Exact simulation of a class of PDMPs

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July 5, 2016

Stochastic Hodgkin-Huxley model (Pakdaman and Al. 2010 [9]).

- **channel-state-tracking** (*Gillespie's first reaction method*) : Clay/Defelice 1983 [3], Rubinstein 1995 [12], Anderson and Al. 2015 [1].
- **channel-number-tracking** (*Gillespie's direct method*) : Skaugen/Walloe 1970 [13], Chow/White 1996 [2], Anderson and Al. 2015 [1].
- **Approximate algorithms** (*Diffusion approximation*) : Orio/Soudry 2012 [8], Goldwyn and Al. 2011 [7].

Let K be a countable set and $d \in \mathbb{N}$.
The set

$$E = \{(\theta, V) : \theta \in K, V \in \mathbb{R}^d\}$$

defined the state space of a PDMP noted $x_t = (\theta_t, V_t)$.

- (θ_t) is a jump process.
- (V_t) is a process which gives the deterministic trajectories.

A PDMP is characterized by the following objects :

- a family of vector fields $f_\theta : \mathbb{R}^d \to \mathbb{R}^d$, $\theta \in K$.
- a non-negative measurable function $\lambda : E \to \mathbb{R}_+$ (rate function).
- a transition measure $Q : E \times \mathcal{B}(E) \to [0, 1]$.

Hypothesis: For $\theta \in K$, the flows $\phi_\theta : \mathbb{R}_+ \times \mathbb{R}^d \to \mathbb{R}^d$ are known explicitly.

Notation: $\forall x = (\theta, V) \in E$, $\forall t \geq 0$

$$\phi_\theta(t, V) = \phi(t, x).$$

Trajectory of (x_t) starting from $x_0 = (\theta_0, V_0) \in E$ (Davis 1984 [4]):

Let

$$F(t, x_0) = e^{-\int_0^t \lambda(\theta_0, \phi(s, x_0)) ds}$$

be the survival function of T_1.

x_{T_1} random variable in E with conditional law $Q\left((\theta_0, \phi(T_1, x_0)), .\right)$.

Then, for $t \leq T_1$,

$$x_t = (\theta_t, V_t) = \begin{cases} (\theta_0, \phi(t, x_0)) & t < T_1, \\ x_{T_1} = (\theta_{T_1}, V_{T_1}) & t = T_1. \end{cases}$$

Then, the PDMP restarts from x_{T_1} at time T_1. The survival function of the inter-jump time S_2 is

$$F(t, x_{T_1}) = e^{-\int_0^t \lambda(\theta_{T_1}, \phi(s, x_{T_1}))ds}$$

The second jump time is $T_2 = T_1 + S_2$.

The conditional law of x_{T_2} is $Q\left((\theta_{T_1}, \phi(S_2, x_{T_1})), .\right)$.

Then, for $T_1 \leq t \leq T_2$

$$x_t = (\theta_t, V_t) = \begin{cases} (\theta_{T_1}, \phi(t - T_1, x_{T_1})) & T_1 \leq t < T_2, \\ x_{T_2} = (\theta_{T_2}, V_{T_2}) & t = T_2 \end{cases}$$

- Inversion of the survival function.
- Resolution of ODE + random hitting time problem (Riedler 2012 [11]).
- Link between a class of PDMPs and the *random time change equations* (Kurtz representation) (Riedler 2013 [10]).
- A probabilistic method using thinning.

Let $i \geq 0$, at time T_i the PDMP is in state x_{T_i}, we want to simulate S_{i+1}.

We have to solve $S(t, x_{T_i}) = U$ where $U \sim U([0,1])$.

$$w(t, x_{T_i}) = -log(S(t, x_{T_i})) = \int_0^t \lambda(\theta_{T_i}, \phi(s, x_{T_i}))ds.$$

Equivalent problem :

$$w'(t, x_{T_i}) = \lambda(\theta_{T_i}, \phi(t, x_{T_i}))$$

$$S_{i+1} = \inf\{s > 0, w(s, x_{T_i}) = -\log(U)\}$$

Equality in law between a class of PDMPs and the processes solution of :

$$X(t) = X(0) + \int_0^t h(X(s))ds + \sum_{k=1}^{r} Y_k\Big(\int_0^t \lambda_k(X(s))ds\Big)\nu_k$$

- $(Y_k)_{k=1,\dots,r}$ independent unit rate Poisson processes.
- $\nu_k \in \mathbb{R}^n$ jump heights.
- $h : \mathbb{R}^n \to \mathbb{R}^n$ contains the vector fields of the PDMP.
- $\lambda_k : \mathbb{R}^n \to \mathbb{R}_+$ such that $\lambda(.) = \sum_{k=1}^r \lambda_k(.)$.

Theorem (Devroye 1986 [6])

Let $(T_n)_{n\geq 0}$ be a Poisson process with jump rate $\lambda(t)$ and let $E \sim \mathcal{E}(1)$, then

$$T_{n+1} \overset{Law}{=} \Lambda^{-1}\left(E + \Lambda(T_n)\right), \qquad n \geq 0$$

where $\Lambda(t) = \int_0^t \lambda(s)ds$.

In applications, we are rarely able to compute Λ et Λ^{-1} explicitly. However, we can compute Λ et Λ^{-1} for specific functions λ.

We want to simulate $(T_n)_{n\geq 0}$ with jump rate $\lambda(t)$.
We choose $(\overline{T}_n)_{n\geq 0}$ a Poisson process with jump rate $\overline{\lambda}(t)$ such that

$$\lambda(t) \leq \overline{\lambda}(t), \qquad \forall t \geq 0.$$

with $\overline{\Lambda}$, $\overline{\Lambda}^{-1}$ explicitly computable.

Idea of the thinning procedure

- Simulate the Poisson process $(\overline{T}_n)_{n\geq 0}$.
- Keep points $\overline{T}_k$ with probability $\frac{\lambda}{\overline{\lambda}}(\overline{T}_k)$.

Let $i \geq 0$, at time T_i the PDMP is in the state x_{T_i}, we want to simulate S_{i+1}.

S_{i+1} is the first jump time of a Poisson process with jump rate $\lambda(\theta_{T_i}, \phi(t - T_i, x_{T_i}))$ for $t \geq T_i$.

Let $\epsilon > 0$,

$$[T_i, +\infty[= \cup_{k \geq 0} P_k^{i,\epsilon}$$

where $P_k^{i,\epsilon} = [T_i + k\epsilon, T_i + (k+1)\epsilon[$.

We define

$$\overline{\lambda}(t) = \sum_{k\geq 0} \overline{\lambda}_k^{i,\epsilon} \mathbf{1}_{P_k^{i,\epsilon}}(t), \qquad t \geq T_i$$

where

$$\overline{\lambda}_k^{i,\epsilon} = sup_{t\in P_k^{i,\epsilon}} \lambda(\theta_{T_i}, \phi(t - T_i, x_{T_i})).$$

Thus, we have

$$\lambda(\theta_{T_i}, \phi(t - T_i, x_{T_i})) \leq \overline{\lambda}(t), \qquad \forall t \geq T_i.$$

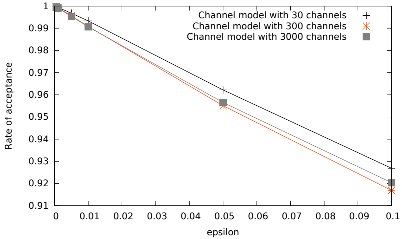
$$\overline{\Lambda}(t) = \sum_{k\geq 0} \overline{\lambda}_k^{i,\epsilon} \Big[(k+1)\epsilon \wedge (t - T_i) - k\epsilon \wedge (t - T_i) \Big]$$

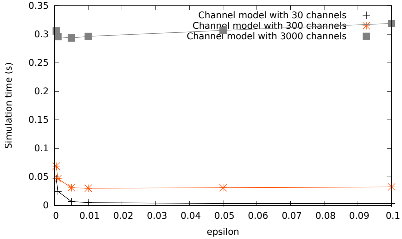
$$\overline{\Lambda}^{-1}(s) = \sum_{p\geq 0} \left(\epsilon \frac{s - \kappa_{p-1}}{\kappa_p - \kappa_{p-1}} + T_i + p\epsilon \right) \mathbf{1}_{[\kappa_{p-1}, \kappa_p[}(s)$$

where

$$\kappa_p = \epsilon \sum_{k=0}^{p} \overline{\lambda}_k^{i,\epsilon}.$$

By convention, $\kappa_{-1} = 0$.


Rate of acceptance
epsilon
Channel model with 30 channels
Channel model with 300 channels
Channel model with 3000 channels
1
0.99
0.98
0.97
0.96
0.95
0.94
0.93
0.92
0.91
0 0.01 0.02 0.03 0.04 0.05 0.06 0.07 0.08 0.09 0.1


Simulation time (s)
epsilon
Channel model with 30 channels
Channel model with 300 channels
Channel model with 3000 channels
0.35
0.3
0.25
0.2
0.15
0.1
0.05
0
0 0.01 0.02 0.03 0.04 0.05 0.06 0.07 0.08 0.09 0.1

We define the global bound

$$\overline{\lambda} = sup_{x \in E} sup_{t \geq 0} \lambda(\theta, \phi(t, x))$$

and the local bound

$$\forall x \in E, \qquad \overline{\lambda} = sup_{t \geq 0} \lambda(\theta, \phi(t, x))$$

Model	Bound	simulation time (sec)	rate of acceptance
Channel	Optimal-$\mathcal{Q}^{\epsilon_n}$	0,003 $(\pm 8.10^{-7})$	0,857 $(\pm 2.10^{-3})$
	Local	0,008 $(\pm 6.10^{-6})$	0,141 $(\pm 2.10^{-3})$
	Global	0,012 $(\pm 3.10^{-6})$	0,065 $(\pm 6.10^{-5})$

Channel model with 30 channels.

Algorithm for the simulation of the first jump time of a non-homogeneous Poisson process

$\tilde{T}_0 \leftarrow 0$
$k \leftarrow 0$
Repeat
  $k \leftarrow k + 1$
  Simulate a uniform random variable U_{2k-1} on $[0, 1]$
  Simulate $E_k = -\log(U_{2k-1})$
  $\tilde{T}_k \leftarrow \tilde{\Lambda}^{-1}\left(E_k + \tilde{\Lambda}(\tilde{T}_{k-1})\right)$
  Simulate a uniform random variable U_{2k} on $[0, 1]$
Until $U_{2k}\tilde{\lambda}(\tilde{T}_k) \leq \lambda(\tilde{T}_k)$
Return $\tilde{T}_k$

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