

Workshop on Particle and Monte Carlo Methods  
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## Particle methods for the simulation of rare events

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## Plan

- examples of rare events
- multilevel Feynman–Kac distributions
- interacting particle system approximations
- combining importance splitting and importance sampling
- extinction of particle system

example in **air-traffic management** (ATM)

studied in the HYBRIDGE european project (IST programme)

partners : NLR, CENA, etc.

- two aircrafts flying over the same area, at the same flight level
- flight plan allows sufficient separation distance between aircrafts
- random perturbations, mainly due to wind, makes actual separation distance smaller than planned separation distance
- risk becomes nonzero, but remains very small
- objective is to evaluate whether flight plan design can be relaxed, so as to increase traffic capacity, without compromising **safety**

two possible measures of risk

- **conflict risk** : probability that separation distance gets smaller than 5 nautical miles, roughly 9260 meters
- **collision risk** : probability that separation distance gets smaller than physical size of aircraft, roughly 100 meters

example in **telecommunication networks**

- buffer at a station, with service rate much larger than customer arrival rate
- empty buffer is a recurrent event
- large enough buffer size so that overflow, resulting in packet loss, is a rare event
- objective is to evaluate the probability that a **buffer overflow** occurs, before the buffer empties again

## Plan

- examples of rare events
- **multilevel Feynman–Kac distributions**
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continuous–time strong Markov process  $\{X_t, t \geq 0\}$ ,  
with values in metric state space  $S$ , and càdlàg trajectories  
for some closed critical region  $B \subset S$ , let

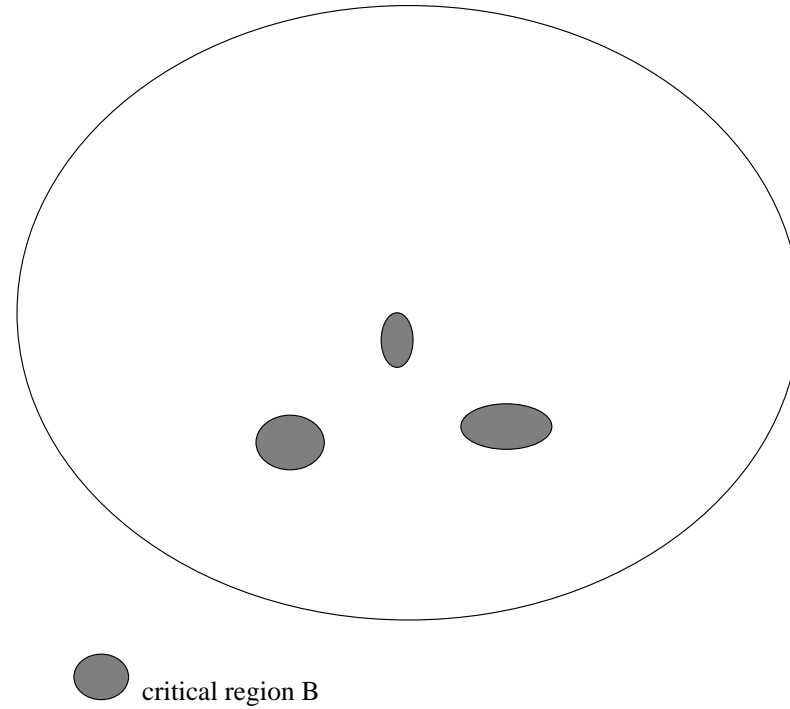
$$T_B = \inf\{t \geq 0 : X_t \in B\}$$

with  $T$  a finite deterministic time, or an a.s.–finite stopping time  
objective is to compute probabilities related with rare (but critical) event

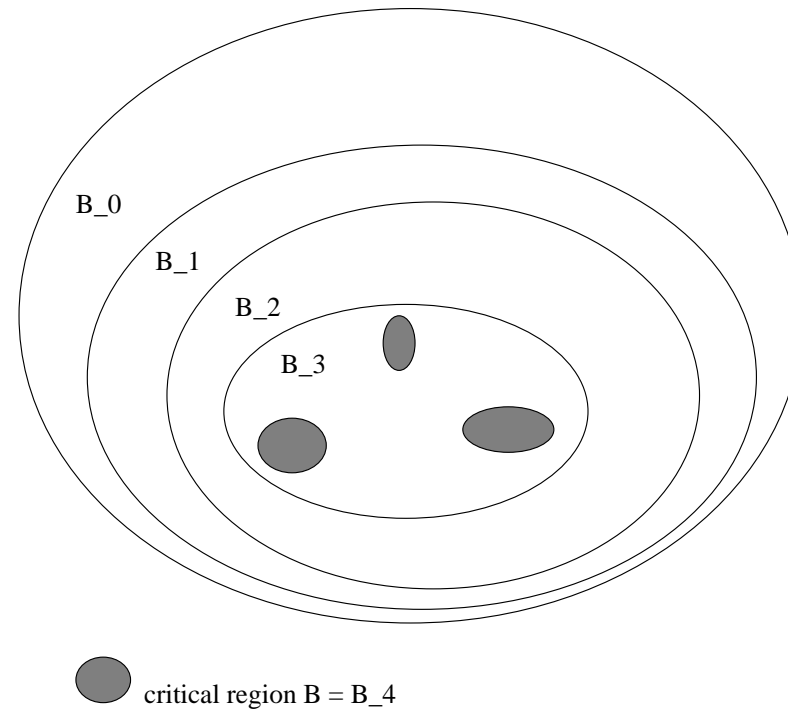
$$\mathbb{P}[T_B \leq T] \quad \text{and} \quad \mathbb{E}[f(X_t, 0 \leq t \leq T_B) \mid T_B \leq T]$$

i.e.

- probability of the rare event  $(T_B \leq T)$
- and probability distribution of the rare trajectories



in practice, none of the simulated trajectories will ever hit the critical region,  
hence naive Monte Carlo method fails



**importance splitting** idea is to select trajectories that approach the critical region



introducing an embedded sequence of closed regions

$$B = B_n \subset \cdots \subset B_1 \subset B_0 = S$$

with corresponding hitting times

$$T_k = \inf\{t \geq 0 : X_t \in B_k\}$$

it holds

$$0 = T_0 \leq T_1 \leq \cdots \leq T_n = T_B$$

clearly

$$\mathbb{P}[T_B \leq T] = \mathbb{P}[T_n \leq T] = \prod_{k=0}^n \mathbb{P}[T_k \leq T \mid T_{k-1} \leq T]$$

but these transition probabilities, from one level to the next, are usually unknown

modelling : discrete–time Markov chain  $\{\mathcal{X}_k, k = 1 \cdots n\}$  induced by discrete–time events from continuous–time Markov process  $\{X_t, t \geq 0\}$

$$\mathcal{X}_k = (X_t, T_{k-1} \wedge T \leq t \leq T_k \wedge T)$$

with values in

$$E = \bigcup_{t' \leq t''} \mathbb{D}([t', t''], S)$$

for any  $e = (x_t, t' \leq t \leq t'') \in E$ , let

$$g_k(e) = 1_{(\pi(e) \in B_k)} \quad \text{where} \quad \pi(e) = x_{t''}$$

clearly

$$(T_k \leq T) \quad \text{iff} \quad (X_{T_k \wedge T} \in B_k) \quad \text{iff} \quad (g_k(\mathcal{X}_k) = 1)$$

hence

$$1_{(T_k \leq T)} = g_k(\mathcal{X}_k) = \prod_{p=1}^k g_p(\mathcal{X}_p)$$

interpretation of rare event probabilities in terms of Feynman–Kac distributions

$$\gamma_k(f) = \mathbb{E}[f(\mathcal{X}_k) \prod_{p=1}^k g_p(\mathcal{X}_p)] = \mathbb{E}[f(X_t, T_{k-1} \leq t \leq T_k) 1_{(T_k \leq T)}]$$

in particular for  $f \equiv 1$

$$\gamma_k(1) = \mathbb{E}[\prod_{p=1}^k g_p(\mathcal{X}_p)] = \mathbb{P}[T_k \leq T]$$

hence

$$\eta_k(f) = \frac{\gamma_k(f)}{\gamma_k(1)} = \mathbb{E}[f(X_t, T_{k-1} \leq t \leq T_k) \mid T_k \leq T]$$

and in particular

$$\eta_k \circ \pi^{-1}(\phi) = \eta_k(\phi \circ \pi) = \mathbb{E}[\phi(X_{T_k}) \mid T_k \leq T]$$

similarly, introducing

$$\gamma_{k|k-1}(f) = \mathbb{E}[f(\mathcal{X}_k) \prod_{p=1}^{k-1} g_p(\mathcal{X}_p)] = \mathbb{E}[f(X_t, T_{k-1} \leq t \leq T_k \wedge T) 1_{(T_{k-1} \leq T)}]$$

it holds

$$\eta_{k|k-1}(f) = \frac{\gamma_{k|k-1}(f)}{\gamma_{k|k-1}(1)} = \mathbb{E}[f(X_t, T_{k-1} \leq t \leq T_k \wedge T) \mid T_{k-1} \leq T]$$

in particular for  $f \equiv g_k$

$$\eta_{k|k-1}(g_k) = \frac{\gamma_k(1)}{\gamma_{k-1}(1)} = \mathbb{P}[T_k \leq T \mid T_{k-1} \leq T]$$

hence

$$\mathbb{P}[T_k \leq T] = \gamma_k(1) = \prod_{p=1}^k \eta_{p|p-1}(g_p) = \prod_{p=1}^k \mathbb{P}[T_p \leq T \mid T_{p-1} \leq T]$$

more generally, introducing path–space Markov chain  $\{\mathcal{X}_{1:k}, k = 1 \cdots n\}$  with  $\mathcal{X}_{1:k} = (\mathcal{X}_1, \cdots, \mathcal{X}_k)$ , and selection function

$$h_p(e_1, \cdots, e_p) = g_p(e_p) \quad \text{for any } (e_1, \cdots, e_p) \in E^p$$

yields

$$\begin{aligned} \gamma_{1:k}(f) &= \mathbb{E}[f(\mathcal{X}_{1:k}) \prod_{p=1}^k h_p(\mathcal{X}_{1:p})] = \mathbb{E}[f(\mathcal{X}_1, \cdots, \mathcal{X}_k) \prod_{p=1}^k g_p(\mathcal{X}_p)] \\ &= \mathbb{E}[f(X_t, 0 \leq t \leq T_k) 1_{(T_k \leq T)}] \end{aligned}$$

and

$$\eta_{1:k}(f) = \frac{\gamma_{1:k}(f)}{\gamma_{1:k}(1)} = \mathbb{E}[f(X_t, 0 \leq t \leq T_k) \mid T_k \leq T]$$

interacting particle methods will provide numerical approximation  
for rare event probabilities

$$\gamma_n(1) = \mathbb{P}[T_B \leq T] \quad \text{and} \quad \eta_{1:n}(f) = \mathbb{E}[f(X_t, 0 \leq t \leq T_B) \mid T_B \leq T]$$

and for transition probabilities, from one level to the next

$$\eta_{k|k-1}(g_k) = \mathbb{P}[T_k \leq T \mid T_{k-1} \leq T]$$

with many estimates and asymptotic results as the number of particles goes to infinity, see Section 12.2 in Del Moral, *Feynman–Kac Formulae* (2004)

notice that the selection functions can take the zero value

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- examples of rare events
- multilevel Feynman–Kac distributions
- **interacting particle system approximations**
- combining importance splitting and importance sampling
- extinction of particle system

## Feynman–Kac flow

$$\eta_{k-1} \xrightarrow{\text{prediction}} \eta_{k|k-1} = \eta_{k-1} Q_k \xrightarrow{\text{update}} \eta_k = g_k \cdot \eta_{k|k-1}$$

where  $\cdot$  denotes projective product, i.e.

$$\eta_k = g_k \cdot \eta_{k|k-1} = \frac{g_k \eta_{k|k-1}}{\eta_{k|k-1}(g_k)}$$

particle approximation of the form

$$\eta_k \approx \eta_k^N = \sum_{i=1}^N w_k^i \delta_{\xi_k^i} \quad \text{where} \quad \xi_k^i = (X_t^i, T_{k-1}^i \wedge T^i \leq t \leq T_k^i \wedge T^i)$$

such that

$$\eta_{k-1}^N \longrightarrow \eta_{k|k-1}^N = S^N(\eta_{k-1}^N Q_k) \longrightarrow \eta_k^N = g_k \cdot \eta_{k|k-1}^N$$



basic (bootstrap) algorithm

- **selection** of particles with nonzero weight : independently for  $i = 1 \cdots N$

$$\tau_{k-1}^i \sim (w_{k-1}^1, \cdots, w_{k-1}^N) \quad \text{with values in index set } \{1, \cdots, N\}$$

and

$$\widehat{\xi}_{k-1}^i = \xi_{k-1}^{\tau_{k-1}^i} \quad \text{and} \quad \widehat{T}_{k-1}^i = T_{k-1}^{\tau_{k-1}^i}$$

- **mutation** : independently for  $i = 1 \cdots N$

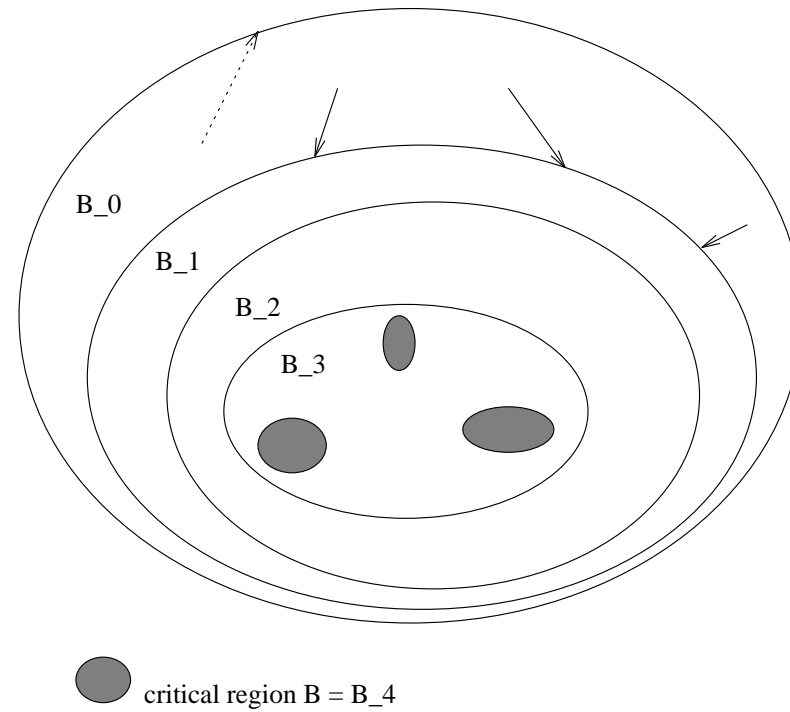
$$\xi_k^i = (X_t^i, \widehat{T}_{k-1}^i \leq t \leq T_k^i \wedge T^i)$$

follows the continuous-time Markov model, starting from  $\pi(\widehat{\xi}_{k-1}^i)$

$$T_k^i = \inf\{t \geq \widehat{T}_{k-1}^i : X_t^i \in B_k\}$$

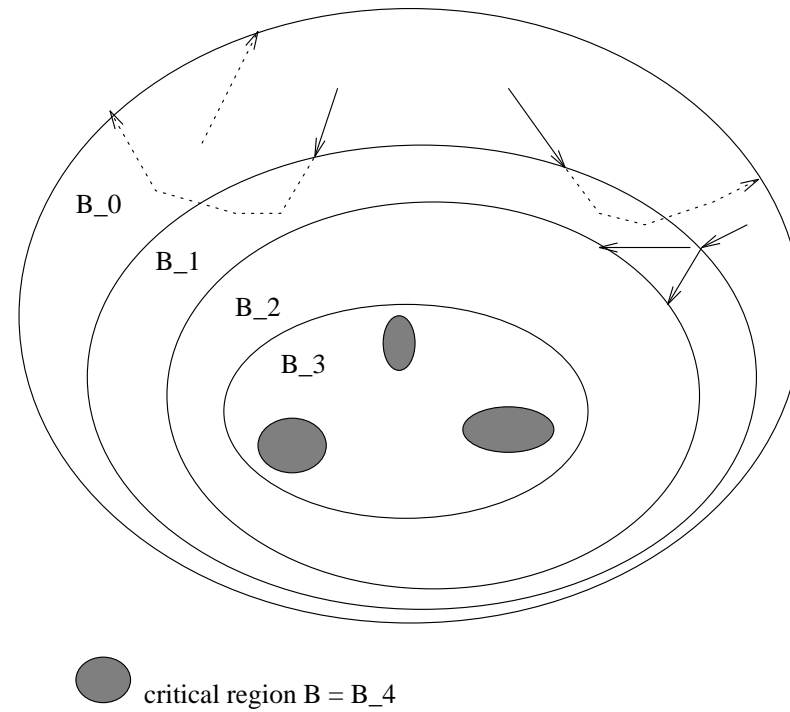
- **weighting** according to success to reach next level : for  $i = 1 \cdots N$

$$w_k^i \propto g_k(\xi_k^i) = 1_{(X_{T_k^i \wedge T^i}^i \in B_k)}$$



between two levels, particles explore the state space

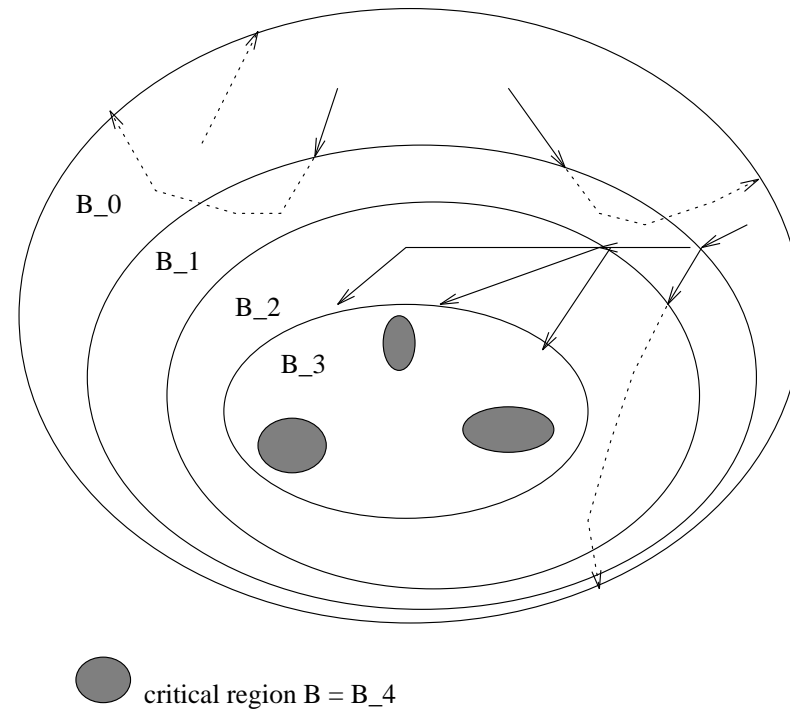
by mimicking the evolution of the continuous-time Markov process  $\{X_t, t \geq 0\}$



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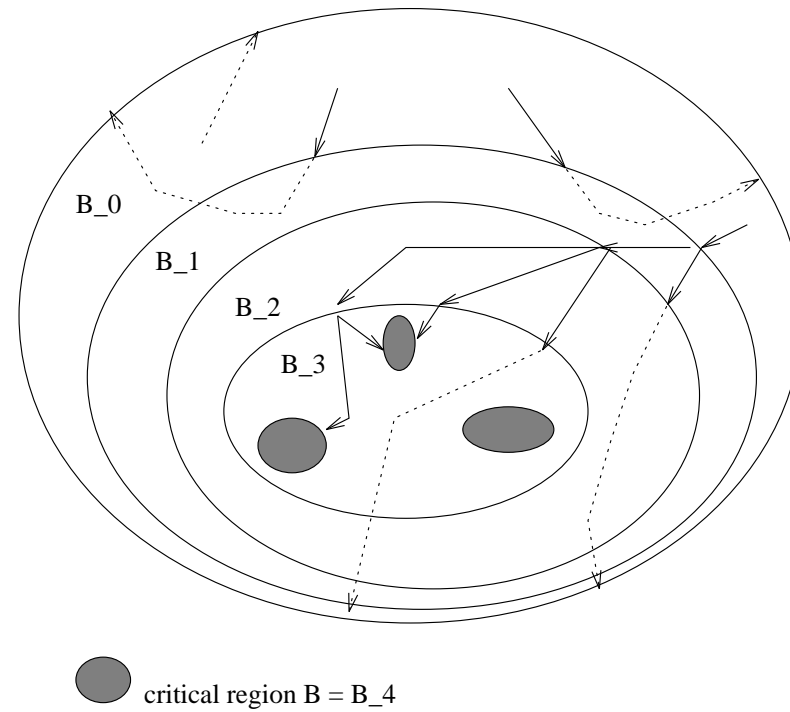
trajectories that succeed to reach the next level before time  $T$  are selected,  
other trajectories are terminated



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between two levels, particles explore the state space

by mimicking the evolution of the continuous-time Markov process  $\{X_t, t \geq 0\}$

trajectories that succeed to reach the next level before time  $T$  are selected,  
other trajectories are terminated

it could happen that all trajectories fail to reach the next level before time  $T$  !

particle approximation of transition probabilities

$$\eta_{k|k-1} \approx \eta_{k|k-1}^N = \frac{1}{N} \sum_{i=1}^N \delta_{\xi_k^i}$$

and in particular for the test-function  $g_k$

$$\mathbb{P}[T_k \leq T \mid T_{k-1} \leq T] = \eta_{k|k-1}(g_k) \approx \eta_{k|k-1}^N(g_k) = \frac{1}{N} \sum_{i=1}^N g_k(\xi_k^i) = \frac{|I_k^N|}{N}$$

where

$$I_k^N = \{i = 1 \cdots N : g_k(\xi_k^i) = 1\} = \{i = 1 \cdots N : T_k^i \leq T\}$$

approximation interpreted as the fraction of trajectories that succeed to reach the next level before time  $T$

particle approximation of rare event probability

$$\gamma_n = \eta_n \prod_{k=1}^n \eta_{k|k-1}(g_k) \approx \gamma_n^N = \eta_n^N \prod_{k=1}^n \eta_{k|k-1}^N(g_k)$$

and in particular

$$\mathbb{P}[T_B \leq T] = \gamma_n(1) \approx \gamma_n^N(1) = \prod_{k=1}^n \eta_{k|k-1}^N(g_k) = \prod_{k=1}^n \frac{|I_k^N|}{N}$$

central limit theorem : as  $N \uparrow \infty$

$$\sqrt{N} \left( \prod_{k=1}^n \frac{|I_k^N|}{N} - \mathbb{P}[T_B \leq T] \right) \Longrightarrow \mathcal{N}(0, \sigma_n^2)$$

provided the particle system does not die !

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change of probability measure (e.g. using the Girsanov theorem)

$$\frac{d\mathbb{P}'}{d\mathbb{P}} \Big|_{\mathcal{F}_{T_k \wedge T}} = \prod_{p=1}^k r_p(\mathcal{X}_p)$$

where

$$\mathcal{F}_t = \sigma(X_s, 0 \leq s \leq t)$$

such that, under new probability measure  $\mathbb{P}'$ , the event  $(T_B \leq T)$  is much less rare

$$\gamma_k(f) = \mathbb{E}[f(\mathcal{X}_k) \prod_{p=1}^k g_p(\mathcal{X}_p)] = \mathbb{E}'[f(\mathcal{X}_k) \prod_{p=1}^k \frac{g_p(\mathcal{X}_p)}{r_p(\mathcal{X}_p)}]$$

another Feynman–Kac formula, with

- another continuous–time Markov process, which hits the critical region  $B$  with higher probability
- modified selection functions  $\frac{g_p}{r_p}$ , which penalizes trajectories of the new continuous–time Markov process that do not look like typical trajectories of the original continuous–time Markov process

combined importance splitting / importance sampling algorithm

- **selection** of particles with higher weights : independently for  $i = 1 \cdots N$

$$\tau_{k-1}^i \sim (w_{k-1}^1 \cdots w_{k-1}^N) \quad \text{with values in index set } \{1, \cdots, N\}$$

and

$$\widehat{\xi}_{k-1}^i = \xi_{k-1}^{\tau_{k-1}^i} \quad \text{and} \quad \widehat{T}_{k-1}^i = T_{k-1}^{\tau_{k-1}^i}$$

- **mutation** : independently for  $i = 1 \cdots N$

$$\xi_k^i = (X_t^i, \widehat{T}_{k-1}^i \leq t \leq T_k^i \wedge T^i)$$

follows **new** continuous-time Markov model, starting from  $\pi(\widehat{\xi}_{k-1}^i)$

$$T_k^i = \inf\{t \geq \widehat{T}_{k-1}^i : X_t^i \in B_k\}$$

- **weighting** according to success to reach next level and to similarity with a typical trajectory of **original** continuous-time Markov model : for  $i = 1 \cdots N$

$$w_k^i \propto \frac{g_k(\xi_k^i)}{r_k(\xi_k^i)} = \frac{1_{(X_{T_k^i \wedge T^i}^i \in B_k)}}{r_k(\xi_k^i)}$$

particle approximation of transition probabilities

$$\mathbb{P}[T_k \leq T \mid T_{k-1} \leq T] \approx \frac{1}{N} \sum_{i=1}^N \frac{g_k(\xi_k^i)}{r_k(\xi_k^i)} = \frac{|I_k^N|}{N} \left[ \frac{1}{|I_k^N|} \sum_{i \in I_k^N} \frac{1}{r_k(\xi_k^i)} \right]$$

particle approximation of rare event probability

$$\mathbb{P}[T_B \leq T] \approx \prod_{k=1}^n \frac{|I_k^N|}{N} \left[ \frac{1}{|I_k^N|} \sum_{i \in I_k^N} \frac{1}{r_k(\xi_k^i)} \right]$$

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**lifetime** of particle system

$$\tau^N = \inf\{k \geq 0 : |I_k^N| = 0\} = \inf\{k \geq 0 : I_k^N = \emptyset\}$$

if  $\mathbb{P}[T_B \leq T] > 0$ , then

$$\mathbb{P}[\tau^N \leq n] \leq c_n \exp\{-a_n N\}$$

for some positive constants  $c_n > 0$  and  $a_n > 0$

central limit theorem : as  $N \uparrow \infty$

$$\sqrt{N} (1_{(\tau^N > n)} \prod_{k=1}^n \frac{|I_k^N|}{N} - \mathbb{P}[T_B \leq T]) \implies \mathcal{N}(0, \sigma_n^2)$$

how to make sure that the particle system never dies ?

if it ever dies, reinitialize it as an  $N$ -sample from an arbitrary probability distribution  $\nu$  on  $E$

particle approximation of the form

$$\eta_k \approx \eta_k^N = \sum_{i=1}^N w_k^i \delta_{\xi_k^i} \quad \text{where} \quad \xi_k^i = (X_t^i, T_{k-1}^i \wedge T^i \leq t \leq T_k^i \wedge T^i)$$

such that

$$\eta_{k-1}^N \longrightarrow \eta_{k|k-1}^N = S^N(\eta_{k-1}^N Q_k) \longrightarrow \eta_k^N = g_k \odot \eta_{k|k-1}^N$$

where

$$g_k \odot \eta_{k|k-1}^N = \begin{cases} \frac{g_k \eta_{k|k-1}^N}{\eta_{k|k-1}^N(g_k)}, & \text{if } \eta_{k|k-1}^N(g_k) > 0 \\ \nu, & \text{otherwise} \end{cases}$$

algorithm with **reinitialization**, Del Moral, Jacod and Protter (PTRF, 2001)

- **selection** of particles with nonzero weight : independently for  $i = 1 \dots N$

$$\tau_{k-1}^i \sim (w_{k-1}^1, \dots, w_{k-1}^N) \quad \text{with values in index set } \{1, \dots, N\}$$

and

$$\widehat{\xi}_{k-1}^i = \xi_{k-1}^{\tau_{k-1}^i} \quad \text{and} \quad \widehat{T}_{k-1}^i = T_{k-1}^{\tau_{k-1}^i}$$

- **mutation** : independently for  $i = 1 \dots N$

$$\xi_k^i = (X_t^i, \widehat{T}_{k-1}^i \leq t \leq T_k^i \wedge T^i)$$

follows the continuous-time Markov model, starting from  $\pi(\widehat{\xi}_{k-1}^i)$

$$T_k^i = \inf\{t \geq \widehat{T}_{k-1}^i : X_t^i \in B_k\}$$

- if  $|I_k^N| \neq 0$ , then **weighting** according to success to reach next level : for  $i = 1 \cdots N$

$$w_k^i \propto g_k(\xi_k^i) = 1_{(X_{T_k^i \wedge T^i}^i \in B_k)}$$

otherwise, if  $|I_k^N| = 0$ , the whole particle system  $\{\xi_k^i, i = 1 \cdots N\}$  is discarded, and **reinitialized** as an  $N$ -sample from an arbitrary probability distribution  $\nu$  on  $E$



another way to make sure that the particle systems never dies

generate a random number  $N_k^H$  of particles (a stopping time) such that exactly  $H$  trajectories succeed to reach the next level

particle approximation of the form

$$\eta_k \approx \eta_k^H = \sum_{i=1}^{N_k^H} w_k^i \delta_{\xi_k^i} \quad \text{where} \quad \xi_k^i = (X_t^i, T_{k-1}^i \wedge T^i \leq t \leq T_k^i \wedge T^i)$$

such that

$$\eta_{k-1}^H \longrightarrow \eta_{k|k-1}^H = S^{N_k^H}(\eta_{k-1}^H Q_k) \longrightarrow \eta_k^H = g_k \cdot \eta_{k|k-1}^H$$

where

$$N_k^H = \inf\{N \geq 0 : |I_k^N| = H\} = \inf\{N \geq 0 : \sum_{i=1}^N g_k(\xi_k^i) = H\}$$

**sequential** algorithm, Oudjane (PhD, 2000), FG and Oudjane (AAP, 2004)

- **selection** of particles with nonzero weight : independently for  $i = 1 \dots N_k^H$

$$\tau_{k-1}^i \sim (w_{k-1}^1, \dots, w_{k-1}^{N_{k-1}^H}) \quad \text{with values in index set } \{1, \dots, N_{k-1}^H\}$$

and

$$\widehat{\xi}_{k-1}^i = \xi_{k-1}^{\tau_{k-1}^i} \quad \text{and} \quad \widehat{T}_{k-1}^i = T_{k-1}^{\tau_{k-1}^i}$$

- **mutation** : independently for  $i = 1 \dots N_k^H$

$$\xi_k^i = (X_t^i, \widehat{T}_{k-1}^i \leq t \leq T_k^i \wedge T^i)$$

follows the continuous-time Markov model, starting from  $\pi(\widehat{\xi}_{k-1}^i)$

$$T_k^i = \inf\{t \geq \widehat{T}_{k-1}^i : X_t^i \in B_k\}$$

- population size  $N_k^H$  is chosen such that  $H$  trajectories exactly succeed to reach the next level, i.e.

$$N_k^H = \inf\{N \geq 0 : |I_k^N| = H\} = \inf\{N \geq 0 : \sum_{i=1}^N g_k(\xi_k^i) = H\}$$

- **weighting** according to success to reach next level : for  $i = 1 \dots N_k^H$

$$w_k^i \propto g_k(\xi_k^i) = 1_{(X_{T_k^i \wedge T^i}^i \in B_k)}$$

given past history of the particle system, the r.v.'s  $\xi_k^i$  are i.i.d. : as  $N \uparrow \infty$

$$\frac{1}{N} \sum_{i=1}^N g_k(\xi_k^i) \longrightarrow \eta_{k-1}^{N_{k-1}^H} Q_k(g_k) = \eta_{k-1}^{N_{k-1}^H} (Q_k g_k)$$

notice that

$$\text{supp } \eta_{k-1}^{N_{k-1}^H} \subset \{e \in E : \pi(e) \in B_{k-1}\}$$

and the strong Markov property yields

$$Q_k g_k(e) = \mathbb{E}[g_k(\mathcal{X}_k) \mid \mathcal{X}_{k-1} = e] = \mathbb{P}[T_k \leq T \mid X_{T_{k-1} \wedge T} = \pi(e)]$$

hence, if

$$\mathbb{P}[T_k \leq T \mid X_{T_{k-1} \wedge T} = x] > 0 \quad \text{for any } x \in B_{k-1}$$

then  $\eta_{k-1}^{N_{k-1}^H} (Q_k g_k) > 0$ , and

$$N_k^H = \inf \left\{ N \geq 0 : \sum_{i=1}^N g_k(\xi_k^i) = H \right\}$$

is an a.s. finite and integrable stopping time

particle approximation of transition probabilities

$$\mathbb{P}[T_k \leq T \mid T_{k-1} \leq T] = \eta_{k|k-1}(g_k) \approx \eta_{k|k-1}^H(g_k) = \frac{|I_k^{N_k^H}|}{N_k^H} = \frac{H}{N_k^H}$$

approximation interpreted as the fraction of trajectories that succeed to reach the next level before time  $T$

particle approximation of rare event probability

$$\mathbb{P}[T_B \leq T] = \gamma_n(1) \approx \gamma_n^H(1) = \prod_{k=1}^n \eta_{k|k-1}^H(g_k) = \prod_{k=1}^n \frac{H}{N_k^H}$$

central limit theorem : as  $H \uparrow \infty$

$$\sqrt{H} \left( \prod_{k=1}^n \frac{H}{N_k^H} - \mathbb{P}[T_B \leq T] \right) \implies \mathcal{N}(0, s_n^2)$$

alternate normalization : average size of particle systems (computing resources)

$$N_{1:n}^H = \frac{1}{n} \sum_{k=1}^n N_k^H$$

central limit theorem : as  $H \uparrow \infty$

$$\frac{N_{1:n}^H}{H} \longrightarrow c_n = \frac{1}{n} \sum_{k=1}^n \frac{1}{\eta_{k|k-1}(g_k)}$$

in probability, hence

$$\sqrt{N_{1:n}^H} \left( \prod_{k=1}^n \frac{H}{N_k^H} - \mathbb{P}[T_B \leq T] \right) \implies \mathcal{N}(0, c_n s_n^2)$$

next steps (future work)

- compare  $\sigma_n^2$  vs.  $c_n s_n^2$
- design intermediate levels so as to minimize asymptotic variance