Journal of Computational and Applied Mathematics 239 (2013) 50–71

Contents lists available at SciVerse ScienceDirect

Journal of Computational and Applied Mathematics

journal homepage: www.elsevier.com/locate/cam

# Almost sure convergence of numerical approximations for Piecewise Deterministic Markov Processes

Martin G. Riedler

*Institute for Stochastics, Johannes Kepler University, Linz, Austria*

ARTICLE INFO

*Article history:*
Received 12 January 2012
Received in revised form 17 September 2012

*MSC:*
60J75
65C20
65L99

*Keywords:*
Piecewise Deterministic Markov Process
Stochastic simulation
Hybrid algorithm
Almost sure convergence

ABSTRACT

Hybrid systems, and Piecewise Deterministic Markov Processes in particular, are widely used to model and numerically study systems exhibiting multiple time scales in biochemical reaction kinetics and related areas. In this paper an almost sure convergence analysis for numerical simulation algorithms for Piecewise Deterministic Markov Processes is presented. The discussed numerical methods arise through discretising a constructive method defining these processes. The stochastic problem of simulating the random, path-dependent jump times of such processes is reformulated as a hitting time problem for a system of ordinary differential equations with random threshold. Then deterministic continuous methods (methods with dense output) are serially employed to solve these problems numerically. We show that the almost sure convergence rate of the stochastic algorithm is identical to the order of the embedded deterministic method. We illustrate our theoretical findings by numerical examples from mathematical neuroscience, Piecewise Deterministic Markov Processes are used as biophysically accurate stochastic models of neuronal membranes.



## 1. Introduction

In recent years the number of applications of hybrid stochastic processes to model systems in biology, (bio-)chemical reaction kinetics and mathematical neuroscience have increased rapidly. These models either stem from a direct modelling approach, e.g., models of excitable biological membranes [1–4], or result from a multiscale approximation to more accurate particle models exhibiting clearly separated time scales, e.g., in biochemical reaction systems [5–8] or in gene regulatory networks [9]. The mathematically correct treatment of these is within the framework of General Stochastic Hybrid Systems [10]. Additional to these novel 'bioscience' applications for hybrid systems there are also more 'classical' applications of high interest in fields such as control and queueing theory, or models in financial mathematics and ecology, cf. [10–14] and references therein. In this paper we focus on Piecewise Deterministic Markov Processes (PDMPs), which are an important class of hybrid systems including most of the hybrid models considered in the literature, see [5,1,2,11,12,6,13,7,3,4,14,9] out of the above mentioned studies. PDMPs are strong Markov processes that combine continuous deterministic time evolution and discontinuous, instantaneous, random 'jump' events. Specifically, the dynamics of the two components are intrinsically intertwined. On the one hand, the continuous time-evolution, defined by ordinary differential equations (ODEs), depends on the outcomes of discrete events via randomly changing parameters and, on the other hand, the probability of the discrete events happening, i.e., a random, instantaneous change in a parameter, depends on the time-evolution – the path – of the continuous variables.

Due to the high complexity of hybrid models, particularly in biochemical applications, they are studied extensively and almost exclusively by numerical means. To this end either so called 'pseudo-exact' algorithms, which are a class of simple

*E-mail address:* martin.riedler@jku.at.

0377-0427/$ – see front matter 
doi:10.1016/j.cam.2012.09.021

statistically approximate algorithms obtained by an ad-hoc model approximation [15], or statistically exact algorithms are employed. Here 'statistically exact' means that in principle the simulation method produces paths that are samples of the distribution of the underlying stochastic process. In contrast pseudo-exact methods produce sample paths (possibly without a discretisation error) from a distribution which, under certain conditions, is expected to be close to the distribution of the underlying stochastic process. Nevertheless convergence, even in law, of these methods to the actual process is unknown. However, even statistically exact algorithms are exact only in theory due to a numerical error which arises inevitably in solving most systems of differential equations in actual implementations. So far model accuracy was primarily of interest as the main source of error and thus considerations regarding the numerical error are in general neglected, cf., e.g., [5–7]. Yet ultimately, even if a theoretically exact PDMP formulation of the model is considered or the model is highly accurate, numerical studies are conducted by numerical approximations to the PDMPs as an analytic representation of the paths is in general not available. Despite the importance and widespread use of numerical studies a numerical analysis, in particular, a thorough analytical investigation of the convergence and error behaviour of algorithms to be used, is still missing. The aim of this article is to provide a – to the best of our knowledge – first contribution towards this goal. We note that the statistically exact algorithms that were introduced in the studies [5,9] fall within the class we consider, however, in the present study a convergence analysis is carried out.

In particular in the present study we are interested in the convergence of statistically exact numerical approximations to PDMPs in a pathwise sense which corresponds to the fact that numerical simulations are carried out path by path. The methods we present for approximating a PDMP incorporate as an integral part continuous ODE methods, also called methods with dense output. Apart from numerically solving the deterministic inter-jump dynamics the key problem in simulating a PDMP is simulating the random, path-dependent jump times. As shown in Section 3 this problem can be reformulated and then, combined with the numerical solution of the inter-jump dynamics, yields a hitting time problem with random threshold. This we solve using continuous ODE methods. The main feature of such a method is that it does not only provide a numerical approximation to the exact solution at discrete grid points but provides an approximation of the whole path over the whole interval. Essentially, continuous methods are approximations on a discrete grid with an interpolation formula for the intervals between the grid points. Hence, these methods are naturally suited for solving hitting time problems. The main result of this paper is that numerical approximations of PDMPs built on continuous ODE methods conserve the order of convergence of the underlying continuous method where an appropriate definition of the error is used which reflects the structure of PDMPs. That is, if an approximation is constructed using, e.g., a continuous Runge–Kutta method of order $p$, then also the almost sure convergence of the stochastic approximation to the PDMP is of order $p$.

As for the PDMPs discussed in the present study we distinguish several types. The main part of the paper is devoted to processes with jumps occurring only in a fixed subset of the components of a vector-valued PDMP which are otherwise piecewise constant. Furthermore we assume that the jump heights are discretely distributed. We consider this particular structure for processes as these arise in applications in mathematical neuroscience, which initially motivated this study, and as a multiscale approximation to certain chemical reaction systems. In these models fast and slow reactions, modelled with reaction rate equations and instantaneous random jumps, respectively, affect a different set of reactants, however, each possesses rates also depending on the other set of reactants. As jumps correspond to an instantaneous event where one or more individual reactants change their state, in these models jump heights are typically integer valued. The second class of PDMPs comprises processes for which jumps may occur in all components and these components need not be necessarily piecewise constant, but jumps are still discretely distributed. These PDMPs include chemical reaction systems where fast and slow reactions may affect the same type of reactants. Finally, we also consider this last general type of processes with continuously distributed jump heights.

The remainder of the paper is organised as follows. In Section 2 we present a brief definition of PDMPs and their construction from sequences of independent, identically distributed (i.i.d.) standard uniform random variables. This provides a theoretically exact simulation algorithm which takes the role of an exact solution for our convergence analysis. Section 3 presents the approximate algorithms we consider in this paper and also contains the main convergence theorem. The proof of the convergence theorem can be found in Section 4. We extend the convergence result to other classes of PDMPs in Section 5. Finally, in Section 6 we present some numerical experiments using examples from the neuroscience literature to illustrate the theoretical findings and draw some conclusions for the usage and implementations of the numerical methods.

## 2. PDMPs and their construction from i.i.d. sequences of uniform random variables

In this section we give a brief introduction to PDMPs, introducing the objects used for their definition and the construction of their paths. In particular, Algorithm A1 defines the process which plays the role of the 'exact solution' for the numerical analysis. For a general discussion of PDMPs we refer to the monographs [12] and, more recently, [13] or the Ph.D. Thesis of the present author [16].

Let $(\Omega, \mathcal{F}, \mathbb{P})$ be a probability space. For the main part of the paper we consider a PDMP $(X(t))_{t\in[0,T]} = (X(t,\omega))_{t\in[0,T]}$ to consist of two qualitatively different components, i.e., $X(t) = (Y(t), \theta(t)) \in \mathbb{R}^{d+m}$. For these we assume that $Y(t)$ possesses continuous paths in a set $D \subseteq \mathbb{R}^d$ and $\theta(t)$ is right continuous and piecewise constant in $K \subset \mathbb{R}^m$, where $K$ is an at most countable set. We denote by $t_n$, $n \geq 1$, the random jump times of the component $\theta(t)$ and by $E = D \times K$ the state space of the process. Such a PDMP is uniquely defined (up to versions) by its characteristic triple $(f, \lambda, \mu)$, where the component