Interacting particle systems for the analysis of rare events

Josselin Garnier (Université Paris Diderot) http://www.proba.jussieu.fr/~garnier

Cf http://www.proba.jussieu.fr/~garnier/expo2.pdf

Problem: estimation of the probability of occurence of a rare event.

Simulation by an Interacting Particle System.

Two versions:

- a rare event in terms of the final state of a Markov chain,
- a rare event in terms of a random variable, whose distribution is seen as the stationary distribution of a Markov chain.

Rare events

- Description of the system: Let E be a measurable space.
- $-(X_p)_{0 \le p \le M}$: a *E*-valued Markov chain:

 $\mathbb{P}(\boldsymbol{X}_p \in A \mid \boldsymbol{X}_{p-1} = \boldsymbol{x}_{p-1}, \dots, \boldsymbol{X}_0 = \boldsymbol{x}_0) = \mathbb{P}(\boldsymbol{X}_p \in A \mid \boldsymbol{X}_{p-1} = \boldsymbol{x}_{p-1})$

- $-V: E \to \mathbb{R}$: the risk function.
- $-a \in \mathbb{R}$: the threshold level.
- Problem: estimation of the probability

 $P = \mathbb{P}(V(\boldsymbol{X}_M) \ge a)$

when a is large $\implies P \ll 1$.

We know how to simulate the Markov chain $(\mathbf{X}_p)_{0 \le p \le M}$.

Rare events

- Description of the system: Let E be a measurable space.
- $-(X_p)_{0 \le p \le M}$: a *E*-valued Markov chain:

 $\mathbb{P}(\boldsymbol{X}_p \in A \mid \boldsymbol{X}_{p-1} = \boldsymbol{x}_{p-1}, \dots, \boldsymbol{X}_0 = \boldsymbol{x}_0) = \mathbb{P}(\boldsymbol{X}_p \in A \mid \boldsymbol{X}_{p-1} = \boldsymbol{x}_{p-1})$

- $-V: E \to \mathbb{R}$: the risk function.
- $-a \in \mathbb{R}$: the threshold level.
- Problem: estimation of the probability

 $P = \mathbb{P}(V(\boldsymbol{X}_M) \ge a)$

when a is large $\implies P \ll 1$.

We know how to simulate the Markov chain $(\mathbf{X}_p)_{0 \le p \le M}$.

• Example: $X_p = X_{p-1} + \theta_p$, $X_0 = 0$, where θ_p is a sequence of independent Gaussian random variables with mean zero and variance one. Here

- $-E = \mathbb{R},$
- -V(x) = x,
- solution known: $X_M = V(X_M) \sim \mathcal{N}(0, M)$.

CEMRACS 2013

Example: Optical communication in transoceanic optical fibers

Optical fiber transmission principle:

- a binary message is encoded as a train of short light pulses.
- the pulse train propagates in a long optical fiber.
- the message is read at the output of the fiber.



Input pulse train

Output pulse train

Transmission is perturbed by different random phenomena (amplifier noise, random dispersion, random birefringence,...).

Question: estimation of the bit-error-rate (probability of error), typically 10^{-6} or 10^{-8} .

Answer: use of a big numerical code (but brute-force Monte Carlo too expensive).

Example: Optical communication in transoceanic optical fibers

• Physical model: $(u_0(t))_{t\in\mathbb{R}}$ = initial pulse profile. $(u(z,t))_{t\in\mathbb{R}}$ = pulse profile after a propagation distance z. $(u(Z,t))_{t\in\mathbb{R}}$ = output pulse profile (after a propagation distance Z).

Propagation from z = 0 to z = Z governed by two coupled nonlinear Schrödinger equations with randomly z-varying coefficients (code OCEAN, Alcatel). \hookrightarrow black box.

→ Truncation of [0, Z] into M segments $[z_{p-1}, z_p), z_p = pZ/M, 1 \le p \le M$. → $X_p = u(z_p, t)_{t \in \mathbb{R}}$ is the pulse profile at distance z_p . Here $(X_p)_{0 \le p \le M}$ is Markov with state space $E = H_0^2(\mathbb{R}) \cap L_2^2(\mathbb{R})$.

CEMRACS 2013

Example: Optical communication in transoceanic optical fibers Question: estimation of the probability of anomalous pulse spreading. Rms pulse width after propagation distance z:

$$\tau(z)^{2} = \int |u(z,t)|^{2} t^{2} dt / \int |u(z,t)|^{2} dt$$

The potential function is $V: \begin{vmatrix} E \to \mathbb{R} \\ V(\mathbf{X}) = \int t^2 |\mathbf{X}(t)|^2 dt / \int |\mathbf{X}(t)|^2 dt$

Problem: estimation of the probability

 $P = \mathbb{P}(\tau(Z) \ge a) = \mathbb{P}(V(X_M) \ge a)$

CEMRACS 2013

Monte Carlo method

• *n* independent copies $((X_0^i, \ldots, X_M^i))_{1 \le i \le n}$ of (X_0, \ldots, X_M) distributed with the original \mathbb{P} .

• Proposed estimator:

$$\hat{P}_n = \frac{1}{n} \sum_{i=1}^n \mathbf{1}_{V(\boldsymbol{X}_M^i) \ge a}$$

Unbiased estimator:

$$\mathbb{E}\left[\hat{P}_n\right] = \mathbb{P}(V(\boldsymbol{X}_M) \ge a) = P$$

Variance:

$$\mathbb{E}\left[\left(\hat{P}_n - P\right)^2\right] = \frac{1}{n}P\left(1 - P\right) \stackrel{P \ll 1}{\simeq} \frac{P}{n}$$

The absolute error $\operatorname{Std}(\hat{P}_n) \simeq \sqrt{P}/\sqrt{n}$. The relative error

$$\frac{\operatorname{Std}(\hat{P}_n)}{P} \simeq \frac{1}{\sqrt{Pn}}$$

 \hookrightarrow We should have $n > P^{-1}$ to get a relative error smaller than one.

Of course: P^{-1} is the minimum size of the sample required for one element to reach the rare level !

CEMRACS 2013

Importance Sampling method

• *n* independent copies $((X_0^i, \ldots, X_M^i))_{1 \le i \le n}$ of (X_0, \ldots, X_M) distributed with a biased distribution \mathbb{Q} .

• Proposed estimator:

$$\hat{P}_n = \frac{1}{n} \sum_{i=1}^n \mathbf{1}_{V(\boldsymbol{X}_M^i) \ge a} \frac{d\mathbb{P}}{d\mathbb{Q}}(\boldsymbol{X}_0^i, \dots, \boldsymbol{X}_M^i)$$

Unbiased estimator:

$$\mathbb{E}_{\mathbb{Q}}\left[\hat{P}_{n}\right] = \mathbb{E}_{\mathbb{Q}}\left[\mathbf{1}_{V(\boldsymbol{X}_{M})\geq a}\frac{d\mathbb{P}}{d\mathbb{Q}}(\boldsymbol{X}_{0},\ldots,\boldsymbol{X}_{M})\right] = P$$

Variance:

$$\mathbb{E}_{\mathbb{Q}}\left[\left(\hat{P}_{n}-P\right)^{2}\right] = \frac{1}{n} \left\{ \mathbb{E}_{\mathbb{P}}\left[\mathbf{1}_{V(\boldsymbol{X}_{M})\geq a}\frac{d\mathbb{P}}{d\mathbb{Q}}(\boldsymbol{X}_{0},\ldots,\boldsymbol{X}_{M})\right] - P^{2} \right\}$$

 \hookrightarrow With a proper choice of \mathbb{Q} , the error-variance can be dramatically reduced. Optimal choice: $d\mathbb{Q} = \frac{\mathbf{1}_{V(\mathbf{X}_{M}) \geq a}}{\mathbb{P}(V(\mathbf{X}_{M}) \geq a)} d\mathbb{P}$. Impossible to apply ! But this result gives ideas (adaptive strategy, ...)

• Critical points: choice of the biased distribution + evaluation of the likelihood ratio + simulation of the biased dynamics (intrusive method).

CEMRACS 2013

Importance Sampling method driven by Large Deviations Principle

• Consider the family of twisted distributions, $\lambda > 0$:

$$d\mathbb{P}^{(\lambda)} = \frac{1}{\mathbb{E}_{\mathbb{P}}(e^{\lambda V(\boldsymbol{X}_{M})})} e^{\lambda V(\boldsymbol{X}_{M})} d\mathbb{P}$$

 $\mathbb{P}^{(\lambda)}$ favors random evolutions with high potential values $V(\mathbf{X}_M)$.

- *n* independent copies $(\mathbf{X}_{M}^{i})_{1 \leq i \leq n}$ distributed with $\mathbb{P}^{(\lambda)}$.
- Estimator:

$$\hat{P}_{n,\lambda} = \frac{1}{n} \sum_{i=1}^{n} \mathbf{1}_{V(\mathbf{X}_{M}^{i}) \geq a} \frac{d\mathbb{P}}{d\mathbb{P}^{(\lambda)}}(\mathbf{X}_{0}^{i}, \dots, \mathbf{X}_{M}^{i})$$

Variance:

$$n\mathbb{E}_{\mathbb{P}^{(\lambda)}}\left[\left(\hat{P}_{n,\lambda}-P\right)^{2}\right] = \mathbb{E}_{\mathbb{P}}\left[\mathbf{1}_{V(\mathbf{X}_{M})\geq a} \ e^{-\lambda V(\mathbf{X}_{M})}\right] \mathbb{E}_{\mathbb{P}}\left[e^{\lambda V(\mathbf{X}_{M})}\right] - P^{2}$$
$$\leq e^{-[\lambda a - \Lambda_{M}(\lambda)]} \ P - P^{2}$$

where $\Lambda_M(\lambda) = \log \mathbb{E}_{\mathbb{P}}[e^{\lambda V(\boldsymbol{X}_M)}]$. For a judicious choice of λ , $\lambda^* a - \Lambda_M(\lambda^*) = \sup_{\lambda>0}[\lambda a - \Lambda_M(\lambda)] \simeq -\ln P$ (large deviations principle), so

$$\mathbb{E}_{\mathbb{P}^{(\lambda)}}[(\hat{P}_{n,\lambda} - P)^2] \lesssim \frac{P^2}{n}$$

Almost optimal: the relative error is $1/\sqrt{n}$ (compare with MC: $1/\sqrt{Pn}$).

CEMRACS 2013

Twisted Feynman-Kac path measures

Question: How to simulate the twisted distribution $\mathbb{P}^{(\lambda)}$?

Answer: We will show a way to simulate the distribution \mathbb{Q} :

$$d\mathbb{Q} = rac{1}{\mathcal{Z}_M} \left\{ \prod_{p=1}^M G_p(\boldsymbol{X}_0, \dots, \boldsymbol{X}_p) \right\} d\mathbb{P}$$

where $(G_p)_{1 \le p \le M}$ is a sequence of positive potential functions on the path spaces E^p , and $\mathcal{Z}_M = \mathbb{E}_{\mathbb{P}}[\prod G_p(\mathbf{X}_0, \dots, \mathbf{X}_p)] > 0$ is a normalization constant. Examples:

-
$$G_p(X_0, ..., X_p) = 1, p < M, \quad G_M(X_0, ..., X_M) = e^{\lambda V(X_M)}.$$

- $G_p(X_0, ..., X_p) = e^{\lambda (V(X_p) - V(X_{p-1}))}.$

- What is a "good" choice for G_p ?
- How to simulate \mathbb{Q} directly from \mathbb{P} ?

Original measures

• $(\mathbf{X}_p)_{0 \le p \le M}$: a *E*-valued Markov chain, starting from $\mathbf{X}_0 = \mathbf{x}_0$, with transition $K_p(\mathbf{x}_{p-1}, d\mathbf{x}_p)$:

$$\mathbb{P}(\boldsymbol{X}_{p} \in A \mid \boldsymbol{X}_{p-1} = \boldsymbol{x}_{p-1}, \dots, \boldsymbol{X}_{0} = \boldsymbol{x}_{0}) = \mathbb{P}(\boldsymbol{X}_{p} \in A \mid \boldsymbol{X}_{p-1} = \boldsymbol{x}_{p-1}) = \int_{A} K_{p}(\boldsymbol{x}_{p-1}, d\boldsymbol{x}_{p})$$

where $K_p(\boldsymbol{x}_{p-1}, \cdot)$ is a probability measure on (E, \mathcal{E}) for any $\boldsymbol{x}_{p-1} \in E$.

• Denote the (partial) path

$$\boldsymbol{Y}_p =_{\text{def.}} (\boldsymbol{X}_0, \dots, \boldsymbol{X}_p) \in E^{p+1}, \qquad p = 0, \dots, M$$

The measure μ_p on E^{p+1} is the distribution of Y_p :

$$\mu_p(f_p) =_{\text{def.}} \int_{E^{p+1}} f_p(\boldsymbol{y}_p) \mu_p(d\boldsymbol{y}_p) = \mathbb{E}[f_p(\boldsymbol{Y}_p)], \qquad f_p \in L^{\infty}(E^{p+1})$$

• Expression of P in terms of μ_M :

 $P = \mu_M(f)$

$$f(\boldsymbol{y}_M) = f(\boldsymbol{x}_0, \dots, \boldsymbol{x}_M) = \mathbf{1}_{V(\boldsymbol{x}_M) \ge a}$$

 \rightarrow If one can compute/estimate μ_M , then one can compute/estimate P.

CEMRACS 2013

• Recursive relation:

$$\mu_p = \Theta_p(\mu_{p-1}) =_{\text{def.}} \int_{E^p} \mu_{p-1}(d\boldsymbol{y}_{p-1}) \mathcal{K}_p(\boldsymbol{y}_{p-1}, \cdot)$$

with $\mu_0 = \delta_{\boldsymbol{x}_0}$. $\mathcal{K}_p(\boldsymbol{y}_{p-1}, d\boldsymbol{y}'_p)$: Markov transitions associated to the chain \boldsymbol{Y}_p :

$$\mathcal{K}_p(\boldsymbol{y}_{p-1}, d\boldsymbol{y}_p') = \delta_{\boldsymbol{y}_{p-1}}(d\boldsymbol{y}_{p,0}', \dots, d\boldsymbol{y}_{p,p-1}')K_p(\boldsymbol{y}_{p-1,p-1}, d\boldsymbol{y}_{p,p}')$$

Here $\boldsymbol{y}_{p-1} = (\boldsymbol{y}_{p-1,0}, \dots \boldsymbol{y}_{p-1,p-1}) \in E^p, \, \boldsymbol{y}_p' = (\boldsymbol{y}_{p,0}', \dots \boldsymbol{y}_{p,p}') \in E^{p+1}):$ \hookrightarrow Linear evolution.

Proof:

$$\begin{split} \mu_{p}(f_{p}) &= \mathbb{E}[f_{p}(\boldsymbol{Y}_{p-1}, \boldsymbol{X}_{p})] \\ &= \int_{E^{p}} \mu_{p-1}(d\boldsymbol{y}_{p-1}) \mathbb{E}[f_{p}(\boldsymbol{y}_{p-1}, \boldsymbol{X}_{p}) | \boldsymbol{Y}_{p-1} = \boldsymbol{y}_{p-1}] \\ &= \int_{E^{p}} \mu_{p-1}(d\boldsymbol{y}_{p-1}) \int_{E} K_{p}(\boldsymbol{y}_{p-1,p-1}, d\boldsymbol{x}_{p}) f_{p}(\boldsymbol{y}_{p-1}, \boldsymbol{x}_{p}) \\ &= \int_{E^{p}} \mu_{p-1}(d\boldsymbol{y}_{p-1}) \int_{E^{p+1}} d\boldsymbol{y}_{p}' \mathcal{K}_{p}(\boldsymbol{y}_{p-1}, d\boldsymbol{y}_{p}') f_{p}(\boldsymbol{y}_{p}') \\ &= \Theta_{p}(\mu_{p-1})(f_{p}) \end{split}$$

CEMRACS 2013

Unnormalized measures

$$\boldsymbol{Y}_p =_{\text{def.}} (\boldsymbol{X}_0, \dots, \boldsymbol{X}_p) \in E^{p+1}, \qquad p = 0, \dots, M$$

FK measure γ_p associated to the pair potentials/transitions (G_p, K_p) :

$$\gamma_p(f_p) = \mathbb{E}\Big[f_p(\mathbf{Y}_p)\prod_{1 \le k < p} G_k(\mathbf{Y}_k)\Big]$$

• Expression of P in terms of γ_M :

 $P = \gamma_M(g)$

$$g(\boldsymbol{y}_M) = g(\boldsymbol{x}_0, \dots, \boldsymbol{x}_M) = \mathbf{1}_{V(\boldsymbol{x}_M) \ge a} \prod_{1 \le p < M} G_p^{-1}(\boldsymbol{x}_0, \dots, \boldsymbol{x}_p)$$

- \rightarrow If one can compute/estimate γ_M , then one can compute/estimate P.
- Recursive relation:

$$\gamma_p = \Psi_p(\gamma_{p-1}) =_{\operatorname{def.}} \int_{E^p} \gamma_{p-1}(d\boldsymbol{y}_{p-1}) G_{p-1}(\boldsymbol{y}_{p-1}) \mathcal{K}_p(\boldsymbol{y}_{p-1}, \cdot)$$

 $\mathcal{K}_p(\boldsymbol{y}_{p-1}, d\boldsymbol{y}_p')$: Markov transitions associated to the chain \boldsymbol{Y}_p

$$\mathcal{K}_p(\boldsymbol{y}_{p-1}, d\boldsymbol{y}'_p) = \delta_{\boldsymbol{y}_{p-1}}(d\boldsymbol{y}'_{p,0}, \dots, d\boldsymbol{y}'_{p,p-1})K_p(\boldsymbol{y}_{p-1,p-1}, d\boldsymbol{y}'_{p,p})$$

 \hookrightarrow Linear evolution.

CEMRACS 2013

Normalized measures

Introduce the normalized measure η_p :

$$\eta_p(f_p) = \gamma_p(f_p) / \gamma_p(1), \qquad p = 0, \dots, M$$

• Expression of P in terms of η_p :

$$P = \eta_M(g) \prod_{1 \le p < M} \eta_p(G_p)$$

Proof:

$$P = \mathbb{E}\Big[g(\mathbf{Y}_M) \prod_{1 \le k < M} G_k(\mathbf{Y}_k)\Big] = \gamma_M(g) = \eta_M(g)\gamma_M(1)$$

Normalizing constant:

$$\gamma_M(1) = \gamma_{M-1}(G_{M-1}) = \eta_{M-1}(G_{M-1}) \ \gamma_{M-1}(1) = \prod_{1 \le p < M} \eta_p(G_p)$$

 \rightarrow If one can compute/estimate $(\eta_p)_{p=1,\dots,M}$, then one can compute/estimate P.

• Recursive relation:

$$\eta_p = \Phi_p(\eta_{p-1}) =_{\text{def.}} \int_{E^p} \eta_{p-1}(d\boldsymbol{y}_{p-1}) G_{p-1}(\boldsymbol{y}_{p-1}) \mathcal{K}_p(\boldsymbol{y}_{p-1}, \cdot) / \eta_{p-1}(G_{p-1}) \mathcal{K}_p(\boldsymbol{y}_{p-1}, \cdot) / \eta_{p-1}(G_{p-$$

 \hookrightarrow Nonlinear evolution.

CEMRACS 2013

Interacting path-particle system

• Goal: simulate the original measures

$$\mu_p = \Theta_p(\mu_{p-1})$$

• Easy: Let $(Y_p^1, \ldots, Y_p^n) \in (E^{p+1})^n$ be independent Markov chains simulated with \mathbb{P} . Then

$$\lim_{n \to \infty} \frac{1}{n} \sum_{i=1}^{n} \delta_{\mathbf{Y}_{p}^{i}} = \mu_{p}$$

Interacting path-particle system

• Goal: simulate the original measures

$$\mu_p = \Theta_p(\mu_{p-1})$$

• Easy: Let $(\mathbf{Y}_p^1, \ldots, \mathbf{Y}_p^n) \in (E^{p+1})^n$ be independent Markov chains simulated with \mathbb{P} . Then

$$\lim_{n \to \infty} \frac{1}{n} \sum_{i=1}^{n} \delta_{\mathbf{Y}_{p}^{i}} = \mu_{p}$$

• Goal: simulate the normalized measures

$$\eta_p = \Phi_p(\eta_{p-1})$$

• Idea: $\mathbb{Y}_p = (\mathbf{Y}_p^1, \dots, \mathbf{Y}_p^n) \in (E^{p+1})^n$ particle system s.t.

$$\lim_{n \to \infty} \frac{1}{n} \sum_{i=1}^{n} \delta_{\mathbf{Y}_{p}^{i}} = \eta_{p}$$

- Key points:
- Nonlinear $\Phi_p \rightarrow$ interacting particle system
- Simulation technique
- Fixed number of particles $(\eta_p(1) = 1)$

CEMRACS 2013

Interacting path-particle system

Question: How to simulate η_M directly from \mathbb{P} ?

$$d\eta_M = \frac{1}{\mathcal{Z}_M} \left\{ \prod_{p=1}^{M-1} G_p(\boldsymbol{X}_0, \dots, \boldsymbol{X}_p) \right\} d\mathbb{P}$$

Answer: System of path-particles, whose empirical measure will be approximately \mathbb{Q} .

- Path-particle: $\mathbf{Y}_p = (\mathbf{X}_0, \dots, \mathbf{X}_p)$ taking values in E^{p+1} , $1 \le p \le M$.
- System with *n* path-particles: $\mathbb{Y}_p = (\mathbf{Y}_p^i)_{1 \le i \le n}$ taking values in $(E^{p+1})^n$.
- Initialization: p = 0: $\mathbf{Y}_0^i = \mathbf{x}_0$ for all $i = 1, \ldots, n$.
- Dynamics: Evolution from generation p to p + 1 as follows:

$$\mathbb{Y}_p \in (E^{p+1})^n \xrightarrow{selection} \widehat{\mathbb{Y}}_p \in (E^{p+1})^n \xrightarrow{mutation} \mathbb{Y}_{p+1} \in (E^{p+2})^n$$



3 particles $\mathbf{Y}_p^1, \mathbf{Y}_p^2, \mathbf{Y}_p^3$ at generation p, with potential weights $G(\mathbf{Y}_p^1) = 1, \ G(\mathbf{Y}_p^2) = 2, \ G(\mathbf{Y}_p^3) = 3.$

CEMRACS 2013

n=3 particles



CEMRACS 2013

n=3 particles



CEMRACS 2013

n=3 particles



CEMRACS 2013



Each particle evolve independently from p to p+1.

CEMRACS 2013



3 particles are selected at generation p + 1.

CEMRACS 2013

n=3 particles 5 4 3 (ک) selection 2 1 0 p+2 p+1 р generation

Each particle evolve independently from p + 1 to p + 2.

CEMRACS 2013

At each generation $p = 0, \ldots, M - 1$:

Selection: from the system $\mathbb{Y}_p = (\mathbf{Y}_p^i)_{1 \leq i \leq n}$, choose randomly and independently n path-particles

$$\widehat{\boldsymbol{Y}}_{p}^{i} = (\widehat{\boldsymbol{Y}}_{0,p}^{i}, \widehat{\boldsymbol{Y}}_{1,p}^{i}, \dots, \widehat{\boldsymbol{Y}}_{p,p}^{i}) \in E^{p+1}$$

according to the Boltzmann-Gibbs particle measure

$$\sum_{i=1}^{n} \frac{G_p(\boldsymbol{Y}_p^i)}{\sum_{j=1}^{n} G_p(\boldsymbol{Y}_p^j)} \,\,\delta_{\boldsymbol{Y}_p^i}$$

Mutation: each selected path-particle \hat{Y}_p^i is extended by an elementary unbiased K_p -transition:

$$\begin{aligned} \mathbf{Y}_{p+1}^{i} &= ((\mathbf{Y}_{0,p+1}^{i}, \dots, \mathbf{Y}_{p,p+1}^{i}) , \mathbf{Y}_{p+1,p+1}^{i}) \\ &= ((\widehat{\mathbf{Y}}_{0,p}^{i}, \dots, \widehat{\mathbf{Y}}_{p,p}^{i}), \mathbf{Y}_{p+1,p+1}^{i}) \in E^{p+1} \end{aligned}$$

where $Y_{p+1,p+1}^{i}$ is a random variable with distribution $K_{p}(\widehat{Y}_{p,p}^{i}, \cdot)$. The mutations are performed independently.

• The occupation measures of the ancestral lines converge to the desired twisted measures:

$$\eta_p^n =_{\text{def.}} \frac{1}{n} \sum_{i=1}^n \delta_{(\mathbf{Y}_{0,p}^i, \dots, \mathbf{Y}_{p,p}^i)} \xrightarrow{n \to \infty} \eta_p$$

In addition, several propagation-of-chaos estimates ensure that the ancestral lines $Y_p^i = (Y_{0,p}^i, \ldots, Y_{p,p}^i)$ are asymptotically i.i.d. with common distribution η_p .

• Estimator of $P = \eta_M(g) \prod_{0 \le p < M} \eta_p(G_p)$:

$$\hat{P}_n = \eta_M^n(g) \prod_{1 \le p < M} \eta_p^n(G_p)$$

$$g(\boldsymbol{x}_0,\ldots,\boldsymbol{x}_M) = \mathbf{1}_{V(\boldsymbol{x}_M) \ge a} \prod_{1 \le p < M} G_p^{-1}(\boldsymbol{x}_0,\ldots,\boldsymbol{x}_p)$$

Proof. asymptotic analysis of genealogical particle models.

cf P. Del Moral, Feynman-Kac formulae, genealogical and interacting particle systems with applications, Springer, New York, 2004.

cf P. Del Moral and J. Garnier, Ann. Appl. Probab. 15 (2005), 2496-2534.

Estimator of the probability of the rare event

Let

$$\hat{P}_{n} = \left[\frac{1}{n}\sum_{i=1}^{n} \mathbf{1}_{V(\mathbf{Y}_{M,M}^{i}) \ge a} \prod_{1 \le p < M} G_{p}^{-1}(\mathbf{Y}_{0,p}^{i}, \dots, \mathbf{Y}_{p,p}^{i})\right] \times \prod_{1 \le p < M} \left[\frac{1}{n}\sum_{i=1}^{n} G_{p}(\mathbf{Y}_{0,p}^{i}, \dots, \mathbf{Y}_{p,p}^{i})\right]$$

 \hat{P}_n is an unbiased estimator of P:

$$\mathbb{E}[\hat{P}_n] = P$$

such that

$$\hat{P}_n \xrightarrow{n \to \infty} P$$
 a.s.

Central limit theorem

• The estimator \hat{P}_n satisfies the central limit theorem

$$\sqrt{n} \left[\hat{P}_n - P \right] \stackrel{n \to \infty}{\longrightarrow} \mathcal{N}(0, \sigma^2)$$

with the asymptotic variance

$$\sigma^2 = \sum_{p=1}^M \mathbb{E}\left[\prod_{j=1}^p G_j\right] \mathbb{E}\left[\prod_{j=1}^p G_j^{-1} (P_{p,M}^a)^2\right] - P^2$$

Here the functions $P_{p,M}^a$ are defined by

$$\boldsymbol{x}_p \in E \mapsto P_{p,M}^a(\boldsymbol{x}_p) = \mathbb{P}(V(\boldsymbol{X}_M) \ge a \mid \boldsymbol{X}_p = \boldsymbol{x}_p)$$

• Useful for

- 1) the choice of "good" functions G_p (variance reduction)
- 2) the design of an estimator of the asymptotic variance.

Sketch of proof

Local errors: introduce the random field \mathcal{W}_p^n given by

$$\mathcal{W}_p^n(f_p) = \sqrt{n} \, [\eta_p^n - \Phi_p(\eta_{p-1}^n)](f_p), \qquad \text{for } f_p \in L^\infty(E)$$

Central limit theorem: The sequence $(\mathcal{W}_p^n)_{1 \leq p \leq M}$ converges in law, as $n \to \infty$, to a sequence of M independent, Gaussian and centered random fields $(\mathcal{W}_p)_{1 \leq p \leq M}$

$$\mathbb{E}\left[\mathcal{W}_p(f_p)\mathcal{W}_p(g_p)\right] = \eta_p\left([f_p - \eta_p(f_p)][g_p - \eta_p(g_p)]\right)$$

Global error: Let $Q_{p,M}$, with $1 \le p \le M$, be the FK semi-group associated to the flow $\gamma_M = \gamma_p Q_{p,M}$. Using the Markov property,

$$Q_{p,M}(f_M)(\boldsymbol{y}_p) = \mathbb{E}\left[f_M(\boldsymbol{Y}_M) \prod_{p \leq k < M} G_k(\boldsymbol{Y}_k) \mid \boldsymbol{Y}_p = \boldsymbol{y}_p
ight]$$

Telescopic decomposition

$$\gamma_M^n - \gamma_M = \sum_{p=1}^M [\gamma_p^n Q_{p,M} - \gamma_{p-1}^n Q_{p-1,M}] = \sum_{p=1}^M [\gamma_p^n - \gamma_{p-1}^n Q_{p-1,p}] Q_{p,M}$$

Use $\gamma_{p-1}^n Q_{p-1,p} = \gamma_{p-1}^n (G_{p-1}) \Phi_{p-1}(\eta_{p-1}^n)$ and $\gamma_{p-1}^n (G_{p-1}) = \gamma_p^n(1)$.

CEMRACS 2013

$$\gamma_M^n - \gamma_M = \sum_{p=1}^M \gamma_p^n(1) [\eta_p^n - \Phi_{p-1}(\eta_{p-1}^n)] Q_{p,M}$$

As a result:

$$\mathcal{W}_M^{\gamma,n}(f_M) =_{\text{def.}} \sqrt{n} [\gamma_M^n - \gamma_M](f_M) = \sum_{p=1}^M \gamma_p^n(1) \ \mathcal{W}_p^n(Q_{p,M} f_M)$$

Consider

$$\sqrt{n} \left[\hat{P}_n - P\right] = \mathcal{W}_M^{\gamma, n}(g)$$

Thus $\mathcal{W}_{M}^{\gamma,n}(g)$ converge in law, as $n \to \infty$, to a centered Gaussian random variable $\mathcal{W}_{M}^{\gamma}(g)$ with the variance

$$\sigma_M^2 =_{\text{def.}} \mathbb{E}(\mathcal{W}_M^{\gamma}(g)^2) = \sum_{p=1}^M \gamma_p(1)^2 \ \eta_p \big([Q_{p,M}(g) - \eta_p Q_{p,M}(g)]^2 \big)$$

CEMRACS 2013

Variance comparisons for the Gaussian model $X_p = X_{p-1} + \theta_p$

where $(\theta_p)_{1 \le p \le M}$ independent, Gaussian, zero-mean, variance one, V(x) = x.

Here X_M is Gaussian, has zero-mean and variance M:

$$P = \mathbb{P}(X_M \ge a) = \frac{1}{\sqrt{2\pi M}} \int_a^\infty \exp\left(-\frac{s^2}{2M}\right) ds \sim \exp\left(-\frac{a^2}{2M}\right)$$

Consider $a \gg \sqrt{M}$ so that $P \ll 1$.

First choice for the potential:

$$G_p(x_0,\ldots,x_p) = \exp(\alpha x_p), \text{ for some } \alpha > 0$$

Calculations show

$$\sigma^{2} \simeq \sum_{p=1}^{M} \left[e^{-\frac{a^{2}}{M}} e^{\frac{p}{M(M+p)} \left[a - \alpha M(p-1)/2\right]^{2} + \frac{1}{12} \alpha^{2} (p-1)p(p+1)} - P^{2} \right]$$

By optimizing, we take $\alpha = 2a/[M(M-1)]$, and we get

$$\sigma^2 \simeq e^{-\frac{a^2}{M} \frac{2}{3} \left(1 - \frac{1}{M-1}\right)}$$

 \hookrightarrow the asymptotic variance is of the order of $P^{4/3}$ \rightarrow relative error $\sim 1/\sqrt{nP^{2/3}}$.

CEMRACS 2013

Consider the same model.

Second choice for the potential:

$$G_p(x_0, \ldots, x_p) = \exp[\alpha(x_p - x_{p-1})], \text{ for some } \alpha > 0$$

We obtain:

$$\sigma^{2} \simeq \sum_{0 \le p < M} \left[e^{-\frac{a^{2}}{M}} e^{\frac{p+1}{M(M+p+1)} \left[a - \alpha \frac{Mp}{p+1} \right]^{2} + \alpha^{2} \frac{p}{p+1}} - P^{2} \right]$$

By optimizing, $\alpha = a/M$, we get

$$\sigma^2 \sim e^{-\frac{a^2}{M}\left(1-\frac{1}{M}\right)}$$

 \hookrightarrow the asymptotic variance is of the order of P^2 .

 \rightarrow relative error $\sim 1/\sqrt{n}$.

By comparing with the previous case: a selection pressure depending only on the state is not efficient !

Numerical simulations with the Gaussian model



 $M = 15, n = 2 \ 10^4$ particles, $\alpha = 1$.

CEMRACS 2013

Optical communication in transoceanic optical fibers

• Physical model:

 $(u_0(t))_{t\in\mathbb{R}}$ = initial pulse profile.

 $(u(z,t))_{t\in\mathbb{R}}$ = pulse profile after a propagation distance z.

 $(u(Z,t))_{t\in\mathbb{R}}$ = output pulse profile (after a propagation distance Z).

 $\tau(z)^2 = \int |u(z,t)|^2 t^2 dt / \int |u(z,t)|^2 dt$ rms pulse width after propagation distance z. Propagation from z = 0 to z = Z governed by two coupled nonlinear Schrödinger equations with randomly z-varying coefficients.

→ Truncation of [0, Z] into M segments $[z_{p-1}, z_p), z_p = pZ/M, 1 \le p \le M$. → $X_p = (u(z_p, t)_{t \in \mathbb{R}})$ is the pulse profile at distance z_p .

Here $(\mathbf{X}_p)_{0 \le p \le M}$ is Markov with state space $E = H_0^2(\mathbb{R}) \cap L_2^2(\mathbb{R})$

The potential function is $V: \begin{vmatrix} E \to \mathbb{R} \\ V(\mathbf{X}) = \int t^2 |\mathbf{X}(t)|^2 dt / \int |\mathbf{X}(t)|^2 dt$

Problem: estimation of the probability

$$P = \mathbb{P}(V(X_M) \ge a) = \mathbb{P}(\tau(Z) \ge a)$$

1) asymptotic model (separation of scales technique)

 \rightarrow the rms pulse width $\tau(z)$ is a diffusion process and its pdf is

$$p_z(\tau) = \frac{\tau^{1/2}}{\sqrt{2\pi} (4\sigma^2 z)^{3/2}} \exp\left(-\frac{\tau}{8\sigma^2 z}\right) \mathbf{1}_{[0,\infty)}(\tau)$$

2) realistic model: impossible to get a closed-form expression for the pdf of $\tau(z)$.

3) experimental observations: the pdf tail of the rms pulse width does not fit with the Maxwellian distribution in realistic configurations.

CEMRACS 2013

Numerical simulations with the PMD model



 $M = 15, n = 2 \ 10^4$ particles, $\alpha = 1$ and $\alpha = 3$.

The solid line stands for the Maxwellian pdf predicted by the asymptotic model.

CEMRACS 2013

Multilevel splitting

- Description of the system:
- Let \boldsymbol{X} be a \mathbb{R}^d -valued random variable with pdf $p(\boldsymbol{x})$.
- Let $V : \mathbb{R}^d \to \mathbb{R}$ be the risk function.
- Let a be the threshold level.

• Problem: estimation of

 $P = \mathbb{P}(V(\boldsymbol{X}) \ge a)$

when a is large $\implies P \ll 1$.

Multilevel splitting

- Splitting strategy:
- Note the decomposition (with $a_M = a > \cdots > a_0 = -\infty$)

$$P = \prod_{j=1}^{M} P_j, \qquad P_j = \mathbb{P}(V(\boldsymbol{X}) > a_j | V(\boldsymbol{X}) > a_{j-1})$$

- Estimate P_j separately.
- Two key issues:
- 1) Algorithm to evaluate each P_j ,
- 2) Selection of the levels a_j .

Answer to 1): use an interacting particle method (based on a Markov process whose invariant distribution has pdf p) $\rightarrow \hat{P}_n$.

Answer to 2): choose a_j such that the P_j 's are all equal to the same $\alpha \in (0, 1)$. Then

$$\operatorname{Var}(\hat{P}_n) = \frac{P^2}{n} \left(\frac{(1-\alpha)\ln P}{\alpha \ln \alpha} \right) + o(n^{-1})$$

 \hookrightarrow one should take $\alpha \to 1$.

CEMRACS 2013

- New strategy with " $\alpha = 1 1/n$ ":
- Generate n particles (with the distribution with pdf p) to create generation zero:

 \hookrightarrow (X_0^1, \dots, X_0^n) independent and identically distributed with the distribution with pdf p(x)

• For $j - 1 \rightarrow j$,

- define the level a_j as the minimum of $V(\boldsymbol{x})$ evaluated on the *n* particles: $a_j = \min_{i=1,...,n} \{ (V(\boldsymbol{X}_{j-1}^i)) \},$

- remove the particle that achieves the minimum,

- generate a new particle with the conditional distribution μ_{a_j} of X knowing that $V(X) > a_j$:

$$\mu_{a_j}(d\boldsymbol{x}) = p_{a_j}(\boldsymbol{x})d\boldsymbol{x}, \qquad p_{a_j}(\boldsymbol{x}) = \frac{\mathbf{1}_{V(\boldsymbol{x}) \ge a_j} p(\boldsymbol{x})}{\int_{\mathbb{R}^d} \mathbf{1}_{V(\boldsymbol{x}') \ge a_j} p(\boldsymbol{x}')d\boldsymbol{x}'}$$

(use the Metropolis-Hastings algorithm).

 \hookrightarrow (X_j^1, \ldots, X_j^n) independent and identically distributed with the distribution μ_{a_j}

• Stop when $a_j > a$. Denote $\hat{J}_n = \min\{j, a_j > a\} - 1$.

CEMRACS 2013

• Result 1: if one knows how to generate the new particle with the distribution μ_{a_j} , then \hat{J}_n follows a Poisson distribution with parameter $-n \ln P$. Proof:

- if $V(\mathbf{X})$ has continuous cumulative distribution function F, then $F(V(\mathbf{X}))$ is a uniform random variable and $-\log(1 - F(V(\mathbf{X})))$ is an exponential random variable.

- the random variables $-\log(1 - F(a_j)), j \ge 1$, are distributed as the successive arrival times of a Poisson process with rate n,

$$-\log(1 - F(a_j)) \stackrel{dist.}{=} \frac{1}{n} \sum_{i=1}^{j} E_i$$

where E_i are i.i.d. exponential random variables.

 $-\mathbb{P}(\hat{J}_n = j) = \mathbb{P}(a_j \le a, a_{j+1} > a) = \mathbb{P}(\sum_{i=1}^j E_i \le -n \ln P < \sum_{i=1}^{j+1} E_i).$

CEMRACS 2013

Proof. Let $\Lambda(y) = -\log(1 - F(y))$. $\Lambda : \mathbb{R} \to (0, \infty)$ is continuous and increasing.

• Generation 0: $(\Lambda(V(X_0^i)))_{i=1,...,n}$ are i.i.d. with the distribution of $\Lambda(V(X))$:

$$\mathbb{P}(\Lambda(V(\boldsymbol{X})) \ge \lambda) = \mathbb{P}(1 - F(V(X_0)) \le 1 - e^{-\lambda}) = e^{-\lambda}$$

Therefore $(\Lambda(V(\mathbf{X}_0^i)))_{i=1,...,n}$ are i.i.d. with the distribution $\mathcal{E}(1)$. Let $a_1 = \min_{i=1,...,n} \{V(\mathbf{X}_0^i)\}$. We have $\Lambda(a_1) = \min_{i=1,...,n} \{\Lambda(V(\mathbf{X}_0^i))\}$.

$$\mathbb{P}(\Lambda(a_1) \ge \lambda) = \mathbb{P}(\Lambda(V(\boldsymbol{X})) \ge \lambda)^n = e^{-n\lambda}$$

Therefore

$$\Lambda(a_1) \sim \frac{1}{n} E_1, \qquad E_1 \sim \mathcal{E}(1)$$

• Generation j. Let $\Lambda_j(y) = -\log(1 - F_j(y))$ where F_j is the cdf of $V(\mathbf{X})$ given $V(\mathbf{X}) \ge a_j$:

$$F_j(y) = \mathbb{P}(V(\boldsymbol{X}) \le y | V(\boldsymbol{X}) \ge a_j) = \frac{\mathbb{P}(a_j \le V(\boldsymbol{X}) \le y)}{\mathbb{P}(V(\boldsymbol{X}) \ge a_j)} = \frac{F(y) - F(a_j)}{1 - F(a_j)}$$

Therefore $\Lambda_j(y) = \Lambda(y) - \Lambda(a_j)$. As above: $(\Lambda_j(V(\mathbf{X}_j^i)))_{i=1,...,n}$ are i.i.d. with the distribution $\mathcal{E}(1)$. Let $a_{j+1} = \min_{i=1,...,n} \{V(\mathbf{X}_j^i)\}$. As above $\Lambda_j(a_{j+1}) \sim \frac{1}{n} E_{j+1}, E_j \sim \mathcal{E}(1)$. Therefore

$$\Lambda(a_{j+1}) = \Lambda(a_j) + \Lambda_j(a_j) \sim \frac{1}{n} \sum_{i=1}^{j+1} E_i, \qquad E_i \sim \mathcal{E}(1)$$

CEMRACS 2013

• Estimator:

$$\hat{P}_n = \left(1 - \frac{1}{n}\right)^{\hat{J}_n}$$

• Result 2: if one knows how to generate the new particle with the distribution μ_{a_i} , then \hat{P}_n is an unbiased estimator of P with variance

$$\operatorname{Var}(\hat{P}_n) = P^2 (P^{-1/n} - 1) \simeq \frac{-P^2 \ln P}{n}$$

In fact

$$\mathbb{P}\left(\hat{P}_n = \left(1 - \frac{1}{n}\right)^j\right) = \mathbb{P}(\hat{J}_n = j) = \frac{P^n(-n\log P)^j}{j!}$$

Moreover, denoting

$$\hat{P}_{n,\pm} = \hat{P}_n \exp\left(\pm \frac{z_{1-\alpha/2}}{\sqrt{n}}\sqrt{-\log\hat{P}_n}\right)$$

where $z_{1-\alpha/2}$ is the $1-\alpha/2$ -quantile of the standard normal distribution, we have

$$\mathbb{P}(P \in [\hat{P}_{n,-}, \hat{P}_{n,+}]) \approx 1 - \alpha.$$

If $\alpha = 0.05$, then $z_{1-\alpha/2} \approx 2$.

CEMRACS 2013

• Aparté: Metropolis-Hastings algorithm.

• Let μ_a be a probability distribution on \mathbb{R}^d with pdf $p_a(\boldsymbol{x})$ (known up to a multiplicative constant). We want to simulate an ergodic Markov chain $(\boldsymbol{X}_t)_{t\geq 0}$ whose invariant distribution is μ_a .

• Preliminary step: choose an instrumental transition density q on \mathbb{R}^d , i.e., for any fixed $\boldsymbol{x}' \in \mathbb{R}^d$, $\boldsymbol{x} \to q(\boldsymbol{x}', \boldsymbol{x})$ is a pdf and we know how to generate a random variable \boldsymbol{X} with this pdf.

• Algorithm:

Step 0: Choose X_0 arbitrarily.

Step t + 1: Choose a candidate \tilde{X}_{t+1} with the distribution with pdf $q(X_t, x)$. Set $X_{t+1} = X_t$ with probability $1 - \rho(X_t, \tilde{X}_{t+1})$ (reject) and $X_{t+1} = \tilde{X}_{t+1}$ with probability $\rho(X_t, \tilde{X}_{t+1})$ (accept). Here

$$\rho(\boldsymbol{x}',\boldsymbol{x}) = \min\left(\frac{p_a(\boldsymbol{x})q(\boldsymbol{x},\boldsymbol{x}')}{p_a(\boldsymbol{x}')q(\boldsymbol{x}',\boldsymbol{x})},1\right)$$

• $(X_t)_{t\geq 0}$ is a Markov chain with transition

$$K(\boldsymbol{x}', d\boldsymbol{x}) = q(\boldsymbol{x}', \boldsymbol{x})\rho(\boldsymbol{x}', \boldsymbol{x})d\boldsymbol{x} + \left(1 - \int q(\boldsymbol{x}', \boldsymbol{y})\rho(\boldsymbol{x}', \boldsymbol{y})d\boldsymbol{y}\right)\delta_{\boldsymbol{x}'}(d\boldsymbol{x})$$

CEMRACS 2013

• We can check (because $p_a(\mathbf{x}')[q(\mathbf{x}', \mathbf{x})\rho(\mathbf{x}', \mathbf{x})] = p_a(\mathbf{x})[q(\mathbf{x}, \mathbf{x}')\rho(\mathbf{x}, \mathbf{x}')])$ $\int d\mathbf{x}' p_a(\mathbf{x}') K(\mathbf{x}', d\mathbf{x}) = p_a(\mathbf{x}) d\mathbf{x}$

 $\hookrightarrow \mu_a$ is stationary for the Markov chain.

• Under mild conditions (for instance, if q is positive), the chain $(X_t)_{t\geq 0}$ is ergodic with stationary distribution μ_a :

$$\sup_{A \in \mathcal{B}(\mathbb{R}^d)} \left| \mathbb{P}(\boldsymbol{X}_t \in A) - \mu_a(A) \right| \stackrel{t \to \infty}{\longrightarrow} 0$$

• In practice:

- after a burn-in phase with some length t_0 , the sequence $(X_t)_{t \ge t_0}$ is stationary with distribution μ_a (but not independent).

- the choice of the instrumental transition density is important to get fast convergence. Ideally the rejection rate should be around 50%.

• If $X_0 \sim \mu_a$, then the chain is stationary. After a few accepted mutations, $X_t \sim \mu_a$ and is quasi-independent from X_0 .

CEMRACS 2013

• Problem: how to generate the new particle with the distribution μ_{a_j} (of X knowing that $V(X) > a_j$)?

Version 1:

- Consider a symmetric transition kernel $q(\mathbf{x}', \mathbf{x})$ such that $q(\mathbf{x}', \mathbf{x}) = q(\mathbf{x}, \mathbf{x}')$.
- Algorithm:
- a_j = minimal value of the *n* particles.
- pick a particle $X_{(1)}$ amongst the n-1 largest particles (larger than a_j).
- for t = 1, ..., T, draw a new particle X^* with the pdf $q(X_{(1)}, \cdot)$; if $V(X^*) > a_j$, then $X_{(1)} = X^*$ with probability $\min(p(X^*)/p(X_{(1)}), 1)$; otherwise keep $X_{(1)}$. - replace the smallest particle by $X_{(1)}$.
- Result 3: the distribution of $X_{(1)}$ is the distribution μ_{a_j} . As $T \to \infty$, the distribution of $X_{(1)}$ becomes independent of the other particles.

• Problem: how to generate the new particle with the distribution μ_{a_j} (of X knowing that $V(X) > a_j$)?

Version 2:

- Consider a transition kernel $q(\mathbf{x}', \mathbf{x})$ such that $p(\mathbf{x}')q(\mathbf{x}', \mathbf{x}) = p(\mathbf{x})q(\mathbf{x}, \mathbf{x}')$.
- Algorithm:
- a_j = minimal value of the *n* particles.
- pick a particle $X_{(1)}$ amongst the n-1 largest particles (larger than a_j).

- for t = 1, ..., T, draw a new particle X^* with the pdf $q(X_{(1)}, \cdot)$; if $V(X^*) > a_j$, then $X_{(1)} = X^*$; otherwise keep $X_{(1)}$.

- replace the smallest particle by $X_{(1)}$.

• Result 3: the distribution of $X_{(1)}$ is the distribution μ_{a_j} . As $T \to \infty$, the distribution of $X_{(1)}$ becomes independent of the other particles. In practice: T = a few tens. Example:



Cf: F. Cerou, A. Guyader (Rennes), P. Glasserman, R. Rubinstein.

CEMRACS 2013

Conclusions

• Importance sampling: bias the input.

Interacting particle system: select the particles based on the output.

 \hookrightarrow No physical insight is required to guess the suitable twisted input distribution. But: need $V(\mathbf{X})$.

• The real distribution is used, not a twisted one.

 \hookrightarrow Non-intrusive method: no need to change the numerical code.

• Number of particles fixed, computational cost (almost) fixed.

• It is possible to make the algorithm partially parallel (not fully parallel as Monte Carlo).

• Also: conditional distributions. The method is efficient for the computation of conditional expectations and for the analysis of the cascade of events leading to a rare event.

CEMRACS 2013