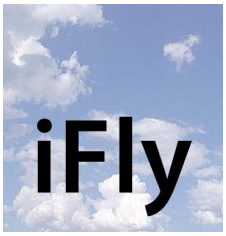

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iFly

Safety, Complexity and Responsibility based design and validation of highly automated Air Traffic Management

Specific Targeted Research Projects (STREP)

Thematic Priority 1.3.1.4.g Aeronautics and Space

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Authors: N. Kantas (UCAM)**, J.M. Maciejowski** (UCAM)

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	J.M. Maciejowski	UCAM	
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Trans-dimensional Simulation for Rare Events Estimation on Stochastic Hybrid Systems

Nikolas Kantas and Jan Maciejowski
Control Group,
Department of Engineering,
University of Cambridge,
Trumpington Street,
Cambridge, CB2 1PZ, UK
{nk234,jmm}@eng.cam.ac.uk

Abstract

In this deliverable we shall consider the problem of rare event simulation on stochastic hybrid processes. We will discuss how a Sequential Monte Carlo samplers formulation of the existing Interacting Particle System algorithm found in [14] can be implemented and how this can benefit from a trans-dimensional Markov Chain Monte Carlo simulation step, in order to achieve rare events estimators of lower variance. The aim is to achieve a simulation speed-up eventually by using less particles that explore the state space more efficiently in areas of lower probabilities.

Contents

List of Acronyms

CLT **C**entral **L**imit **T**heorem

FK **F**eynman **K**ac

IPS **I**nteracting **P**article **S**ystem

IS **I**mportance **S**ampling

MC **M**onte **C**arlo

MCMC **M**arkov **C**hain **M**onte **C**arlo

MH **M**etropolis **H**astings

PF **P**article **F**ilter

RJ **R**eversible **J**ump

RJMCMC **R**eversible **J**ump **M**arkov **C**hain **M**onte **C**arlo

RM **R**esample **M**ove

SMC **S**equential **M**onte **C**arlo

1 Introduction

In this deliverable we shall consider the problem of using rare events simulation for a continuous time stochastic hybrid process in the context of estimating conflicts or collision risk. We will entirely focus on the methodological aspects when Sequential Monte Carlo (SMC) [16, 17, 23] is used to estimate the risk factors of the continuous state part enters some rare set, which represents the collision or conflict. As much work has been done on implementing generic SMC algorithms for the particular application, [9, 12, 8] we shall propose an algorithmic setting that can be used in the same context and for the present not discuss any consideration regarding the application.

In the applied probability literature, particle implementations of genealogical and branching interacting processes, which admit a Feynman-Kac (FK) flow representation [16], have been used to estimate low probabilities ($\sim 10^{-10}$ or less) in [20] and [21] respectively. In Cérou et al [14] these results have been generalised for the case of using strong Markov continuous time processes. The authors present a generic Interacting Particle System algorithm (IPS), prove convergence and provide a Central Limit Theorem (CLT).

The generic algorithm of [14] has been extended for stochastic hybrid systems in [28, 29] by employing advanced Importance Sampling (IS) techniques. These extensions have been applied successfully at complex Air Traffic Management problems in [9, 11]. In this deliverable we aim to give a SMC samplers interpretation of the methodology found in [14], which has first appeared in [27] and propose a suitable extension, which uses a reversible jump Markov Chain Monte Carlo (MCMC) simulation step [25, 24]. Although the algorithm we propose is essentially different than [14], the computational tools developed in [11, 9, 28, 29] can be trivially reapplied. Therefore, this alternative algorithm will be easy to implement and applied at the same complex Air Traffic Management problems.

In the context of iFly objectives this deliverable contains extensions and modifications of the algorithm proposed in iFly deliverable D7.2e [10], so that trans-dimensional MCMC simulation can be used along with the IPS algorithm of D7.2e [10]. Although in our approach we shall use a slightly different framework based on SMC samplers [17, 18] and propose an alternative problem formulation so that MCMC steps can be implemented, we emphasise that the specific routines and methodological developments D7.2e [10] can be reapplied trivially.

The organisation of the rest of the deliverable shall be as follows. In Section 2 the basic principles of using Sequential Monte Carlo Samplers for rare event estimation are discussed. In Section 3 we formulate the problem and in Section 4 we propose a generic algorithmic solution. In Section 5 we discuss specific implementation issues related to stochastic hybrid systems and in Section 6 we outline some open research issues. Finally, in Section 7 we provide a few concluding remarks.

2 SMC Samplers for Rare Events Simulation

In this section we shall briefly describe the basic principles of using Sequential Monte Carlo Samplers for rare event estimation. The ideas we propose are based on the work in [27]. We shall not present any details on the general SMC samplers methodology, as this lies beyond the scope of this deliverable, but instead highlight the basic features of the approach. We refer the interested reader to [17] and [18] for a complete treatment on the topic.

In order to obtain estimates of the probability of a rare event, we will define a sequence of distributions defined over the same path space of an appropriate discrete time Markov process. Note that this formulation is slightly different to traditional SMC algorithms found in [23] and are also known as Particle Filters (PF) in the context of optimal state estimation, where inference is performed recursively on spaces of increasing dimension. The difference lies in that rhe first of the distributions corresponds to the law of the Markov chain up to a stopping time and subsequent distributions are distorted according to a sequence of indicator function potentials, which ultimately cause the distributions of the path to concentrate their mass on the rare events of interest. This iterative approach makes it possible to obtain weighted samples with weights of low variance from the target distribution from which it would otherwise be extremely difficult to sample. Then, we can estimate the rare event probabilities as estimates of the normalisation constants via SMC.

The SMC samplers approach can improve the sample diversity dramatically relative to that of the samples obtained by methods which iteratively extend the path and apply importance resampling in the context of [23]. This is due to the well known degeneracy of the resampling step, which after a few iterations causes the particle samples to become more dependent to a very small set of particles or even a single particle instead of most of the population at the beginning of the path. The result is that after a few iterations the particle approximation of the path tends to deteriorate and the variance increases in a geometric rate. In the context of static parameter estimation this is well explained in [2] and in the context of rare event simulation one can refer to [20]. Furthermore, as noted by [3], if the transition kernel of the Markov chain admits heavy tails, then rare events are likely to be driven by single large shocks rather than an accumulation of small ones and, therefore working on the path space is likely to produce much better results in such setting.

The law of the Markov process up to a stopping time is a trans-dimensional distribution since the dimension of the state of interest is itself a random variable. The general framework for trans-dimensional problems has been presented in the seminal work of P.J. Green in [25],[24] and a popular computational approach is that of reversible jump Markov Chain Monte Carlo simulation (MCMC). In this deliverable, we aim to provide a straight forward extension to the work of [27], by presenting appropriate trans-dimensional Metropolis-Hastings (MH) kernels that can explore the space of varying dimension.

3 Problem Formulation

3.1 Dynamical Model

Consider the bivariate stochastic process $\{Y_t\} = \{(X_t, \Theta_t)\}_{t\in\mathbb{R}_+}$ defined on a complete stochastic basis $(\Omega, \mathcal{F}, \mathbb{F}, \mathbb{P}, \mathbb{T})$ with $(\Omega, \mathcal{F}, \mathbb{P})$ being a complete probability space, and $\mathbb{F}$ being a right continuous filtration, i.e. a increasing sequence of sub-σ-algebras of $\mathcal{F}$. Let also $(x_t, \theta_t) \in E'$, where $E' = \mathbb{R}^{d_x} \times \mathbb{M}$, with $\mathbb{M}$ being a finite discrete set and denote $\mathcal{E}' = \mathcal{B}(E')$ as the Borel σ-algebra of E'. We will assume that $\{(X_t, \Theta_t)\}_{t\in\mathbb{R}_+}$ is a switching diffusion varying according to

$$dX_t = a(X_t, \Theta_t)dt + b(X_t, \Theta_t)dW_t, \quad (1)$$

$$P_{\theta_{t+\delta|\theta_t, x_t}}(\theta|\Theta_t = \eta, X_t = x) = \lambda_{\eta\theta}(x)\delta + o(\delta), \quad \forall \eta \neq \theta \quad (2)$$

where W_t is a Wiener process in $\mathbb{R}^{d_x}$ independent of $\{\Theta_t\}_{t\in\mathbb{R}_+}$ and the initial condition (x_0, θ_0) can be both deterministic or distributed according to $\eta_0 \times \mu_0$.
Assumption (A1) *We will assume that η_0, μ_0, a, b, $\lambda_{i,j}$ are such that (1-2) admits an a.s. pathwise unique solution and $\{Y_t\}$ is a strong Markov process.*

This stochastic hybrid model was adopted in the work of [28] and [29], and in the references within one can find conditions on $\eta_0, \mu_0, a, b, \lambda_{i,j}$ for which (A1) is true.

3.2 Advanced Sampling Methods for Stochastic Hybrid Systems

In practice in order to sample from $\{Y_t\}$ one can adopt various sampling schemes. For the diffusion a popular choice for dicretising in time is the Euler discretisation

$$x_{t_{j+1}} = x_{t_j} + a(x_{t_j}, \theta_{t_j})h + b(x_{t_j}, \theta_{t_j})(W_{t_{j+1}} - W_{t_j}),$$

where $W_{t_{j+1}} - W_{t_j} \sim \mathcal{N}(0, t_{j+1} - t_j)$. In [12] the authors implement this for the algorithm of [14] to solve a complex Air Traffic Management problem, where the aircrafts were modelled according to *(1-2)*. The authors noted that a naive implementation might suffer in the case of rare switchings between the modes of θ. In [28] they proposed a solution by sampling a fixed number of particles for each mode and using an Importance Sampling (IS) estimator with a proposal that admitted more frequent switchings. This solution was further refined in [11] and [29] by employing a Rao-Blackwellised approach and using IS proposals whose discrete part consisted of an aggregation mode process of smaller discrete state space. This was further refined in [9] with the use of importance switching for the aggregation process. A summary of these refinements can be found in iFly deliverable D7.2e [10].

Although we will not present this sampling approach here, throughout this deliverable we shall assume that it is possible to use the advanced sampling methods contained in these papers and especially in the most recent, [9]. Then we shall be able to simulate a discrete time inhomogeneous Markov chain $\{Y_n\}_{n\geq 0} = \{(X_n, \Theta_n)\}_{n\in\mathbb{N}_+}$ that approximates $\{Y_t\}_{t\in\mathbb{R}_+}$ consistently with respect to the size of the discretisation intervals. In addition, for the discrete Markov chain $\{Y_n\}_{n\geq 0}$ we will use the same initial distribution $\eta_0 \times \mu_0$ as for the continuous time process $\{Y_n\}_{n\geq 0}$.

We do not require that $\{Y_n\}_{n\geq 0}$ should be sampled directly from the law of the Markov chain. This could be done indirectly using Importance Sampling proposals assuming that the likelihood ratios involved are well defined. For the rest of this deliverable we will be using mostly $\{Y_n\}_{n\geq 0}$ instead of its continuous time counterpart, but having said this we emphasise that this does not alter the underlying methodology critically and was this choice was adopted for the sake of simplicity.

3.3 Trans-dimensional Rare Event description

For notational convenience, let $E = \mathbb{R}^{d_x}$ and $\mathcal{E} = \mathcal{B}(\mathbb{R}^{d_x})$. We will consider the rare events corresponding to the probability that the continuous part $\{X_t\}_{t\in\mathbb{R}_+}$ of the Markov process $\{Y_t\}_{t\in\mathbb{R}_+}$ enters some rare set, $\mathcal{T} \subset E$, before it next enters some recurrent set, $\mathcal{R}$,

$$\mathbb{P}_{\eta_0}(X_\tau \in \mathcal{T}),$$

where the stopping time τ is defined as

$$\tau = inf\{s \in \mathbb{N}_+^* : X_s \in \mathcal{R} \cup \mathcal{T}\}.$$

The set $\mathcal{R}$ is assumed to be a recurrent set and we also assume that $\mathcal{R} \cap \mathcal{T} = \emptyset$. This construction is required only to make the stopping time τ almost surely finite, [31]. This framework corresponds to the classes of problems considered in [14, 15]. Note that in the case where $s \in \mathbb{R}_+^*$ we obtain a similar definition of τ for the continuous time process. Although in this paper we shall not explicitly deal with this case, the continuous time problem formulation is very similar.

Here we illustrate that it is possible to employ our approach for solving the same class of problem as the various multi-level splitting algorithms. We employ a Feynman-Kac formulation which is very different to that used by [14]. In our case the flow is entirely synthetic, whereas the evolution of the flow is fundamentally related to the dynamical structure of the chain of interest in the previously proposed algorithm by [14].

We are interested in the possible paths of $\{X_{0:p}\}_{p\geq 0}$, which is the continuous part of the discrete time Markov chain path $\{Y_{0:p}\}_{p\geq 0}$, starting somewhere in the support of η_0 and then evolving according to the law of $\{Y_n\}_{n\geq 0}$ until X_τ eventually intersects with $\mathcal{R} \cup \mathcal{T}$. Assuming these paths of interest exist, let F be the space defined as

$$F = \bigcup_{p=2}^{\infty} \{p\} \times \ supp(\eta_0) \times \ (E\backslash(\mathcal{R} \cup \mathcal{T}))^{p-1} \times \ \mathcal{R} \cup \mathcal{T},$$

where $supp(\psi)$ denotes the support of a measure ψ and for notational convenience we assume that the support of the initial distribution does not include either the rare set nor the recurrent set, i.e.

$$supp(\eta_0) \cap (\mathcal{R} \cup \mathcal{T}) = \emptyset.$$

It becomes apparent from this representation that computing $\mathbb{P}_{\eta_0}(X_\tau \in \mathcal{T})$ is

actually a trans-dimensional estimation problem since we have

$$\begin{aligned}\mathbb{P}_{\eta_0}(X_\tau \in \mathcal{T}) &= \mathbb{P}_{\eta_0}\left((\tau, X_{0:\tau}) \in F\right) \\ &= \sum_{p=2}^{\infty} \int_{E^p} \mathbb{P}_{\eta_0}(X_{0:p} \in dx_{0:p}) \mathbb{I}_{\mathcal{T}}(x_p) \prod_{s=0}^{p-1} \mathbb{I}_{E\setminus(\mathcal{R}\cup\mathcal{T})}(x_s),\end{aligned}$$

where we denote for any set B, the indicator function as $\mathbb{I}_B(x) = 1$ if $x \in B$ and $\mathbb{I}_B(x) = 0$ otherwise. Note that we are summing over trajectories $X_{0:p}$ of all possible lengths. Also, to simplify presentation from now on we shall drop the subscript of $\mathbb{P}$.

In common with many techniques for solving this problem, we employ a decreasing sequence of nested sets which concentrate themselves on the rare set of interest:

$$\mathcal{T} = \mathcal{T}_T \subset \mathcal{T}_{T-1} ... \mathcal{T}_2 \subset \mathcal{T}_1. \tag{3}$$

Our approach differs slightly in that we try to arrange these sets such that the majority of paths reaching $\mathcal{T}_k$ before $\mathcal{R}$ also reach $\mathcal{T}_{k+1}$ before $\mathcal{R}$. Essentially this means that the sets are somehow closer together than normal splitting approaches. For simplicity we construct a sequence of distributions which place all of their mass on one of these sets, although it is easy to extend this setting to situations in which other smoother potential functions instead of $\mathbb{I}_{\mathcal{T}}(x_p)$ are employed to produce better results as done in [20, 27]. We define our synthetic distributions[1] as

$$\begin{aligned}\pi_k(Y_{1:\tau_k} \in dy_{1:\tau_k}) &= \mathbb{P}(X_{1:\tau_k} \in dx_{1:\tau_k}, \Theta_{1:\tau_k} = \theta_{1:\tau_k} | X_{\tau_k} \in \mathcal{T}_k) \\ &= \frac{1}{Z_k} \mathbb{P}(X_{1:\tau_k} \in dx_{1:\tau_k}, \Theta_{1:\tau_k} = \theta_{1:\tau_k}, X_{\tau_k} \in \mathcal{T}_k),\end{aligned}$$

with the stopping times being

$$\tau_k = inf\{s : X_s \in \mathcal{T}_k \cup R\}$$

and the normalising constant

$$Z_k = \mathbb{P}(X_{\tau_k} \in \mathcal{T}_k).$$

Given that we are able to obtain samples from this sequence of distributions, we can obtain an estimate of the ratio of normalising constants. These can be done by recursively estimating the product of ratio of normalising constants.

4 Generic Algorithm

In this section we present the algorithm found in [27] as a path based reinterpretation of multi-level splitting using SMC samplers framework found in [17, 18]. The flexibility of this sampling scheme makes it possible to apply much more general sampling strategies. In the remainder of this deliverable we shall propose how the algorithm of [27] can include a reversible jump MCMC step and discuss how some advanced sampling strategies found in [11] and [29] can be incorporated to this approach.

[1] Note that are considering the part of the chain $\{Y_n\}$ for $n \geq 1$. This is a simplification ignores the effect of $\eta_0 \times \mu_0$ and considers that Y_0 as deterministic. This was done to simplify presentation and in practice is not a problem.

4.1 SMC Sampler algorithm of [27]

We will present an SMC algorithm that approximates π_k by a set of particles obtained by simulation. We denote the particle set at level k as $\Xi_k = \left\{\Xi_k^{(i)}\right\}_{i=1}^N$, where each particle $\Xi_k^{(i)} = \left(\tau_k^{(i)}, X_{1:\tau_k^{(i)}}^{(i)}, \Theta_{1:\tau_k^{(i)}}^{(i)}\right)$. Also, we refer to $\left\{W_k^{(i)}, \Xi_k^{(i)}\right\}_{i=1}^N$ as the weighted particle set, where $W_k^{(i)}$ is the weight of the i-th particle. At level k we will assume that $\left\{W_{k-1}^{(i)}, \Xi_{k-1}^{(i)}\right\}_{i=1}^N$ is available and the weighted particle set is updated recursively. The particle sets at each level can be thought of evolving through the following recursion:

$$\cdots \longrightarrow \Xi_{k-1} \overset{\text{resampling}}{\longrightarrow} \widehat{\Xi}_{k-1} \overset{\text{reversible jump}}{\longrightarrow} \widetilde{\Xi}_{k-1} \overset{\text{extend path}}{\longrightarrow} \Xi_k \longrightarrow \cdots$$

where $\widehat{\Xi}_{k-1}$, $\widetilde{\Xi}_{k-1}$ follow the same notation as Ξ_k.

To monitor the performance of the algorithm we define the effective sampling size (ESS) at level k:

$$ESS_k = \left(\sum_{i=1}^N \left(W_k^i\right)^2\right)^{-1},$$

where ESS_k is always less than N and can be interpreted as the number of perfect samples from the target distribution that would lead the same estimator variance.

We proceed by describing the algorithm as follows:

Algorithm 1 ***SMC Sampler for rare event simulation:***

`Initialise at` $k = 1$ `an ensemble of N weighted path-particles:`
for $i = 1, ...N$:

- `Sample the path` $\Xi_1^{(i)}$ `from the law of the discretised Markov chain until it hits either` $\mathcal{T}_1$ `or` $\mathcal{R}$`, at stopping time` $\tau_1^{(i)}$`, i.e.` $\Xi_1 = \left\{\tau_1^{(i)}, X_{1:\tau_1^{(i)}}^{(i)}, \Theta_{1:\tau_1^{(i)}}^{(i)}\right\}_{i=1}^N$.
- `Set` $W_1^{(i)} = \mathbb{I}_{\mathcal{T}_1}(X_{\tau_1^{(i)}}^{(i)})$
- `Normalise weights` $W_1^{(i)} = \frac{W_1^{(i)}}{\sum_{j=1}^N W_1^{(j)}}$

end for

`Proceed for k >` 1
for $k = 2, ..., T$:

1. `Resample from` $\left\{W_{k-1}^{(i)}, \Xi_{k-1}^{(i)}\right\}_{i=1}^N$ `if` $ESS_k < N_{thresh}$`, to obtain the weighted particle set` $\left\{\widehat{W}_{k-1}^{(j)}, \widehat{\Xi}_{k-1}^{(j)}\right\}_{j=1}^N$`, where` $\widehat{W}_{k-1}^{(i)} = \frac{1}{N}$ `and` $\Pr(j = \varphi(i)) = W_{k-1}^{(\varphi(i))}$`, where` $\varphi(i)$ `is determined from the resampling scheme. If resampling is not used, set` $\left\{\widehat{W}_{k-1}^{(i)}, \widehat{\Xi}_{k-1}^{(i)}\right\}_{i=1}^N = \left\{W_{k-1}^{(i)}, \Xi_{k-1}^{(i)}\right\}_{i=1}^N$.

2. Apply a reversible jump M-H kernel, $\widetilde{K}_{k-1}$, of invariant distribution π_{k-1} to each path-particle $\widehat{\Xi}_{k-1}^{(i)}$:
for $i = 1, ..., N$:
apply a reversible jump move to the i-th path-particle sample

$$\widetilde{\Xi}_{k-1}^{(i)} \sim \widetilde{K}_{k-1}(\widehat{\Xi}_{k-1}^{(i)}, \cdot).$$

end for

3. Extend the path if necessary until it hits either $\mathcal{T}_k$ or $\mathcal{R}$, at stopping time $\tau_k^{(i)}$ and reweight the particles:
for $i = 1, ..., N$:
I) Extend the i-th path-particle $\widetilde{\Xi}_{k-1}^{(i)}$ to get $\Xi_k^{(i)}$ as follows

$$\Xi_k^{(i)} \sim K_k(\widetilde{\Xi}_{k-1}^{(i)}, \cdot),$$

where $K_k(\widetilde{\Xi}_{k-1}^{(i)}, \Xi_k^{(i)})$ follows from simulating $\left(X^{(i)}_{\widetilde{\tau}_{k-1}^{(i)}+1:\tau_k^{(i)}}, \Theta^{(i)}_{\widetilde{\tau}_{k-1}^{(i)}+1:\tau_k^{(i)}}\right)$ using the transition law of the chain $\{Y_n\}_{n\geq 1}$ from time $\widetilde{\tau}_{k-1}^{(i)}$ to $\tau_k^{(i)}$ using $\left(\widetilde{X}^{(i)}_{\widetilde{\tau}_{k-1}^{(i)}}, \widetilde{\Theta}^{(i)}_{\widetilde{\tau}_{k-1}^{(i)}}\right)$ as the initial condition and then augmenting the new simulated path with the previous path $\left(\widetilde{X}^{(i)}_{1:\widetilde{\tau}_{k-1}^{(i)}}, \widetilde{\Theta}^{(i)}_{1:\widetilde{\tau}_{k-1}^{(i)}}\right)$.
II) Weight the particle ensemble using $W_k^{(i)} = \widehat{W}_{k-1}^{(i)} \mathbb{I}_{\mathcal{T}_k}(X^{(i)}_{\tau_k^{(i)}})$.
end for

III) Normalise weights $W_k^{(i)} = \frac{W_k^{(i)}}{\sum_{j=1}^{N} W_k^{(j)}}$.

end for
Estimate the quantity of interest as $p^{\bigstar} = \prod_{k=1}^{T} \widehat{Z}_k$ with $\widehat{Z}_k = \frac{1}{N} \sum_{i=1}^{N} W_k^{(i)}$.

Algorithm 1 is identical to the one found in [27] apart from step 2, which has been added. It has to be noted that resampling should be avoided if not necessary. This can be done by monitoring the effective sampling size (ESS) and resampling only when the ESS drops beneath a certain preset threshold, i.e. $ESS_k < N_{thresh}$. For example one could set $N_{thresh} = \frac{N}{2}$; for more details see [23]. In addition, we refer the reader to [22] for a comparison of various resampling schemes and to [30] for general details on the ESS and resampling.

For convenience we have assumed that K_k is the law of the discretised Markov chain conditioned upon hitting $\mathcal{T}_k$ before $\mathcal{R}$. One might wish to consider situations in which the proposal kernels, $\{K_k\}_{k\geq 1}$ are able to modify that part of the path which has been proposed thus far in addition to extending it. This can be relatively simple to accomplish, and simply leads to a slightly more complex weight expression. Similarly if an IS proposal were to be used the weights should be modified according to the Importance Ratio. In the interests of clarity we have presented only the simpler case here. IS will be discussed further in Section 5.1.

4.2 Generic Reversible Jump moves for $\widetilde{K}_k$

In the algorithm above $\widetilde{K}_k$ has been introduced to improve the sample diversity. In this section we shall describe how dimension-changing moves can be implemented by Reversible Jump Metropolis Hastings (MH) kernels $\widetilde{K}_k$. We remind the reader that the invariant distribution $\pi_k(Y_{1:\tau_k})$ of $\widetilde{K}_k$ depends explicitly on τ_k. We propose first to update each particle $\widehat{\tau}_k^{(i)}, \widehat{\Xi}_k^{(i)}$ conditional upon using a combination of birth, death and update moves using the reversible jump MCMC algorithm of [24, 25]. This is achieved using the following simple Metropolis-Hastings (MH) algorithm [32]. In contrast with presentation so far, we shall be using $Y^{(i)}_{1:\tau_k^{(i)}}$ to denote $\left(X^{(i)}_{1:\tau_k^{(i)}}, \Theta^{(i)}_{1:\tau_k^{(i)}}\right)$ for the sake of simplicity.

The procedure is as follows

Algorithm 2 ***Reversible Jump MCMC:***

1. `At level` k `we have the particle set` $\widehat{\Xi}_k = \left\{\widehat{\tau}_k^{(i)}, \widehat{X}^{(i)}_{1:\tau_k^{(i)}}, \widehat{\Theta}^{(i)}_{1:\tau_k^{(i)}}\right\}_{i=1}^{N}$

2. `for` $i = 1, ..., N$:
   `Sample` $u \sim U[0,1]$.

   - `if` $u \leq b_{\widehat{\tau}_k^{(i)}}$: `Carry out a birth move, set` $\widetilde{\tau}_k^{(i)} = \widehat{\tau}_k^{(i)} + 1$ `and insert a new state in the path of` $\widehat{Y}^{(i)}_{1:\widehat{\tau}_k^{(i)}}$ `to obtain` $\widetilde{\Xi}_k^{(i)}$, `where` $\widetilde{\Xi}_k^{(i)} = \left(\widetilde{\tau}_k^{(i)}, \widetilde{X}^{(i)}_{1:\widetilde{\tau}_k^{(i)}}, \widetilde{\Theta}^{(i)}_{1:\widetilde{\tau}_k^{(i)}}\right)$.
   - `elseif` $u \leq b_{\widehat{\tau}_k^{(i)}} + d_{\widehat{\tau}_k^{(i)}}$: `Carry out a death move, set` $\widetilde{\tau}_k^{(i)} = \widehat{\tau}_k^{(i)} - 1$ `and kill an existing state of the path of` $\widehat{Y}^{(i)}_{1:\widehat{\tau}_k^{(i)}}$ `to obtain` $\widetilde{\Xi}_k^{(i)}$.
   - `else: Carry out an update move, set` $\widetilde{\tau}_k^{(i)} = \widehat{\tau}_k^{(i)}$ `and generate an updated version of the path of` $\widehat{Y}^{(i)}_{1:\widehat{\tau}_k^{(i)}}$ `to obtain` $\widetilde{\Xi}_k^{(i)}$.

   `end for`

3. `Iterate step 2` κ `times for each new particle set.`

The birth, death and terms derived above can be thought of as ratios between the distribution over the newly proposed state of the chain and the current state. These terms must also ensure reversibility and the dimension-matching requirement for reversible jump MCMC, [24],[25]. In order to satisfy the detailed balanced condition one has to ensure that for any i, $b_i + d_i + u_i = 1$, where u_i is the update probability. For example, in practice one could set the birth and death probabilities such that $b_{\tau_k} = d_{\tau_k} = u_{\tau_k} = 1/3$. We will proceed by presenting this simple reversible jump method, by considering separately the birth, death, and update moves. We will be assuming that the current state of the Markov chain is targeting the invariant distribution $\pi_k(Y_{1:\tau_k})$ and

that appropriate proposal distributions $q_u(y,\cdot)$ and $q_b(\cdot)$ can be designed in the context of Section 3.2.

Birth move:

A birth move is carried out with probability $b_{\widehat{\tau}_k^{(i)}}$. The new candidate state is constructed by sampling a location uniformly in the interval $\{1,...,\widehat{\tau}_k^{(i)}\}$, i.e. $J \sim \mathcal{U}\{1,...,\widehat{\tau}_k^{(i)}\}$, and sampling $\widetilde{Y}^* \sim q_b(\cdot)$. The proposed candidate $(\widehat{\tau}_k^{(i)}+1, \widehat{Y}_{1:J-1}^{(i)}, \widetilde{Y}^*, \widehat{Y}_{J:\widehat{\tau}_k^{(i)}}^{(i)})$ is accepted with probability

$$\alpha_{birth} = min\{1, \frac{\pi_k(\widehat{Y}_{1:J-1}^{(i)}, \widetilde{Y}^*, \widehat{Y}_{J:\widehat{\tau}_k^{(i)}}^{(i)}) d_{\widehat{\tau}_k^{(i)}+1}}{\pi_k(\widehat{Y}_{1:\widehat{\tau}_k^{(i)}}^{(i)}) q_b(\widetilde{Y}^*) b_{\widehat{\tau}_k^{(i)}}}\}. \tag{4}$$

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Death move:

With probability $d_{\widehat{\tau}_k^{(i)}}$, we propose a death move; Sample $J \sim \mathcal{U}\{1,...,\widehat{\tau}_k^{(i)}\}$. The candidate state $(\widehat{\tau}_k^{(i)}-1, \widehat{Y}_{1:J-1}^{(i)}, \widehat{Y}_{J+1:\widehat{\tau}_k^{(i)}}^{(i)})$, is accepted with probability

$$\alpha_{death} = min\{1, \frac{\pi_k(\widehat{Y}_{1:J-1}^{(i)}, \widehat{Y}_{J+1:\widehat{\tau}_k^{(i)}}^{(i)}) q_b(\widehat{Y}_J) b_{\widehat{\tau}_k^{(i)}-1}}{\pi_k(\widehat{Y}_{1:\widehat{\tau}_k}^{(i)}) d_{\widehat{\tau}_k^{(i)}}}\}. \tag{5}$$

Update move:

With probability $1 - b_{\widehat{\tau}_k^{(i)}} - d_{\widehat{\tau}_k^{(i)}}$, we propose a standard fixed dimensional move where we could update all or a subset of the components $\widehat{Y}_{1:\widehat{\tau}_k^{(i)}}^{(i)}$ using Metropolis-Hastings or Gibbs moves. Blocking some of the variables can improve the mixing time of the Markov chain. In our simple Metropolis-Hastings scheme sample $J \sim \mathcal{U}\{1,...,\widehat{\tau}_k^{(i)}\}$ and then $\widetilde{Y}_J^* \sim q_u(\widehat{Y}_J^{(i)},\cdot)$ then the candidate $(\widehat{\tau}_k^{(i)}, \widehat{Y}_{1:J-1}^{(i)}, \widetilde{Y}_J^*, \widehat{Y}_{J+1:\widehat{\tau}_k^{(i)}}^{(i)})$ is accepted with probability

$$\alpha_{update} = min\{1, \frac{\pi_k(\widehat{Y}_{1:J-1}^{(i)}, \widetilde{Y}_J^*, \widehat{Y}_{J+1:\widehat{\tau}_k^{(i)}}^{(i)}) q_u(\widetilde{Y}_J^*, \widehat{Y}_J^{(i)})}{\pi_k(\widehat{Y}_{1:\widehat{\tau}_k^{(i)}}^{(i)}) q_u(\widehat{Y}_J^{(i)}, \widetilde{Y}_J^*)}\} \tag{6}$$

Under weak assumptions on the model, the Markov chain generated by this transition kernel will be irreducible and aperiodic and hence will generate asymptotically samples from the target distribution $\pi_k(Y_{1:\tau_k})$.

The proposed algorithm is related to the Resample Move (RM) algorithm in [4] and the one in [1] both used for parameter estimation. Compared to [4] our approach is different as it incorporates reversible jumps to enable variable dimension moves. Compared to [1] the difference of our algorithm lies in the problem formulation and application used it is used for. In this sense the drawbacks illustrated in [1] regarding the convergence of the algorithm are relevant only for estimating static parameters of state space models and for rare event estimation.

5 Implementation Details

This approach, which was initiated in [27], can be developed further. In particular, the sequence of distributions could be refined to make it more effective for the case of stochastic hybrid systems. More specifically practical considerations can lead to design of appropriate proposal distributions for both K_k and $\widetilde{K}_k$. In the previous section we presented the algorithm in a general format so that it can be used generically for a variety of dynamical models. In this section we we will consider the class of models defined by (1)-(2) and briefly explain how earlier work in D7.2e [10] can be reused in this setting.

5.1 Importance sampling and aggregation of modes

In the exposition of Algorithm 1 K_k was assumed to be the law of the discretised Markov chain conditioned upon hitting $\mathcal{T}_k$ before $\mathcal{R}$. In [11, 9, 28, 29] the authors use Importance sampling and Rao-Blackwellisation to account for large discrete state spaces and rare switchings that may be critical for the performance of a rare event estimator. The work in the previously mentioned papers is summarised in iFly deliverable D7.2e [10]. The same issues apply also for Algorithm 1 and implementing these extensions is part of specifically designing K_k and modifying the expression of the weights in step 3 II of Algorithm 1 accordingly.

We proceed by sketching how the improvements of D7.2e [10] can be incorporated in our approach. The methodology is almost identical. Steps 1-3 in Section 7 of D7.2e are essentially equivalent with a recursion of step 3 followed by step 1 of Algorithm 1. The only difference is that in our case we store and perform a recursion on the complete path $Y^{(i)}_{1:\tau_k}$ rather than the marginals $Y^{(i)}_{\tau_k}$ so that step 2 of Algorithm 1 can be implemented. Therefore if the Hierarchical Hybrid IPS is modified to store and propagate the complete genealogy of the particles and is then followed by Algorithm 2 we will obtain an approach equivalent to the one described in this deliverable.

Finally one might wish to consider situations in which the proposal kernels, $\{K_k\}_{k\geq 1}$ are able to modify that part of the path which has been proposed thus far in addition to extending it. This can be relatively simple to accomplish, and simply leads to a slightly more complex weight expression. For more details, see [10].

5.2 Designing the Reversible Jump-MH kernel $\widetilde{K}_k$

The main benefit of the RJMCMC move is to explore the path space of $Y_{1:\tau_k}$ both in time and in space so that the particles stay in more promising regions, where the transitions between level sets can be made more likely. In Section 4.2 we presented RJMCMC in the most generic way. Here we will provide recommendations for designing q_b, q_u both for the presented general case as well as for the specific problem of rare event estimation after taking into account some practical considerations.

5.2.1 Generic case: exploring the path space of $Y_{1:\tau_k}$

In the update step of Algorithm 2 the approach is as in traditional MCMC rejuvenation moves presented in [4] for parameter estimation. In [4] the authours

propose an algorithm like Algorithm 1 to perform joint filtering of fixed and varying parameters, where $\widetilde{K}_k$ consisted only of the update step (i.e. there were no transdimensional birth and death moves). This is known in the literature as the Resample Move (RM) Particle Fiter (PF). With reference to our problem, the purpose of q_u is to modify the trajectory of $\widehat{Y}_{1:\tau_k}^{(i)}$ by proposing moves in $(E')^{\tau_k}$ so that an accepted change can bridge the gap between π_k and π_{k+1} by propagating at level $k+1$ a more diverse particle population. For the context of rare events estimation this means that the previous simulated path $\widehat{Y}_{1:\tau_k}^{(i)}$ is modified so that at level $k+1$ the probability of the particles reaching $\mathcal{T}_{k+1}$ is increased. q_u can be a symmetrical kernel with the centre being $\widehat{Y}_{1:\tau_k}^{(i)}$ and the bandwidth being either constant or decreasing with level k. A Gaussian shaped kernel can be used, but more choices are possible; for more details see [33].

As regards to the birth and death moves, it allows the exploration to be made with respect to τ_k as well. The proposal distribution q_b acts in a similar manner to the proposal distributions of IS. With reference to the presentation in Section 4.2, q_b could be a low bandwidth kernel extending $\widehat{Y}_{1:J-1}^{(i)}$, so that is $\widetilde{Y}^*$ very likely to hit level set $\mathcal{T}_J$. The birth move will be accepted if $\widehat{Y}_{\widehat{\tau}_k^{(i)}}^{(i)}$ is then more likely to be in $\mathcal{T}_k$ using an added intermediate step. It is more clear now that the level sets need to be rather close for this approach to work.

5.2.2 Practical considerations for Rare Event Simulation

There are certain drawbacks when the approach of the previous section is used. The first is that the memory requirements for storing $Y_{1:\tau_k}$ is not scalable with the level number k, therefore T cannot be very large. In [4] a fixed lag technique was proposed where instead only $Y_{\tau_k-L+1:\tau_k}$ is renewed through the MH kernel, where $L>0$ and small. Even so, proposing new paths $Y_{\tau_k-L+1:\tau_k}$ through some modified proposal distributions q_b, q_u, would be useful if the SMC potential g_k was a function of $Y_{1:\tau_k}$ or $Y_{\tau_k-L+1:\tau_k}$. In our case in Algorithm 1 g_k is given by

$$g_k(Y_{1:\tau_k}) = \mathbb{I}_{\mathcal{T}_k}(X_{\tau_k}).$$

When using a potential with such a form (i.e. an indicator function) it is clear that rejuvenating the path of $Y_{1:\tau_k}^{(i)}$ will not contribute to the weights at all unless we manually set $J=\tau_k$ for the death step, $J=\tau_k+1$ for the birth step and $J=\tau_k$ for the update step. This solution seems suitable for the rare events simulation problem we are considering. We propose to set J to these values for each case and use

$$\begin{aligned}\widetilde{Y}^*_{\tau_k^{(i)}+1} &\sim q_b(\widehat{Y}^{(i)}_{\tau_k^{(i)}},\cdot),\\ \widetilde{Y}^*_{\tau_k^{(i)}} &\sim q_u(\widehat{Y}^{(i)}_{\tau_k^{(i)}},\cdot),\end{aligned}$$

as proposals for the birth and update cases respectively. Designing q_b and q_u should follow in the same context as before only this time we modify only the last part of the path, which is of particular interest given the form of g_k.

When such a proposal mechanism is employed the MH kernel $\widetilde{K}_k$ is no longer ergodic. Note that in contrast to standard RJMCMC this is not required when MH moves are used along with SMC [4]. The resulting particle approximation

obtained will be still closer to $\pi_k(Y_{1:\tau_k})$ (e.g. when compared with a total variation norm) than the case when $\widetilde{K}_k$ is not used. Also, we suspect that the structure of the distributions $\pi_k(Y_{1:\tau_k})$ may not vary significantly with τ_k and we might often have

$$\pi_k(Y_{1:\tau_k}) \approx \pi_k(Y_{1:\tau_k+1}).$$

Hence the probability of having the reversible moves accepted will be reasonable. Standard Bayesian applications of reversible jump MCMC usually do not enjoy this property and it makes it more difficult to design fast mixing algorithms.

When standard SMC is used T is usually of an order ranging from $10^2 - 10^5$ [23]. In this case $\kappa = 1$ should suffice when designing $\widetilde{K}_k$, i.e. we propose using only a single MH step. In [10] the authors use $T = 8$. In that case, if RJMCMC moves are used we would suggest κ to be larger ranging from $10^2 - 10^3$.

6 Open Research Issues

Eventually the challenge to be addressed is to balance on the competing demands on computational power of using a large number of particles and using a large number of intermediate distributions. In this section we briefly outline a few other possible research directions that can provide extensions to our approach, which might improve the performance of the algorithm.

6.1 Smooth potentials

In practice it might be very expensive to consider a dense sequence of nested level sets for this approach to work. An alternative would be to use a smoother potential function $g_k(x)$ instead of $\mathbb{I}_{\mathcal{T}_k}(x)$ in the expression of the weights in step 3 II of Algorithm 1. The potential g_k can be dependent to an increasing parameter β_k, which plays the role of an inverse temperature. Annealing can be used so that as β_k increases then resembles closer $\mathbb{I}_{\mathcal{T}_k}(x)$. For example $g_k(x)$ can be defined as

$$g_k(x) = \left(1 + \exp(-\beta_k(V_k(x) - c_k))\right)^{-1},$$

where V_k is an arbitrary continuous function defined as

$$V_k : \begin{cases} \mathcal{T}_k & \rightarrow & [c_k, +\infty) \\ E \backslash \mathcal{T}_k & \rightarrow & (-\infty, c_k] \end{cases}$$

Note that until now we have been using $x = X_{\tau_k}$ as the argument of the level potential g_k. This is not restrictive and g_k can be also modified as a function of the previous path $X_{1:\tau_k}$. In addition, the SMC sampler can use a more smooth path sampling approach instead estimating the normalisation constants product of estimators directly. For more details see [27].

6.2 Continuous time RJMCMC

In case π_k is hard to compute, one could investigate more advanced reversible jump methods found in [13] and [34] that might suit our problem in better fashion. It is clear that continuous time formulation of Algorithm 2 might resolve implementation issues related to having to use a the time discretised

process $\{Y_n\}_{n\geq 0}$ explicitly in the problem formulation. Algorithm 1 can be easily extended for the continuous time formulation. In addition employing a Rao Blackwellisation for (1)-(2) can be combined with exact simulation algorithms for continuous time processes [5, 6, 7], leading to a lower bias due to time discretisation.

6.3 Adaptive selection of levels

An alternative multilevel splitting context that uses adaptive selection of the sequence of distributions to be employed has been presented in [15]. It might be worth investigating if this can be incorporated in the current approach and combining adaptation of the level sets with the effective sample size of SMC. Similar approaches have been used in Approximate Bayesian Computation for problems in Biology [19].

6.4 Replacing RJMCMC steps by SMC sampling

Also a trans-dimensional SMC approach can be considered without the use of MCMC [26]. Currently, this is a direction that is more useful to consider in the long term as it would require a completely new analysis.

6.5 Theoretical Analysis

Although we have not performed a theoretical analysis of the algorithm presented here, it is possible to establish a broad range of theoretical results by the application of the techniques found in [16]. Note that we can obtain a central limit theorem using these techniques, and that it will have the form presented in [18]. The resulting asymptotic variance of the estimates produced by the algorithm presented here will be closely related to the mixing properties of the proposal kernels used to move around the state space. Further analysis may include establishing reasonable conditions under which the particle system is stable, as well as to determine computable bounds upon the variance and bias associated with the SMC algorithm presented above.

7 Conclusions

In this deliverable we have attempted to discuss how an SMC sampler with trans-dimensional MCMC steps can be used for a rare events simulation problem that is useful for conflict or collision risk assessment. Our aim is to use this approach so that the generic algorithm can be implemented for this application using earlier powerful tools developed in previous formulations of the problem. Hopefully, this will lead to a more efficient simulation procedure that can use less particles and achieve a significant speed up.

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