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Importance sampling of Piecewise Deterministic Markov Processes for rare event simulation



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Estimation of the probability of failure of industrial systems involved in the operation of nuclear power plants and dams.



• A computer code simulates the operation of the system.

 \longrightarrow Piecewise Deterministic Markov Processes.

- Typical probabilities of failure are very small (about 10⁻⁵).
- Each simulation is numerically expensive.
- \hookrightarrow Crude Monte-Carlo methods are not feasible.

Piecewise Deterministic Markov Processes

PDMP	Rare event simulation	Mean hitting times	AIS—CE	Numerical results
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Definition of	a PDMP			Sedf

Piecewise Deterministic Markov Process (M.H.A Davis 1984)

Hybrid process: $Z_t = (X_t, M_t) \in E$

- position $X_t \in \mathcal{X}$ is continuous
- mode $M_t \in \mathcal{M}$ is discrete
- $\blacksquare \begin{tabular}{ll} Flow Φ \rightarrow deterministic dynamics between two jumps \end{tabular}$
- **2** Jump intensity $\lambda \rightarrow$ law of the time of the random jumps
- 3 Jump kernel K → law of the state of the process after a jump





Take home message:

- explicit computation of the pdf of a PDMP trajectory,
- no need to recalculate the flow.

Rare event simulation

PDMP	Rare event simulation	Mean hitting times	AIS—CE	Numerical results
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Objective: estimate

$$\mathrm{P}_{\mathcal{F}} = \mathbb{P}_{f_0}\left(\mathbf{Z} \in \mathcal{T}_{\mathcal{F}}\right) = \mathbb{P}_{f_0}\left(\exists t \in [0, t_{\mathsf{max}}] : Z_t \in \mathcal{F}\right)$$

- $\mathbf{Z} = (Z_t)_{t \in [0, t_{max}]}$ is a PDMP trajectory of fixed duration t_{max} ,
- **\mathbf{Z} \sim f_0** the reference distribution of the PDMP trajectory,
- $T_{\mathcal{F}}$ is the set of feasible PDMP trajectories that reach a critical region \mathcal{F} of the state space before time t_{max} .

Crude Monte-Carlo :
$$\widehat{\mathrm{P}}_{\mathcal{F}}^{\mathsf{CMC}} = \frac{1}{N} \sum_{k=1}^{N} \mathbb{1}_{\mathbf{Z}_k \in \mathcal{T}_{\mathcal{F}}}$$
 with $\mathbf{Z}_1, \ldots, \mathbf{Z}_N \stackrel{\text{i.i.d.}}{\sim} f_0$

 $\label{eq:requires on average 1/P_{\mathcal{F}} simulations to obtain one realization of the event.}$ $\hookrightarrow \mbox{High relative variance of } \widehat{P}_{\mathcal{F}}^{\mbox{CMC}} \mbox{ when } P_{\mathcal{F}} \mbox{ is small.}$



Idea: simulate trajectory Z according to an alternative distribution g which gives more weight on T_F than f_0 , then fix the bias with the likelihood ratio $w = f_0/g$.

Importance sampling trick with alternative distribution g :

$$P_{\mathcal{F}} = \mathbb{P}_{f_0} \left(\mathbf{Z} \in \mathcal{T}_{\mathcal{F}} \right) = \mathbb{E}_{f_0} \left[\mathbb{1}_{\mathbf{Z} \in \mathcal{T}_{\mathcal{F}}} \right] = \int \mathbb{1}_{\mathbf{z} \in \mathcal{T}_{\mathcal{F}}} f_0(\mathbf{z}) d\zeta(\mathbf{z})$$
(2)

$$= \int \mathbb{1}_{\mathbf{z}\in\mathcal{T}_{\mathcal{F}}} \frac{f_0(\mathbf{z})}{g(\mathbf{z})} g(\mathbf{z}) d\zeta(\mathbf{z}) = \mathbb{E}_g \left[\mathbb{1}_{\mathbf{Z}\in\mathcal{D}} \frac{f_0(\mathbf{Z})}{g(\mathbf{Z})} \right]$$
(3)

IS estimator:
$$\widehat{\mathrm{P}}_{\mathcal{F}}^{\mathsf{IS}} = \frac{1}{N} \sum_{k=1}^{N} \mathbb{1}_{\mathbf{Z}_k \in \mathcal{T}_{\mathcal{F}}} \frac{f_0(\mathbf{Z}_k)}{g(\mathbf{Z}_k)} \quad \text{with } \mathbf{Z}_1, \dots, \mathbf{Z}_N \overset{\text{i.i.d.}}{\sim} g \qquad (4)$$

 \hookrightarrow Variance of $\widehat{\mathrm{P}}_{\mathcal{F}}^{\mathsf{IS}}$ relies on the choice of g



- Optimal IS distribution: $g_{opt} : z \mapsto \frac{1}{P_{\mathcal{F}}} \mathbb{1}_{z \in \mathcal{T}_{\mathcal{F}}} f_0(z)$ produces a zero-variance IS estimator.
- PDMP case: the optimal IS distribution g_{opt} is fully determined by the so-called committor function U_{opt} of the process. Knowing U_{opt} is sufficient to generate PDMP trajectories under g_{opt}.
- **Committor function:** probability of realizing the rare event {**Z** ∈ *T*_{*F*}} knowing the state of the process at any given time *s* ∈ [0, *t*_{max}].

$$U_{\text{opt}}(Z_s) = \mathbb{P}_{f_0}(\mathbf{Z} \in \mathcal{T}_{\mathcal{F}} | Z_s)^{\mathbb{I}_{\mathbf{Z}_s \notin \mathcal{T}_{\mathcal{F}}}} \quad \text{with} \quad \mathbf{Z}_s = (Z_t)_{t \in [0,s]}.$$
(5)

• General committor function: when estimating $\mathbb{E}_{f_0} [\varphi(\mathbf{Z})]$ we have $\bigcup_{\text{opt}} (\mathbf{Z}_s) = \mathbb{E}_{f_0} [\varphi(\mathbf{Z}) \mid \mathbf{Z}_s]$ with $\mathbf{Z}_s = (Z_t)_{t \in [0,s]}$.



Edge committor function U_{opt}^- : mean value of the committor function knowing the process is about to jump with reference jump kernel K_0 .

$$^{II} U_{opt}^{-}(Z_{s}^{-}) = \mathbb{E}_{\mathcal{K}_{\mathbf{0}}(Z_{s}^{-}, \cdot)} [U_{opt}(Z_{s})]^{II}.$$

$$\tag{6}$$

Optimal jump intensity and jump kernel: (Thomas Galtier 2019)

$$"\lambda_{\rm opt} = \lambda_0 \times \frac{U_{\rm opt}^-}{U_{\rm opt}}" \quad \text{and} \quad "K_{\rm opt} = K_0 \times \frac{U_{\rm opt}}{U_{\rm opt}^-}".$$
(7)

If the process is *c* times more likely to realize the event:

- **1** by jumping now from state z, then $\lambda_{opt}(z)$ should be c times $\lambda_0(z)$,
- 2 by jumping to state z from state z^- rather than jumping randomly from z^- , then $K_{opt}(z^-, z)$ should be c times $K_0(z^-, z)$.

PDMP 000	Rare event simulation 00000●	Mean hitting times	AIS—CE 000	Numerical results 00000
Our method	in a nutshell			Sede

- Chennetier, Chraibi, Dutfoy, Garnier (2022), Adaptive importance sampling based on fault tree analysis for piecewise deterministic Markov process. *arXiv preprint arXiv:2210.16185*.
- **1** Building a family of approximations of the committor function U_{opt}.
 - First contribution: Fault tree analysis (minimal path sets and cut sets),
 - *Current work:* Mean hitting times of a random walk on a graph.
- The best representative of this family is sequentially determined using a cross-entropy procedure coupled with a recycling scheme for past samples.
- 3 A consistent and asymptotically normal post-processing estimator of the final probability $P_{\mathcal{F}}$ is returned.

Approximating U_{opt} with graph-based mean hitting times





Figure 1: PDMP with 64 modes, $\mathcal{M}_\mathcal{F}$ in dark blue.

 $\mathbf{Z}\in\mathcal{T}_{\mathcal{F}}$ only if the trajectory stays long enough in a mode of $\mathcal{M}_{\mathcal{F}}.$



- Let $(Y_t)_t$ be a time-continuous random walk on the mode set \mathcal{M} with an infinitesimal generator matrix Q.
- We note $h_m = \mathbb{E}[\tau_m(\mathcal{M}_{\mathcal{F}})]$ with $\tau_m(\mathcal{M}_{\mathcal{F}}) = \inf_{t \ge 0} \{Y_t \in \mathcal{M}_{\mathcal{F}} \mid Y_0 = m\}.$
- If the random walk is time-homogeneous then (h_m)_{m∈M} the vector of mean hitting times of M_F is explicit and solution of the linear system:

$$h_{m_1} = 0 \ \forall m_1 \in \mathcal{M}_F \text{ and } \sum_{m_2 \notin \mathcal{M}_F} Q[m_1, m_2] h_{m_2} = -1 \ \forall m_1 \notin \mathcal{M}_F.$$
 (8)

Idea: compute $(h_m)_{m \in \mathcal{M}}$ for a matrix Q chosen such that $(Y_t)_t$ "behaves like" $(M_t)_t$ the mode part of the PDMP trajectory $(Z_t)_t$.

 \hookrightarrow In practice even using the simple random walk gives good results.

Minimal support condition: for any $m_1, m_2 \in \mathcal{M}$, $Q[m_1, m_2] > 0$ only if there are $x_1, x_2 \in \mathcal{X}$ such that $K((x_1, m_1), (x_2, m_2)) > 0$.

 PDMP
 Rare event simulation
 Mean hitting times
 AIS—CE
 Numerical results

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Proximity score and approximation of U_{opt}

I For each mode $m \in \mathcal{M}$, we set ρ_m the proximity score to the set $\mathcal{M}_{\mathcal{F}}$:

$$\rho_m = 1 - \frac{h_m}{\max_{m' \in \mathbb{M}} \{h_{m'}\}} \in [0, 1].$$

We define a family (U_θ)_{θ∈Θ} of approximations of U_{opt} parameterized by a vector θ ∈ Θ ⊂ ℝ^{d_Θ} of arbitrary size d_Θ.

$$U_{\theta}\left((x,m)\right) = \exp\left(\sum_{k=1}^{d_{\Theta}} \theta_k \times \psi_{k,d_{\Theta}}\left(\rho_m\right)\right)$$
(9)

The sequence $(\psi_{k,\infty})_{k\in\mathbb{N}^*}$ is typically a basis of $L^2([0,1])$. For example:

- Polynomial: $\psi_{k,d_{\Theta}}(\rho) = \rho^k$.
- Piecewise linear: $\psi_{k,d_{\Theta}}(\rho) = \rho \mathbb{1}_{\rho > \frac{k-1}{d_{\Theta}}}$.



Figure 2: Scores on a graph with 64 vertices. M_F is given by the vertices with score 1.

Recycling adaptive IS



How to find the best candidate within the family $(U_{\theta})_{\theta \in \Theta}$?

To each candidate $U_{\theta} \in (U_{\theta})_{\theta \in \Theta}$ corresponds an importance distribution $g_{\theta} \in (g_{\theta})_{\theta \in \Theta}$. We look for the closest distribution g_{θ} to g_{opt} in the sense of the Kullback-Leibler divergence.

$$\begin{aligned} \underset{\theta \in \Theta}{\arg\min \mathcal{D}_{\mathsf{KL}}} \left(g_{\mathsf{opt}} \| g_{\theta} \right) &= \underset{\theta \in \Theta}{\arg\min} \ \mathbb{E}_{g_{\mathsf{opt}}} \left[\log \left(\frac{g_{\mathsf{opt}}(\mathbf{Z})}{g_{\theta}(\mathbf{Z})} \right) \right] \\ &= \underset{\theta \in \Theta}{\arg\min} \ \int -\log \left(g_{\theta}(\mathbf{Z}) \right) \frac{\mathbb{1}_{\mathbf{Z} \in \mathcal{T}_{\mathcal{F}}} f_{0}(\mathbf{Z})}{\mathcal{P}_{\mathcal{F}}} d\zeta \left(\mathbf{Z} \right) \\ &= \underset{\theta \in \Theta}{\arg\max} \ \mathbb{E}_{f_{0}} \left[\mathbb{1}_{\mathbf{Z} \in \mathcal{T}_{\mathcal{F}}} \log \left(g_{\theta}(\mathbf{Z}) \right) \right]. \end{aligned}$$

This last quantity can be minimized iteratively by successive Monte-Carlo approximations with importance sampling.



Start with an initial parameter $\theta^{(1)}$. At iteration $j = 1, \dots, J$:

Simulation step: generate a new sample of n_j trajectories

$$\mathbf{Z}_{j,1},\ldots,\mathbf{Z}_{j,n_j} \overset{ ext{i.i.d.}}{\sim} g_{oldsymbol{ heta}^{(j)}}$$

2 Optimization step: compute the next iterate $\theta^{(j+1)}$ by solving:

$$\boldsymbol{\theta}^{(j+1)} \in \operatorname*{arg\,max}_{\boldsymbol{\theta} \in \Theta} \sum_{i=1}^{j} \sum_{k=1}^{n_{j}} \mathbb{1}_{\mathbf{Z}_{i,k} \in \mathcal{T}_{\mathcal{F}}} \frac{f_{0}(\mathbf{Z}_{i,k})}{g_{\boldsymbol{\theta}^{(i)}}(\mathbf{Z}_{i,k})} \log \left[g_{\boldsymbol{\theta}}(\mathbf{Z}_{i,k})\right]$$
(10)

Estimation step: at iteration J, the final estimator of the probability $P_{\mathcal{F}}$ is:

$$\widehat{\mathbf{P}}_{\mathcal{F}} = \frac{1}{\sum_{j=1}^{J} n_j} \sum_{j=1}^{J} \sum_{k=1}^{n_j} \mathbb{1}_{\mathbf{Z}_{j,k} \in \mathcal{T}_{\mathcal{F}}} \frac{f_0(\mathbf{Z}_{j,k})}{g_{\boldsymbol{\theta}^{(j)}}(\mathbf{Z}_{j,k})}$$
(11)

Recycling scheme: past samples are reused during optimization and estimation. We proved **consistency** and **asymptotic normality** of $\widehat{P}_{\mathcal{F}}$ for the PDMP case.

Numerical results



Performances on the spent fuel pool

Test case: Spent fuel pool from nuclear industry. The corresponding graph has 32,768 vertices.

Method	Ν	$\widehat{P}_{\mathcal{F}}$	$\widehat{\sigma}/\widehat{\mathbf{P}}_{\mathcal{F}}$	95% confidence interval
	10 ⁵	2×10^{-5}	223.60	$\left[0 \text{ ; } 4.77 imes 10^{-5} ight]$
СМС	10 ⁶	1.3×10^{-5}	277.35	$\left[5.93 imes10^{-6}\ ;\ 2.01 imes10^{-5} ight]$
	10 ⁷	1.77×10^{-5}	237.68	$\left[1.51 imes10^{-5}\ ;\ 2.03 imes10^{-5} ight]$
AIS-MHT	10 ³	1.86×10^{-5}	1.62	$\left[1.67 imes10^{-5}\ ;\ 2.04 imes10^{-5} ight]$
	10 ⁴	2.01×10^{-5}	0.86	$\left[1.98 imes10^{-5}\ ;\ 2.05 imes10^{-5} ight]$

Table 1: Comparison between crude Monte-Carlo (CMC) and our adaptive importance sampling method with mean hitting times (AIS-MHT).

 \hookrightarrow Variance reduction by a factor of 10,000.



Figure 3: 15 confidence intervals with AIS–MHT method and sample size of 1000 vs 1 confidence interval with CMC method and sample size of 10^7 .

PDMP 000	Rare event simulation	Mean hitting times	AIS—CE 000	Numerical results ○○○●○
References				5 edf
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Thank you for your attention.

Supplementary material

Committor function

FTA—MPS

Adaptive algorithm

Example: the spent fuel pool



If the system does not cool the pool, the nuclear fuel evaporates the water then damages the structure and contaminates the outside.



Aim: estimating the probability of the water level falling below a set threshold.



Flow Φ : solution of differential equations. Can be costly to solve. When no jump between time *s* and *s* + *t* :

$$Z_{s+t}=\Phi_{Z_s}(t).$$

Deterministic jumps : when the position reaches ∂E the boundaries of E.

$$\tau_z^{\partial} = \inf\{t > 0 : \Phi_z(t) \in \partial E\}.$$

Jump intensity λ : parameter of the distribution of the time T_z of the next random jump knowing current state z.

$$\mathbb{P}(\tau_z > t \mid Z_s = z) = \mathbb{1}_{t < t_z^{\partial}} \exp\left(-\int_0^t \lambda\left(\Phi_z(u)\right) du\right).$$
(12)

Jump kernel K: for any departure state z^- , density $z \mapsto K(z^-, z)$ of a Markovian kernel \mathcal{K}_{z^-} with respect to some measure ν_{z^-} on E.

Committor function

FTA—MPS 00000 Adaptive algorithm



Likelihood of a PDMP trajectory

Let $\mathbf{Z} := (Z_t)_{t \in [0, t_{max}]}$ be a PDMP trajectory of duration t_{max} on E.

Density function of a PDMP trajectory (*Thomas Galtier 2019*)

There is a dominant measure ζ for which a PDMP trajectory **Z** with $n_{\mathbf{Z}}$ jumps, inter-jump times $t_1, \ldots, t_{n_{\mathbf{Z}}}$ and arrival states $z_1, \ldots, z_{n_{\mathbf{Z}}}$ admits a probability density function f.

$$f(\mathbf{Z}) = \prod_{k=0}^{n_{\mathbf{Z}}} \left[\lambda\left(\Phi_{z_{k}}(t_{k})\right) \right]^{\mathbb{1}_{t_{k} < \tau_{z_{k}}^{\partial}}} \exp\left[-\int_{0}^{t_{k}} \lambda\left(\Phi_{z_{k}}(u)\right) \, \mathrm{d}u \right] K\left(\Phi_{z_{k}}(t_{k}), z_{k+1}\right)^{\mathbb{1}_{k < n_{\mathbf{Z}}}}.$$
(13)

Take home message:

- explicit computation of the pdf of a PDMP trajectory,
- \blacksquare no need to recalculate the flow.

Committor function for importance sampling



Committor function: probability of realizing the rare event $\{\mathbf{Z} \in \mathcal{T}_{\mathcal{F}}\}$ knowing that at a fixed time s > 0 the process is in a given state z.

$$U_{\rm opt}(z,s) = \mathbb{P}_{f_0} \left(\mathbf{Z} \in \mathcal{T}_{\mathcal{F}} \,|\, Z_s = z \right). \tag{14}$$

(in general $U_{opt}(\mathbf{Z}) = \mathbb{E}_{f_0} \left[\varphi(\mathbf{Z}) \mid \mathbf{Z}_s \right]$ with $\mathbf{Z}_s = (Z_t)_{t \in [0,s]}$ when estimating $\mathbb{E}_{\pi_0} \left[\varphi(\mathbf{Z}) \right]$)

Knowing U_{opt} is sufficient to build the optimal IS estimator.

To lighten the future equations we also note the variant committor function U_{opt}^- :

$$U_{\rm opt}^{-}(z^{-},s) = \int_{z \in E} U_{\rm opt}(z,s) \, K\left(z^{-},z\right) \, d\nu_{z^{-}}.$$
 (15)

 U_{opt}^- is the probability of realizing the rare event $\{\mathbf{Z} \in \mathcal{T}_F\}$ knowing that at a fixed time s > 0 the process jumps from a given state z^- .



Optimal jump intensity and jump kernel: (Thomas Galtier 2019)

$$\lambda_{\text{opt}}(\Phi_{z}(t); s) = \lambda_{0}(\Phi_{z}(t)) \times \frac{U_{\text{opt}}^{-}(\Phi_{z}(t), s+t)}{U_{\text{opt}}(\Phi_{z}(t), s+t)},$$

$$K_{\text{opt}}(z^{-}, z; s) = K_{0}(z^{-}, z) \times \frac{U_{\text{opt}}(z, s)}{U_{\text{opt}}^{-}(z^{-}, s)}.$$
(16)
(17)

If the process is k times more likely to realize the event:

- **1** by jumping now from state z, then $\lambda_{opt}(z)$ should be k times λ_0 ,
- 2 by going to state z after a jump from state z^- , then $K_{opt}(z^-, z)$ should be k times $K_0(z^-, z)$.

Approximation with MPS

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The path sets of a system are the sets of components such that:

Approximation of the committor function with minimal path sets

- I keeping all components of any path set intact prevents system failure.
- 2 keeping one component broken in each path set ensures system failure.

A $M\mbox{inimal}\ P\mbox{ath}\ S\mbox{et}$ is a path set that does not contain any other path set. We note:

- d_{MPS} the number of MPS (they are unique if the system is coherent),
- $\beta^{(MPS)}(z)$ the number of MPS with at least one broken component.

A good U_{θ} should therefore be increasing in $\beta^{(MPS)}(z)$.



Figure 4: Physical representation of the SFP

Figure 5: Functionnal diagram of the SFP

8 MPS in the spent fuel pool system: (with $L_j = (L_{i,j})_{i=1}^3$ for j = 1, 2, 3) $(G_0, S_1, L_1), (G_1, S_1, L_1), (G_0, S_1, L_2), (G_2, S_1, L_2),$ $(G_0, S_1, L_3), (G_3, S_1, L_3), (G_0, S_2, L_3), (G_3, S_2, L_3).$

Supplementary material	Committor function	FTA—MPS 000●0	Adaptive algorithm
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Our MPS-based proposition

For $oldsymbol{ heta} \in \mathbb{R}^{d_{\mathsf{MPS}}}_+$ we propose:

$$I_{\theta}^{(\text{MPS})}(z) = \exp\left[\left(\sum_{i=1}^{\beta^{(\text{MPS})}(z)} \theta_i\right)^2\right].$$
 (18)

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Flexible dimension of θ : imposing equality on some coordinates of θ reduce its effective dimension and simplify the search for a good θ when d_{MPS} is large.

 \rightarrow Example for dimension 1 with $\theta_1 = \cdots = \theta_{d_{MPS}}$:

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$$U_{\theta}^{(\mathsf{MPS})}(z) = \exp\left[\left(\theta_1 \,\beta^{(\mathsf{MPS})}(z)\right)^2\right]. \tag{19}$$

The form $x \mapsto \exp(x^2)$ garantees that the ratios U_{θ}^-/U_{θ} are strictly increasing in $\beta^{(MPS)}$. Without this condition, it is increasingly difficult to break new components and they are repaired faster and faster as they are lost.

Minimal cut sets

Committor function

FTA—MPS 0000● Adaptive algorithm



Minimal cut sets: smallest sets of components that if left broken ensure system failure. (permanent repair of one component in each group prevents the failure)

In this system: there is 69 minimal cut sets for 15 components.



Figure 6: Functionnal diagram of the SFP

Adaptive algorithm

FTA—MPS



Asymptotic confidence interval

Assumptions

- The functions λ , K, and $(U_{\theta})_{\theta \in \Theta}$ are bounded on their support below and above by strictly positive constants,
- $2 \ \theta_{\rm opt} \in \Theta \text{ is the unique maximizer of } \theta \mapsto \mathbb{E}_{f_0} \left[\mathbbm{1}_{\mathbf{Z} \in \mathcal{T}_{\mathcal{F}}} \ \log g_{\theta} \left(\mathbf{Z} \right) \right],$
- 3 there is $t_{\varepsilon} > 0$ such that $t_z^{\partial} \ge t_{\varepsilon}$ for any $z^- \in \partial E$ and any $z \in \text{supp } K(z^-, \cdot)$.

Under these assumptions, with $\widehat{\sigma}^2 = \frac{1}{\sum_{j=1}^J n_j} \sum_{j=1}^J \sum_{k=1}^{n_j} \mathbb{1}_{\mathbf{Z}_{j,k} \in \mathcal{T}_{\mathcal{F}}} \frac{f_0(\mathbf{Z}_{j,k})^2}{g_{\theta(j)}(\mathbf{Z}_{j,k})^2} - \widehat{P}_{\mathcal{F}}^2$ the estimator of the asymptotic variance $\mathbb{E}_{f_0} \left[\mathbb{1}_{\mathbf{Z} \in \mathcal{T}_{\mathcal{F}}} \frac{f_0(\mathbf{Z})}{g_{\theta_{opt}}}(\mathbf{Z}) \right] - \mathcal{P}_{\mathcal{F}}^2$, and with $v_{1-\alpha/2}$ the $(1 - \alpha/2)$ -quantile of the $\mathcal{N}(0, 1)$ distribution, we have :

$$\mathbb{P}\left(\mathbf{P}_{\mathcal{F}} \in \left[\widehat{\mathbf{P}}_{\mathcal{F}} - \mathbf{v}_{1-\alpha/2}\sqrt{\widehat{\sigma}^2/N_J}; \, \widehat{\mathbf{P}}_{\mathcal{F}} + \mathbf{v}_{1-\alpha/2}\sqrt{\widehat{\sigma}^2/N_J}\right]\right) \xrightarrow[N_J \to \infty]{} 1 - \alpha.$$

Bandit problem

Committor function

FTA—MPS

Adaptive algorithm



Off-policy best arm identification in multi-armed bandit

Several nominal distributions π₁,..., π_d,
 μ_i := E_{πi} [φ(Z)] for i = 1,..., d and a function φ (example: φ = 1_D).

Objective: find the best distribution $\underset{i \in \{1,...,d\}}{\arg\min} \mathbb{E}_{\pi_i} \left[\varphi(\mathbf{Z}) \right]$

Reverse importance sampling: if we draw $(\mathbf{Z}_1, \dots, \mathbf{Z}_N) \sim \left(\otimes_{k=1}^N q_k \right)$ then:

$$\widehat{\mu}_i = rac{1}{N} \sum_{k=1}^N arphi(\mathbf{Z}_k) rac{\pi_i(\mathbf{Z}_k)}{q_k(\mathbf{Z}_k)} \quad ext{for any } i = 1, \dots, d$$

Best sequential sampling policy?

Supp	material

Stability of the method

Committor function

FTA—MPS 00000 Adaptive algorithm



1e-5 3.5 Estimated probability for CMC method with $N = 10^7$. Estimated probability for AIS method with $N = 10^3$. CI for CMC method with $N = 10^7$. 3.0 CI for AIS method with $N = 10^3$. Probability 5.2 2.0 1.5 0 10 20 30 40 50 Confidence interval nº

Figure 7: 50 confidence intervals with AIS–MPS method and sample size of 1000 vs 1 confidence interval with CMC method and sample size of 10^7 .