Rare Event Simulation for Piecewise Deterministic Markov Processes

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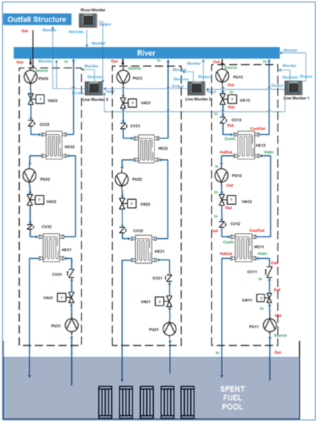
Reliability assessment

- Motivation: Reliability assessment of power generation systems
- Simulation tool: PyCaTSHOO developed by EDF
- Rare event issue: Monte-Carlo is inefficient
- Example: spent fuel pool $\longrightarrow$



- Variance reduction method needed, possible solutions:
  - Importance sampling (IS) $\rightarrow$ Intrusive method modifies the law of the random dynamical system.
    Problem: Choice of the importance distributions.
  - Interacting particle system method (IPS) $\rightarrow$ Non-intrusive method that uses selection steps to favor the "best" simulations.
    Problem: Choice of the potential functions.

Power generation system modeled by a PDMP

- Dynamical system characterized by physical variables (temperature, pressure, water level, ...)
- System failure = physical variables hit a critical region.
- Components are in different statuses (On, Off, Broken, ...), which determine the (deterministic) dynamics of the physical variables
- Partial failures / repairs / control mechanisms.
- State of the system:

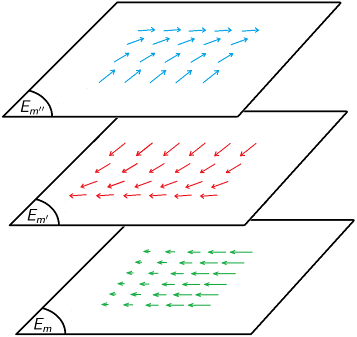
$$Z_t = (M_t, X_t)$$

M_t = statuses of the components = mode (discrete, $M_t \in \mathbb{M}$),
X_t = physical variables = position (continuous, $X_t \in \mathbb{R}^d$).
$\to$ Piecewise deterministic Markov processes (PDMP) (Davis 1984).

$\hookrightarrow$ We need to adapt variance reduction methods for PDMP.

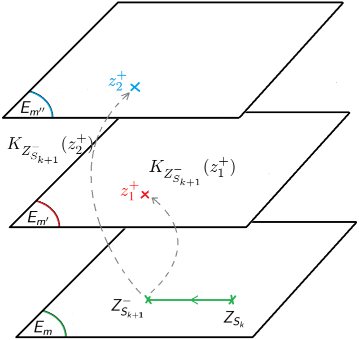
PDMP without boundary

- State space $E = \mathbb{M} \times \mathbb{R}^d = \cup_{m \in \mathbb{M}} E_m$,
  $$E_m = \{(m, x), x \in \mathbb{R}^d\}.$$
- If there is no jump and $Z_0 = (m, x)$, then $Z_t = (m, \phi_{(m,x)}(t))$.
  Typically,
  $$\begin{cases} \frac{d}{dt}\phi_{(m,x)}(t) = V_m(\phi_{(m,x)}(t)), \\ \phi_{(m,x)}(0) = x \end{cases}$$



PDMP without boundary and with random jumps

- State space $E = \cup_{m \in \mathbb{M}} E_m$,
  $E_m = \{(m, x), x \in \mathbb{R}^d\}$.
- Between jumps:
  $Z_{S_k+t} = (M_{S_k}, \phi_{(M_{S_k}, X_{S_k})}(t))$.
- Random jump times:
  $\mathbb{P}(S_{k+1} - S_k \leq t | Z_{S_k})$
  $= 1 - \exp\Big[- \int_0^t \lambda(Z_{S_k+u}) du \Big]$
- Random jump destinations:
  $\mathbb{P}(Z_{S_{k+1}} \in A | Z_{S_k}, S_{k+1} - S_k) = \mathcal{K}_{Z^-_{S_{k+1}}}(A)$
  where $Z^-_{S_{k+1}} = (M_{S_k}, \phi_{Z_{S_k}}(S_{k+1} - S_k))$.



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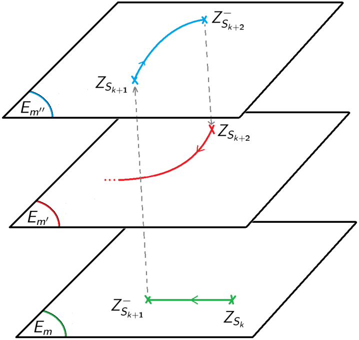
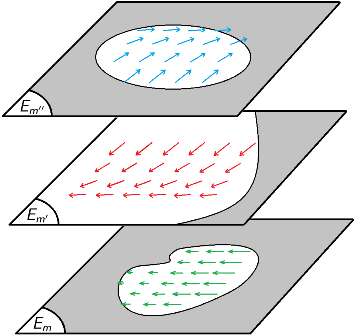


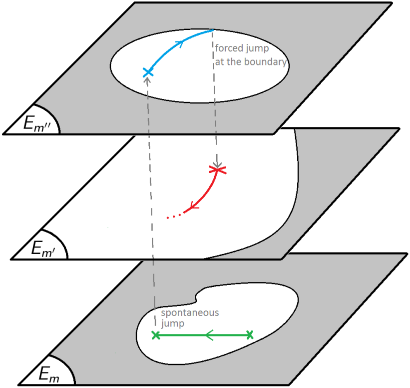
PDMP with boundaries

- State space $E = \cup_{m \in \mathbb{M}} E_m$,
  $E_m = \{(m,x), x \in \Omega_m\}$, Ω_m open.
- If there is no random jump,
  if $Z_0 = (m,x)$,
  then $Z_t = (m, \phi_{(m,x)}(t))$,
  until Z_t hits a boundary at $t = t^*(m,x)$,
  $t^*(m,x) = \inf\{s > 0,\ \phi_{(m,x)}(s) \in \partial\Omega_m\}$
  and then it jumps.



PDMP with boundaries and with random jumps

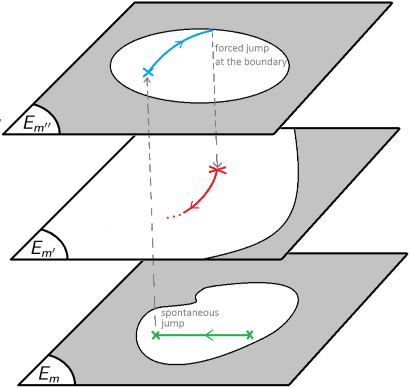
- State space $E = \cup_{m\in\mathbb{M}} E_m$,
  $E_m = \{(m,x), x \in \Omega_m\}$.
- Between jumps:
  $Z_{S_k+t} = (M_{S_k}, \phi_{(M_{S_k},X_{S_k})}(t))$.
- Random jump times:
  if $t < t^*(Z_{S_k})$, then
  $\mathbb{P}(S_{k+1} - S_k \leq t | Z_{S_k})$
  $= 1 - \exp\Big[- \int_0^t \lambda(Z_{S_k+u})du \Big]$
  if $t \geq t^*(Z_{S_k})$, then
  $\mathbb{P}(S_{k+1} - S_k \leq t | Z_{S_k}) = 1$.



- Random jump destinations:
  $\mathbb{P}(Z_{S_{k+1}} \in A | Z_{S_k}, S_{k+1} - S_k) = \mathcal{K}_{Z^-_{S_{k+1}}}(A)$
  for $z^- \in \partial E$, $\mathcal{K}_{z^-}$: destination for a forced jump at boundary
  for $z^- \in E$, $\mathcal{K}_{z^-}$: destination for a random (spontaneous) jump

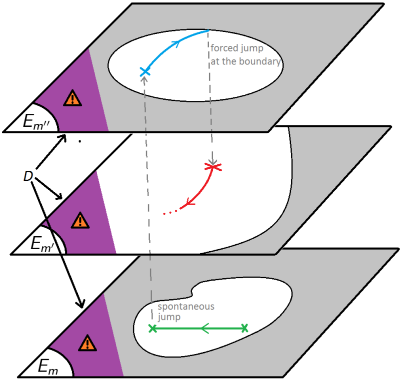
Model a power generation system by a PDMP

- State space $E = \cup_{m \in \mathbb{M}} E_m$,
  $E_m = \{(m, x), x \in \Omega_m\}$.
- $Z_t = (M_t, X_t)$ with
  M_t statuses of the components (off, ...)
  X_t physical variables (temperature, ...)
- ϕ is deduced from physics laws
- spontaneous jumps model failures and repairs
- jumps at boundaries model control mechanisms (with possible failure on demand).



Reliability assessment for a PDMP with boundaries

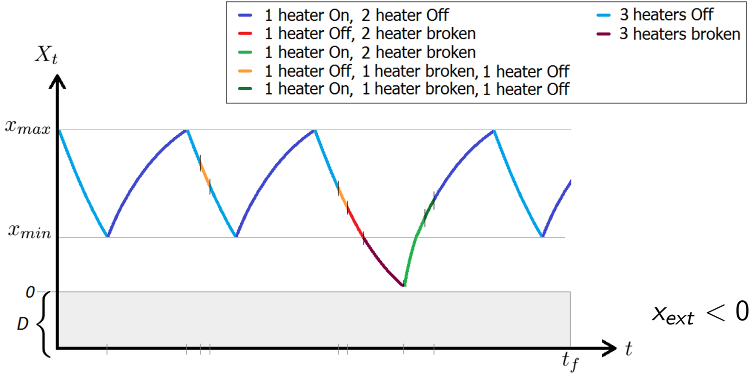
- State space $\cup_{m \in \mathbb{M}} E_m$,
  $$E_m = \{(m, x), x \in \Omega_m\}.$$
- Failure domain $D \subset \mathbb{R}^d$.
- Goal: estimate
  $$p = \mathbb{P}(\exists t \in [0, t_f], Z_t \in D).$$



An example: a heated room system

- System heated by three redundant components.
- $M_t \in \mathbb{M} = \{Off, On, Broken\}^3$ and $X_t \in \mathbb{R}$ room temperature.
- X_t is governed by an ODE parameterized by m:

$$\frac{dX_t}{dt} = \kappa(x_{ext} - X_t) + \sum_{j=1}^{3} q_j \mathbf{1}_{m_j=On}$$



An example: a heated room system

- System heated by three redundant components (heaters).
- $M_t \in \mathbb{M} = \{Off, On, Broken\}^3$ and $X_t \in \mathbb{R}$ room temperature.
- X_t is governed by an ODE parameterized by m.
- For heater $j = 1, 2, 3$:
  λ_j=failure rate when heater j is On,
  κ_j=failure rate when heater j is Off,
  μ_j=repair rate when heater j is Broken,
  π_j=probability of failure on demand of heater j.
- Jump intensity rate:

$$\lambda(z = (m, x)) = \sum_{j, m_j = On} \lambda_j + \sum_{j, m_j = Off} \kappa_j + \sum_{j, m_j = Broken} \mu_j$$

- Jump destination kernel: if $x \in (x_{min}, x_{max})$ and $m^- = (Off, Off, Off)$

$$\mathcal{K}_{(x,m^-)}(\{x, m\}) = \begin{cases} \frac{\kappa_1}{\kappa_1+\kappa_2+\kappa_3} & \text{if } m = (Broken, Off, Off) \\ \frac{\kappa_2}{\kappa_1+\kappa_2+\kappa_3} & \text{if } m = (Off, Broken, Off) \\ \frac{\kappa_3}{\kappa_1+\kappa_2+\kappa_3} & \text{if } m = (Off, Off, Broken) \end{cases}$$

and so on.

Importance sampling (IS) with PDMPs

Denote $\mathbf{Z} = (Z_t)_{t \in [0,t_f]}$. We want to estimate $p = \mathbb{P}(\mathbf{Z} \in \mathcal{D})$.

Idea: Determine an importance process (PDMP) $\mathbf{Z}'$ such that

- $p = \mathbb{E}[\mathbf{1}_{\mathcal{D}}(\mathbf{Z}')\mathcal{L}(\mathbf{Z}')]$ where $\mathcal{L}$ is the likelihood ratio of the distribution of $\mathbf{Z}'$ wrt the distribution of $\mathbf{Z}$,
- $\mathbb{E}\big[\mathbf{1}_{\mathcal{D}}(\mathbf{Z}')\mathcal{L}(\mathbf{Z}')^2\big]$ is small.

Indeed, if $(\mathbf{Z}'_j)_{j=1}^N$ is an iid sample with the distribution of $\mathbf{Z}'$, then

$$\hat{p}_{IS} = \frac{1}{N} \sum_{j=1}^{N} \mathbf{1}_{\mathcal{D}}(\mathbf{Z}'_j)\mathcal{L}(\mathbf{Z}'_j)$$

is an unbiased estimator of p with variance

$$\mathrm{Var}\big(\hat{p}_{IS}\big) = \frac{1}{N}\Big[\mathbb{E}\big[\mathbf{1}_{\mathcal{D}}(\mathbf{Z}')\mathcal{L}(\mathbf{Z}')^2\big] - p^2\Big]$$

Ideally, for the optimal importance process, we have $\mathbb{E}[\mathbf{1}_{\mathcal{D}}(\mathbf{Z}')\mathcal{L}(\mathbf{Z}')^2] = p^2$ and $\mathrm{Var}\big(\hat{p}_{IS}\big) = 0$.

Reference measure for PDMPs

With simple hypotheses: λ is bounded and $\mathcal{K}_{z^-}(A) = \int_A K_{z^-}(z)\nu_{z^-}(dz)$

- Denote by S_k the time and by Z_{S_k} the arrival state of the k-th jump.
- Denote $\mathbf{Z} = (Z_t)_{t\in[0,t_f]}$ with $S_0 = 0$, $Z_0 = z_0$,
  $\Theta(\mathbf{Z}) = \big(S_1, Z_{S_1}, S_2 - S_1, Z_{S_2}, \dots\big)$.
- Θ is one-to-one.
- It is possible to write a reference measure (with $t_j = s_j - s_{j-1}$):

$$\zeta(\cdot) = \int_{\Theta(\cdot)} \mu_{z_0}(dt_1)\nu_{z_1^-}(dz_1)\cdots\mu_{z_{n-1}}(dt_n)\nu_{z_n^-}(dz_n)\mu_{z_n}(dt_{n+1})$$

  with $z_{j+1}^- = \phi_{z_j}(t_{j+1})$ and $\mu_z(dt) = \lambda(dt) + \delta_{t^*(z)}(dt)$.
- The density of a trajectory is (with $t_k = s_k - s_{k-1}$):

$$f(\mathbf{z}) = \prod_{k=0}^{n} \lambda(\phi_{z_k}(t_{k+1}))^{\mathbf{1}_{t_{k+1}<t^*(z_k)}} \exp\Big[-\int_0^{t_{k+1}} \lambda(\phi_{z_k}(u))du\Big] \prod_{k=1}^{n} K_{z_k^-}(z_k)$$

  Note: There are trajectories $\mathbf{z}$ such that $\mathbb{P}(\mathbf{Z} = \mathbf{z}) > 0$.

Optimal importance process

The optimal importance process is a PDMP.

- Do not modify the flows $\phi_z(t)$ and the boundaries $\partial\Omega_m$.
- Modify the jump time intensity

$$\lambda^*(z,t) = \lambda(z)\frac{U^{*,-}(z,t)}{U^*(z,t)}$$

- Modify the jump destination kernel

$$K^*_{z^-}(z,t) = K_{z^-}(z)\frac{U^*(z,t)}{U^{*,-}(z^-,t)}$$

where

$$\begin{aligned} U^*(z,t) &= \mathbb{P}(\exists s \in [t,t_f], Z_s \in D | Z_t = z) \\ U^{*,-}(z^-,t) &= \mathcal{K}_{z^-} U^*(\cdot,t) \\ &= \mathbb{P}(\exists s \in [t,t_f], Z_s \in D | Z_{t^-} = z^-, \text{ jump at } t) \end{aligned}$$

$U^*(z,t)$ = committor function (promixity to the failure domain).

Practical importance process

- Let $U_\alpha(z,t)$ be a a parametric function family (that is intended to approximate $U^*(z,t)$)
- Consider the PMDP (depending on α) with the original flows and

$$\lambda_\alpha(z,t) = \lambda(z)\frac{U_\alpha^-(z,t)}{U_\alpha(z,t)}$$

$$K_{\alpha,z^-}(z,t) = K_{z^-}(z)\frac{U_\alpha(z,t)}{U_\alpha^-(z^-,t)}$$

with $U_\alpha^-(z^-,t) = \mathcal{K}_{z^-} U_\alpha(\cdot,t)$.

- Implement IS with the PDMP built with $(\lambda_\alpha, K_\alpha)$.
- Determine α by a cross-entropy method (for instance).

Empirical results on the heated room system

- Let $b(z)$ be the number of broken heaters.
- Let $U_\alpha(z,t) = \exp[\alpha b(z)^2]$, $\alpha > 0$ (a unique parameter !).
- Then

	N_{sim}	$\hat{p}_{IS}$	$\hat{\sigma}^2_{IS}/N_{sim}$	Conf. interval
MC	10^6	$0.4\,10^{-5}$	$4.0\,10^{-12}$	$[0.01\,10^{-5}, 0.79\,10^{-5}]$
	10^7	$1.3\,10^{-5}$	$1.3\,10^{-12}$	$[1.07\,10^{-5}, 1.51\,10^{-5}]$
IS	10^3	$1.28\,10^{-5}$	$4.37\,10^{-13}$	$[1.15\,10^{-5}, 1.41\,10^{-5}]$
	10^6	$1.288\,10^{-5}$	$5.05\,10^{-16}$	$[1.283\,10^{-5}, 1.292\,10^{-5}]$

H. Chraibi, A. Dutfoy, T. Galtier, and J. Garnier, Optimal importance process for piecewise deterministic Markov process, ESAIM P&S **23**, pp. 893-921 (2019).

Interacting particle system (IPS)

- Discretize the trajectories $\mathbf{z} = (z_t)_{t \in [0,t_f]}$:

$$\tau_k = k t_f / n, \qquad \mathbf{z}_k = (z_0, z_{\tau_1}, \ldots, z_{\tau_k})$$

- Consider:

$$p = \mathbb{P}(\mathbf{Z}_n \in \mathcal{D}) = \mathbb{P}\big(\exists k \in \{0, \ldots, n\},\, Z_{\tau_k} \in D\big)$$

Principle:

- Use the original Markovian dynamics (i.e., the original λ and K).
- Select the good "particles" using potential functions $G_k(\mathbf{z}_k)$ (forget low-potential trajectories, multiply high-potential trajectories).

P. Del Moral and J. Garnier, Genealogical particle analysis of rare events, Ann. Appl. Probab. **15**, pp. 2496-2534 (2005).

IPS: algorithm

- For given potential functions $G_k(\mathbf{z}_k)$, $k = 0, \ldots, n-1$.
- IPS generator of a system of N particles $(\mathbf{Z}_n^j)_{j=1}^N$:

Initialization $k = 0$**:** $\forall j = 1, \ldots, N$, $\mathbf{Z}_0^j \stackrel{i.i.d.}{\sim} \pi_0$.
while $k < n$ **do**
Selection:
$(\tilde{N}_k^j)_{j=1,\ldots,N} \sim Mult\big(N, (W_k^j)_{j=1,\ldots,N}\big)$, $W_k^j = \frac{G_k(\mathbf{Z}_k^j)}{\sum_{s=1}^N G_k(\mathbf{Z}_k^s)}$
$\tilde{\mathbf{Z}}_k^j = \mathbf{Z}_{\tilde{N}_k^j}^j$, $\tilde{W}_k^j = W_{\tilde{N}_k^j}^j$.
Propagation:
for $j = 1, \ldots, N$ **do**
continue the trajectory $\tilde{\mathbf{Z}}_k^j$ to get $\mathbf{Z}_{k+1}^j$
using the original Markov dynamics,
set $W_{k+1}^j = \tilde{W}_k^j$

IPS: properties

- The estimator:

$$\hat{p}_{IPS} = \Big[\frac{1}{N}\sum_{j=1}^{N}\frac{\mathbf{1}_{\mathcal{D}}(\mathbf{Z}_n^j)}{\prod_{k=0}^{n-1} G_k(\mathbf{Z}_k^j)}\Big]\prod_{k=0}^{n-1}\Big[\frac{1}{N}\sum_{j=1}^{N} G_k(\mathbf{Z}_k^j)\Big]$$

  is unbiased and strongly consistent.

- When the potential functions are positive-valued, we have

$$\sqrt{N}(\hat{p}_{IPS} - p) \xrightarrow[N\to\infty]{d} \mathcal{N}\big(0, \sigma^2_{IPS,G}\big),$$

  with

$$\sigma^2_{IPS,G} = \sum_{k=0}^{n}\left\{\mathbb{E}\Big[\prod_{i=0}^{k-1} G_i(\mathbf{Z}_i)\Big]\mathbb{E}\Big[\mathbb{P}(\mathbf{Z}_n \in \mathcal{D}|\mathbf{Z}_k)^2 \prod_{s=0}^{k-1} G_s^{-1}(\mathbf{Z}_s)\Big] - p^2\right\}$$

  Empirical estimators of the asymptotic variance are available (Lee and Whiteley 2018).

IPS: Optimal potential functions

σ^2_{IPS} is minimized for the following potential functions:

$$G_k^*(\mathbf{z}_k) = \sqrt{\frac{g_k(z_{\tau_k})}{g_{k-1}(z_{\tau_{k-1}})}}, \qquad \mathbf{z}_k = (z_0, z_{\tau_1}, \ldots, z_{\tau_k})$$

for $k = 0, \ldots, n-1$, with $g_{-1}(z) = 1$,

$$g_k(z) = \mathbb{E}\big[U^*(Z_{\tau_{k+1}}, \tau_{k+1})^2 | Z_{\tau_k} = z\big]$$

and $U^*(z, \tau_k) = \mathbb{P}(\exists j \in \{k, \ldots, n\}, \, Z_{\tau_j} \in D | Z_{\tau_k} = z)$.
Note that

- G^* is defined in terms of the committor function U^*.
- G^* depends on k, z_{τ_k} and $z_{\tau_{k-1}}$ only.
- The minimal variance is (usually) positive (IPS not as efficient as IS).

H. Chraibi, A. Dutfoy, T. Galtier, and J. Garnier, Optimal potential functions for the interacting particle system method, Monte Carlo Methods Appl., mcma-2021-2086 (2021).

IPS for PDMP

- Concentrated PDMP: low jumps rates and concentrated jump kernels.
- Example: Reliable energy production systems are concentrated PDMPs.
- The process is likely to follow deterministic paths, jumping only at boundaries.
- If possible, use a version of the memorization method (Labeau 1996) in the IPS method (weakly intrusive method).
- $\hat{p}_{IPS+M}$ is unbiased, strongly consistent, asymptotically normal and

$$\sigma^2_{IPS+M} \leq \sigma^2_{IPS}$$

H. Chraibi, A. Dutfoy, T. Galtier, and J. Garnier, Application of the interacting particle system method to piecewise deterministic Markov processes used in reliability, Chaos **29**, 063119 (2019).