Multilevel Hybrid Chernoff Tau-Leap

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Abstract

Markovian pure jump processes can model many phenomena, e.g. chemical reactions at molecular level, protein transcription and translation, spread of epidemics diseases in small populations and in wireless communication networks, among many others. In this work [6] we present a novel multilevel algorithm for the Chernoff-based hybrid tau-leap algorithm. This variance reduction technique allows us to: (a) control the global exit probability of any simulated trajectory, (b) obtain accurate and computable estimates for the expected value of any smooth observable of the process with minimal computational work.

Statement of the problem

Let X be a Pure Jump Process

$$X = (X_1, \ldots, X_d) : [0,T] \times \Omega \to \mathbb{Z}_+^d$$

described by

- Finite number of possible reactions, $\nu_j \in \mathbb{Z}^d, x \in \mathbb{Z}_+^d$,

$$x \to x + \nu_j, \quad j{=}1, ..., J$$

- and propensity (jump intensity) functions, $a_j : \mathbb{R}^d \to \mathbb{R}^+$ such that

$$\mathrm{P}\left(X(t+\mathrm{d}t) = x + \nu_j \,\middle|\, X(t) = x\right) = a_j(x)\mathrm{d}t + o(\mathrm{d}t)\,, \qquad (1)$$

Typically, $X_k(t)$ is the population size at time t of the $k-th$ species in the chemical kinetics jargon.
Goal: accurately approximate the Quantity of Interest (QoI)

$$\mathrm{E}\left[g(X(T))\right],$$

for some real observable $g : \mathbb{R}^d \to \mathbb{R}$.
The process X can be characterized by

$$X(t) = X(0) + \sum_{j=1}^{J} \nu_j Y_j \left(\int_0^t a_j(X(s))\,\mathrm{d}s \right),$$

where $Y_j : \mathbb{R}_+ \times \Omega \to \mathbb{Z}_+$ are indep. unit-rate Poisson processes [3].

Idea: Multilevel simulation of hybrid paths

- **Multivel Monte Carlo (MLMC)**. Use a control variate multilevel approach to reduce the computational work (runtime) of the standard Monte Carlo method.
- **Coupled Hybrid Paths**. The MLMC method requires the generation of coupled hybrid paths. The exact method used in the MLMC hybrid algorithm is the Modified Next Reaction Method [2].

The modified next reaction method

- This is an algorithm for simulating exact trajectories of the process X based on the random time change representation.
- Uses explicitly the firing times of the involved independent Poisson process.
- Advantages: (i) is faster than the SSA since we only need only one uniform r.v. at each step. (ii) We can sample in the cases where the rate functions depend on time and there are delayed reactions.
- Finally, it is possible to simulate correlated (tau-leap, pure jump) trajectories, and also nested (tau-leap, tau-leap) trajectories. In [1] this technique is used to develop a uniform step MLMC algorithm.

Coupling algorithm

Couplig idea [1]. Let Y_1, Y_2 be two independent unit-rate Poisson processes. Set

$$Z_1(t) = Y_1(\lambda_1 t) + Y_2(\lambda_2 t)$$
$$Z_2(t) = Y_1(\lambda_1 t)$$

where $\lambda_1, \lambda_2 \in \mathbb{R}_+$. The idea is to use Y_1 to generate simultaneous jumps and Y_2 to model the extra jumps. Then, Z_1 and Z_2 are coupled homogeneous Poisson processes. By construction,

$$\mathrm{Var}\left[Z_1(t) - Z_2(t)\right] = \mathrm{Var}\left[Y_2(\lambda_2 t)\right] = \lambda_2 t\,.$$

In the non-homogeneous case, where $\lambda_1 = \lambda_1(t), \lambda_2 = \lambda_2(t)$, we have

$$Z_1(t) = Y_1\left(\int_0^t \hat{\lambda}(s)ds\right) + Y_2\left(\int_0^t \lambda_1(s) - \hat{\lambda}(s)ds\right)$$
$$Z_2(t) = Y_1\left(\int_0^t \hat{\lambda}(s)ds\right) + Y_3\left(\int_0^t \lambda_2(s) - \hat{\lambda}(s)ds\right)$$

where $\hat{\lambda}(t) \equiv \min\{\lambda_1(t), \lambda_2(t)\}$. We observe that $Z_1(t) \overset{\mathcal{D}}{=} Y\left(\int_0^t \lambda_1(s)ds\right)$ with Y a unit-rate Poisson process.

Couplig of hybrid trajectories. The MLMC estimator requires the generation of $[g_\ell - g_{\ell-1}](\omega_m)$. This is a functional of two coupled hybrid paths.

- Given two grids,
  1. a coarse grid, $(t_i, t_{i+1})_{i=1..N}$, $t_N{=}T$
  2. a finer grid, $(s_j, s_{j+1})_{j=1..K}$, such that $s_1{=}t_1$, $s_K{=}t_N$ and i is a subsequence of j,

the idea is to generate two coupled hybrid paths, using 4 algorithms as building blocks:

Algorithm	at coarser grid	at finer grid
1	TL	TL
2a	TL	MNRM
2b	MNRM	TL
3	MNRM	MNRM

- Given current time t:

1: $\bar{t} \leftarrow$ next grid point in $(t_i)_{i=0}^N$ larger than t
2: $\bar{a} \leftarrow a(\bar{X})$
3: $(\bar{m}, \bar{\tau}) \leftarrow$ method and Chernoff tau size given $(\bar{X}, \bar{t}, \bar{\delta})$
4: $\bar{H} \leftarrow \min\{t{+}\bar{\tau}, T\}$
5: $\bar{\bar{t}} \leftarrow$ next grid point in $(s_j)_{j=0}^{N'}$ larger than t
6: $\bar{\bar{a}} \leftarrow a(\bar{\bar{X}})$
7: $(\bar{\bar{m}}, \bar{\bar{\tau}}) \leftarrow$ method and Chernoff tau size given $(\bar{\bar{X}}, \bar{\bar{t}}, \bar{\bar{\delta}})$
8: $\bar{\bar{H}} \leftarrow \min\{t{+}\bar{\bar{\tau}}, T\}$
9: **while** $t < T$ **do**
10: $H \leftarrow \min\{\bar{H}, \bar{\bar{H}}\}$
11: **if** $\bar{m} =$ TL **and** $\bar{\bar{m}} =$ TL **then**
12: Apply algorithm 1.
13: $t \leftarrow H$
14: **else**
15: **while** $t < H$ **do**
16: **if** $\bar{\bar{m}} =$ MNRM **then**
17: $\bar{\bar{a}} \leftarrow a(\bar{\bar{X}})$
18: **end if**
19: **if** $\bar{m} =$ MNRM **then**
20: $\bar{a} \leftarrow a(\bar{X})$
21: **end if**
22: Apply algorithm 2a, 2b or 3.
23: **end while**
24: **end if**
25: **if** $t < T$ **then**
26: **if** $\bar{H} \leq \bar{\bar{H}}$ **then**
27: Update $\bar{t}, \bar{a}, \bar{m}, \bar{\tau}$, and $\bar{H}$
28: **end if**
29: **if** $\bar{H} \geq \bar{\bar{H}}$ **then**
30: Update $\bar{\bar{t}}, \bar{\bar{a}}, \bar{\bar{m}}, \bar{\bar{\tau}}$, and $\bar{\bar{H}}$
31: **end if**
32: **end if**
33: **end while**

Multivel Monte Carlo

Multivel by Giles [4]. In order to reduce the variance of the standard Monte Carlo estimator $\hat{\theta}_1 := \frac{1}{M}\sum_{n=1}^{M} X(\omega_m)$ of $\mathrm{E}[X]$, we define another estimator which uses a control variate Y, correlated with X, where $\mathrm{E}[Y]$ is known. In fact, we assume that we can generate pairs $(X(\omega), Y(\omega))$ in such way that the cost of generating $Y(\omega)$ is less than the corresponding cost of generating $X(\omega)$.

$$\hat{\theta}_2 := \frac{1}{M}\sum_{m=1}^{M}\{X(\omega_m) - (Y(\omega_m) - \mathrm{E}[Y])\}\,.$$

We have that $\mathrm{Var}\left[\hat{\theta}_2\right] \leq \mathrm{Var}\left[\hat{\theta}_1\right]$.

- 2 levels: estimate $\mathrm{E}\left[g(\bar{\bar{X}}(T))\right]$, using $g(\bar{X}(T))$ as a control variate.

$$\mathrm{E}\left[g(\bar{\bar{X}}(T))\right] = \mathrm{E}\left[g(\bar{X}(T))\right] + \mathrm{E}\left[g(\bar{\bar{X}}(T)) - g(\bar{X}(T))\right]$$

its Monte Carlo estimator is

$$\frac{1}{M_0}\sum_{m=1}^{M_0} g(\bar{X}(T,\omega_m)) + \frac{1}{M_1}\sum_{m=1}^{M_1} g(\bar{\bar{X}}(T,\omega_m)) - g(\bar{X}(T,\omega_m))\,.$$

- in the case of L levels:

$$\mathrm{E}[g_L] = \mathrm{E}[g_0] + \sum_{\ell=1}^{L}\mathrm{E}[g_\ell - g_{\ell-1}]\,,$$

where $g_\ell \equiv g(\bar{X}_{\Delta t_\ell}(T))$, where Δt_ℓ represents the step-size at mesh level ℓ. Its MLMC estimator is

$$\frac{1}{M_0}\sum_{m=1}^{M_0} g_0(\omega_m) + \sum_{\ell=1}^{L}\frac{1}{M_\ell}\sum_{m=1}^{M_\ell}[g_\ell - g_{\ell-1}](\omega_m)\,.$$

Multivel Monte Carlo estimator

In order to estimate the QoI, we consider the following telescopic decomposition

$$\mathrm{E}[g_0 \mathbf{1}_{A_0}] + \sum_{\ell=1}^{L}\mathrm{E}\left[g_\ell \mathbf{1}_{A_\ell} - g_{\ell-1}\mathbf{1}_{A_{\ell-1}}\right].$$

Here $A_\ell = A_\ell(\omega)$ is the event in which the $\bar{X}_{\Delta t_\ell}$-trajectory arrived to the final time T, without exiting the state space of X, at level ℓ.
We can use the MLMC estimator

$$\frac{1}{M_0}\sum_{m=1}^{M_0} g_0\mathbf{1}_{A_0}(\omega_m) + \sum_{\ell=1}^{L}\frac{1}{M_\ell}\sum_{m=1}^{M_\ell}[g_\ell\mathbf{1}_{A_\ell} - g_{\ell-1}\mathbf{1}_{A_{\ell-1}}](\omega_m)\,.$$

Global Error Decomposition. $\mathrm{E}[g(X(T))]$ − MLMC Estimator =

$$\mathrm{E}\left[(g(X) - g(\bar{X}_L))\mathbf{1}_{A_L}\right] + \mathrm{E}\left[g(X)\mathbf{1}_{\bar{A}_L}\right] + \frac{1}{M_0}\sum_{m=1}^{M_0}(\mathrm{E}[g_0\mathbf{1}_{A_0}] - g_0\mathbf{1}_{A_0}(\omega_m))$$
$$+ \sum_{\ell=1}^{L}\frac{1}{M_\ell}\sum_{m=1}^{M_\ell}\left([g_\ell\mathbf{1}_{A_\ell} - g_{\ell-1}\mathbf{1}_{A_{\ell-1}}](\omega_m) - \mathrm{E}\left[g_\ell\mathbf{1}_{A_\ell} - g_{\ell-1}\mathbf{1}_{A_{\ell-1}}\right]\right)\,.$$

that is,

$$\underbrace{\text{time discretiz. error}}_{\approx \mathcal{E}_{I,L} := \sum_k \mathrm{E}[\varphi_k err_k]} + \underbrace{\text{global exit error}}_{\approx \mathcal{E}_{E,L} := \delta\ \hat{\mathrm{E}}[g(X(T))]\ \hat{\mathrm{E}}[N_{TL}(\Delta t_L, \delta)]} + \underbrace{\text{statistical error}}_{\approx \mathcal{E}_S := 2\sqrt{\sum_{\ell=0}^{L}\frac{\mathcal{V}_\ell}{M_\ell}}}$$

Dual error estimation. Using duals (see [5]) we accurately estimate the difference of two very close quantities. We define and estimate the weak and strong errors, for each level, as follows:

$$\mathcal{E}_{I,L} : = \mathrm{E}\left[g(X(T)) - g(\bar{X}_L(T))\right] \approx \mathcal{A}\left(\sum_k \mathrm{E}\left[(\varphi_k e_k)\right]; \cdot\right),\ L \geq 0$$
$$\mathcal{V}_0 := \mathrm{Var}\left[g(\bar{X}_0(T))\right]$$
$$\mathcal{V}_L := \mathrm{Var}\left[g(\bar{X}_L(T)) - g(\bar{X}_{L-1}(T))\right] \approx \mathcal{A}\left(\sum_k \mathrm{E}\left[(\varphi_k e_k)^2\right]; \cdot\right),\ L \geq 1$$

Here $\{\varphi_k(\omega)\}_k$ are discrete duals obtained from the variational equation of the mean field associated with the process X.
Finally, $\{e_k(\omega)\}_k$ are computable approximations of the local errors.

Estimation procedure

We have a two step algorithm:

Step 1: We define

$$\Psi_0 := \mathrm{E}[\text{cost of a 0 - level path}]$$
$$\Psi_L := \mathrm{E}[\text{cost of coupled paths at levels } L-1 \text{ and } L]\,,\ L \geq 1$$

and optimize for the variables M_ℓ and L, the computational cost $\sum_{\ell=0}^{L}\Psi_\ell M_\ell$, subject to $|\mathcal{E}_{I,L}| + 2\sqrt{\sum_{\ell=0}^{L}\frac{\mathcal{V}_\ell}{M_\ell}} \leq TOL{-}TOL^2$. Here we chose the one-step exit probability bound δ in such way that the global exit error is less than TOL^2.

Step 2: Computation of the MLMC estimation of $\mathrm{E}[g(X(T))]$.

Numerical results for the GTT model

Here is one realization of the estimation procedure:

TOL	$\delta(TOL)$	$h_L(TOL)$	L	C_{ML} (sec)	C_{SSA} (sec)	$\frac{C_{ML}}{C_{\text{SSA}}}$
1.00e-01	1.00e-05	6.3e-03	3	1.9e+00	2.1e+01	0.09
5.00e-02	1.25e-06	6.3e-03	3	7.1e+00	8.3e+01	0.09
2.50e-02	1.56e-07	1.6e-03	4	2.7e+01	2.6e+02	0.11
1.25e-02	1.95e-08	3.9e-04	5	1.4e+02	1.3e+03	0.11
6.25e-03	2.44e-09	3.9e-04	5	6.7e+02	5.2e+03	0.13
3.13e-03	3.05e-10	9.8e-05	6	3.1e+03	2.2e+04	0.14

where C_{ML} and C_{SSA} are the actual runtimes of the Hybrid MLMC and the SSA methods respectively.

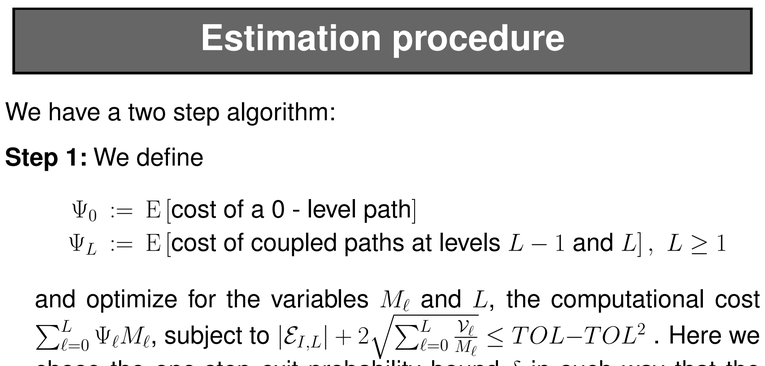

Figure 1: *Left Panel: Five realizations of the calibration phase, for the single level (SL) Chernoff hybrid method and the multilevel (ML) one. As TOL goes to zero, the error bound goes to zero. In the SL case, the predicted runtime of the Hybrid method approaches the predicted runtime of the SSA. Right Panel: Actual work (runtime) versus estimated error bound, for the SL Chernoff hybrid method and the ML one.*

Conclusions

- We developed a new multilevel approach for the Chernoff-based hybrid tau-leap algorithm. It can estimate the expected value of an observable of the process X at a final time T within a certain prescribed tolerance TOL and with high probability.
- Our methodology provides the parameter choices for the simulation *i.e.*one-step exit probability bound, number of levels, time mesh and the number of simulations for each level such that optimizes the computational work.
- The computational complexity of our method is of order $\mathcal{O}\left(TOL^{-2}\right)$.

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