standard SMC implementation with a proposal distribution that includes a drift term, similar to that proposed by Durham and Gallant (2002). Specifically, the proposal distribution $q(x_{m,t} \mid x_{m,1:t-1})$ used follows

$$x_{m,t} = x_{m,t-1} + \frac{c}{T} + \sigma_{m,t}\varepsilon_{m,t}, \tag{B.17}$$

and the same evolution law of $\sigma_{m,t}$, with $\varepsilon_{m,t} \sim N(0,1)$ and $t = 1, \cdots, T-1$. Note that $c < 0$, we included a negative drift term $\frac{c}{T}$ in the proposal distribution to force $x_{m,t}$ towards the constraint region. At the end, the samples are weighted by $w_T^{(i)} = \mathbb{I}(x_{m,T}^{(i)} <$

$c) \prod_{t=1}^{T} p(x_{m,t}^{(i)} \,|\, x_{m,0:t-1}^{(i)}) / \prod_{t=1}^{T} q(x_{m,t}^{(i)} \,|\, x_{m,1:t-1}^{(i)})$.

[SMCc-PA]: Samples are generated using the SMCc method in Algorithm 1, with a parametric priority score function, with $t_+ = T$ for all t. The propagation equation (4.13) is used as the proposal distribution. The priority score used is $\beta_t^{(i)} = w_t^{(i)} \widehat{p}(x_{m,T} < c \,|\, x_{0:t}^{(i)})$ with $\widehat{p}(x_{m,T} < c \,|\, x_{0:t}^{(i)}) = \Phi\big(c; x_t^{(i)}, (T-t)\overline{\sigma}_m^2\big)$, where $\Phi(c; \mu, \sigma^2)$ is the CDF of $N(\mu, \sigma^2)$ evaluated at the value c and $\overline{\sigma}_m^2$ is the long-term average of $\sigma_{m,t}^2$.

[SMCc-FP] Samples are generated using the SMCc method with priority scores estimate based on forward pilots. All settings are similar to SMCc-PA, except that $p(C_T \,|\, x_{m,0:t}^{(i)}, C_t) = p(x_{m,T} < c \,|\, x_{m,0:t}^{(i)})$ is estimated by forward pilots. The model is not Markovian, but the statistic $S(x_{m,0:t}) = (x_{m,t}, \sigma_{m,t+1})$ can be used and satisfies (3.10). Furthermore, since $p(x_{m,T} < c \,|\, x_{m,t}, \sigma_{m,t+1}) = p(x_{m,T} - x_{m,t} < c - x_{m,t} \,|\, \sigma_{m,t+1})$, we estimate the conditional cumulative distribution function $p(x_{m,T} - x_{m,t} < \Delta \,|\, \sigma_{m,t+1})$, using a histogram estimator with partition $\mathcal{S}_\sigma = \cup_d \{0.005(d-1) < \sigma_{m,t+1} \leq 0.005d\}$.

In the above approaches (except Rejection), we force the samples to satisfy the constraint $x_{m,T} < c$ in the last step, by letting $x_{m,T}^{(i)} \sim N(x_{m,T-1}^{(i)}, \sigma_T^{2(i)})$ truncated on $(-\infty, c)$, and updated their importance weight accordingly.

Appendix C. Dynamic system of Acrobot used in Section 4.3

The dynamics of Acrobot can be described by the following differential equation.

$$\begin{bmatrix} \dot{\theta}_1 \\ \dot{\theta}_2 \\ \ddot{\theta}_1 \\ \ddot{\theta}_2 \end{bmatrix} = \xi(\boldsymbol{\theta}, \kappa) := \begin{bmatrix} \dot{\theta}_1 \\ \dot{\theta}_2 \\ \frac{d_{22}(u_1 - c_1 - g_1) - d_{12}(u_2 - c_2 - g_2)}{d_{11}d_{22} - d_{12}d_{21}} \\ \frac{d_{11}(u_2 - c_2 - g_2) - d_{21}(u_1 - c_1 - g_1)}{d_{11}d_{22} - d_{12}d_{21}} \end{bmatrix}, \tag{C.18}$$

with

$$\begin{aligned}
d_{11} &= I_1 + I_2 + 2m_0 l_c^2 + m_0 l^2 + 2m_0 l l_c \cos\theta_2, \\
d_{22} &= I_2 + m_0 l_c^2, \\
d_{12} &= d_{21} = I_2 + m_0 l_c^2 + m_0 l l_c \cos\theta_2, \\
c_1 &= -m_0 l l_c \dot{\theta}_2^2 \sin\theta_2 - 2m_0 l l_c \dot{\theta}_1 \dot{\theta}_2 \sin\theta_2, \\
c_2 &= m_0 l l_c \dot{\theta}_1^2 \sin\theta_2, \\
g_1 &= m_0(l + l_c) g \cos\theta_1 + m_0 l_c g \cos(\theta_1 + \theta_2), \\
g_2 &= m_0 l_c g \cos(\theta_1 + \theta_2), \\
u_1 &= -\mu\dot{\theta}_1, \\
u_2 &= \kappa - \mu\dot{\theta}_2,
\end{aligned}$$

where m_0, l, l_c are the mass, length and distance between the center of mass and pivot for both arms correspondingly, I_1 and I_2 are their moments of inertia, μ is the friction coefficient, and g is the acceleration of gravity. We set $m_0 = 1.0$, $l = 1.0$, $l_c = 0.5$, $I_1 = I_2 = \frac{1}{12}$ and

$g = 9.8$ as in the international standard of units.

We discretize the time with interval length $\delta = 0.02$ seconds and let $x_t = \boldsymbol{\theta}_{t\delta} = (\theta_{t\delta,1}, \theta_{t\delta,2}, \dot{\theta}_{t\delta,1}, \dot{\theta}_{t\delta,2})$. Using the fourth order Runge-Kutta method (DeVries and Wolf, 1994), we approximate the equation (C.18) by a discrete-time model as follows.

$$x_t = x_{t-1} + v(x_{t-1}, \kappa_{t-1})\delta, \tag{C.19}$$

where $v(x_{t-1}, \kappa_{t-1}) = (v^{(1)} + 2v^{(2)} + 2v^{(3)} + v^{(4)})/6$ with

$$\begin{aligned} v^{(1)} &= \xi(x_{t-1}, \kappa_{t-1}), \\ v^{(2)} &= \xi(x_{t-1} + v^{(1)}\delta/2, \kappa_{t-1}), \\ v^{(3)} &= \xi(x_{t-1} + v^{(2)}\delta/2, \kappa_{t-1}), \\ v^{(4)} &= \xi(x_{t-1} + v^{(3)}\delta, \kappa_{t-1}), \end{aligned} \tag{C.20}$$

where $\xi(\cdot)$ is in (C.18) and κ_t is the torque imposed at time $t\delta$.

Appendix D. Formulation of the Acrobot example as a constrained problem

The Acrobot problem is a typical example of Case 5 in Appendix A. As a stopping time problem, a standard rejection sampling procedure would generate $x_0, x_1, \cdots$ using the forward propagation equation until the sample path reaches the target region Γ before the maximum duration time T. This approach may not be efficient as the probability to reach Γ before T could be extremely small. To find the shortest sample path to reach Γ, we consider SMCc in Algorithm 1 with certain modification as follows. To find the shortest sample path to reach Γ, we consider generating sample paths properly weighted with respect to the target distribution

$$\pi_T(x_{0:T}) \;\propto\; p(x_{0:T}\,|\,C)\,e^{-a\tau} \propto p(x_{0:T})\mathbb{I}(\tau \le T)\,e^{-a\tau}, \tag{D.21}$$

where τ is the stopping time defined in (A.15), $C = \{\tau \le T\}$ and $\mathbb{I}(\cdot)$ is an indicator function. Here an additional term $e^{-a\tau}$, $a > 0$, is added to the target distribution to encourage faster stopping. Set the intermediate target distribution as

$$\tilde{p}_t(x_{0:t}) = p(x_{0:t}), \quad t < T,$$

and let $p_t^+(x_{0:t}) = \pi_T(x_{0:T})$. Similar to (2.8), to effectively generated properly weighted samples with respect to $\pi_T(x_{0:T})$, the optimal priority score in SMCc is

$$\begin{aligned}
\beta_t \;&=\; w_t\,\frac{p_t^+(x_{0:t})}{\tilde{p}_t(x_{0:t})} \propto w_t\,\frac{\int p(x_{0:T})\mathbb{I}(\tau \le T)e^{-a\tau}\,dx_{t+1:T}}{p(x_{0:t})} \\
&=\; w_t\,\mathbb{E}\big[\mathbb{I}(\tau \le T)\,e^{-a\tau}\,|\,x_{0:t}\big]
\end{aligned}$$

In implementation, when a sample path $x_{0:t}^{(i)}$ reaches the target region Γ, it is "accepted" without further propagation.

Now we discuss how to approximate the term $E\big[\mathbb{I}(\tau \le T)\,e^{-a\tau}\,|\,x_{0:t}\big]$. Since the state sequence is a homogeneous Markovian process, that is, $p(x_t\,|\,x_{0:t-1}) = p(x_t\,|\,x_{t-1}) = p(x_1\,|\,x_0)$, β_t can be estimated using the backward pilots as in Algorithm 3, with $t_1 = 0$, $t_2 = T$, $I_T = \{x_T \in \Gamma\}$ and $I_t = \Omega$ for $t < T$. Particularly, we use

$$\beta_t^{(i)} = w_t^{(i)} f_t(x_{0:t}^{(i)}) \tag{D.22}$$

with

$$f_t(x_{0:t}) = \begin{cases} e^{-\tau}, & \text{if } \tau(x_{0:t}) \le t; \\ \sum_{d=1}^{D} \eta_{t,d} \mathbb{I}\big(x_t \in \mathcal{X}_d\big), & \text{if } \tau(x_{0:t}) > t, \end{cases}$$

where

$$\eta_{t,d} = \sum_{s=t}^{T-1} \left[\frac{1}{m|\mathcal{X}_d|} \sum_{j=1}^{m} e^{-a(t+T-s)} \widetilde{w}_s^{(j)} \mathbb{I}(\widetilde{x}_s^{(j)} \in \mathcal{X}_d) \right].$$

Here $\frac{1}{m|\mathcal{X}_d|} \sum_{j=1}^{m} e^{-a(t+T-s)} \widetilde{w}_s^{(j)} \mathbb{I}(\widetilde{x}_s^{(j)} \in \mathcal{X}_d)$ is an approximation of $\mathbb{E}\big[\mathbb{I}(\tau = t+T-s)\, e^{-a\tau} \,|\, x_{0:t}\big]$ if $\tau(x_{0:t}) > t$.

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