An introduction to particle simulation of rare events

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Outline

Summary

Rare event analysis

- **Stochastic process** $X \oplus$ **Rare event** A **:**

$$\mathrm{Proba}(X \in A) \quad \& \quad \mathrm{Law}((X_0, \ldots, X_t) \mid X \in A)$$

$\supset$ engineering/physics/biology/economics/finance :

  - *Finance :* ruin/default probabilities, financial crashes, eco. crisis,...
  - *engineering :* networks overload, breakdowns, engines failures,...
  - *Physics :* climate models, directed polymer conformations, particle in absorbing medium, ground states of Schroedinger models.
  - *Statistics :* tail probabilities, extreme random values.
  - *Combinatorics :* Complex enumeration problems.

- **Process strategies** $\in$ **Rare event** $\Rightarrow$ Control and prediction.

$$X_t = F_t(X_{t-1}, W_t) \rightarrow \mathrm{Law}((W_0, \ldots, W_t) \mid X \in A)$$

Stochastic models

Only 2 Ingredients

- 1 Physical/biological/financial process : queuing network, portfolio, volatility process, stock market evolutions, interacting/exchange economic models ...
- 1 Potential function (energy type, indicator, restrictions): critical level crossing, penalties functions, constraints subsets, performance levels, long range dependence...

Objectives

- Estimation of the probability of the rare event.
- Computing the full distributions of the path of the process evolving in the critical regime $\rightsquigarrow$ prediction $\oplus$ control.

Twisted Monte Carlo methods

$$\mathbb{P}(X \in A) = 10^{-10} \rightsquigarrow \text{Find } \mathbb{Q} \text{ s.t.} \quad \mathbb{Q}(A) \simeq 1$$

Elementary Monte Carlo estimate X^i iid $\mathbb{Q}$

$$\mathbb{P}(A) := \int \frac{d\mathbb{P}}{d\mathbb{Q}}(x)\ 1_A(x)\ \mathbb{Q}(dx) \simeq \mathbb{P}^N(A) := \frac{1}{N} \sum_{1 \leq i \leq N} \frac{d\mathbb{P}}{d\mathbb{Q}}(X^i)\ 1_A(X^i)$$

$$\text{Variance} \simeq \int \frac{d\mathbb{P}}{d\mathbb{Q}}(x)\ 1_A(x)\ \mathbb{P}(dx) \quad (\text{ex. cross-entropy} : \mathbb{Q} \in \{\mathbb{Q}_a, a \in \mathcal{A}\})$$

Drawbacks

- Huge variance if $\mathbb{Q}$ badly chosen $\rightsquigarrow$ optimal choice $\mathbb{Q}(dx) \propto 1_A(x)\mathbb{P}(dx)$.
- Need to twist the original reference process X.
- Stochastic evolution $X = (X_0, \ldots, X_n)$

$$\frac{d\mathbb{P}_n}{d\mathbb{Q}_n}(X) := \prod_{k=0}^{n} \frac{p_k(X_k|X_{k-1})}{q_k(X_k|X_{k-1})} \quad \text{degenerate product martingale w.r.t. } n$$

Summary

Flow of measure with increasing sampling complexity

- Rare event = cascade/series of intermediate less-rare events
  ($\uparrow$ energy levels, physical gateways, index level crossings).
- Conditional probability flow = flow of optimal twisted measures

$$n \rightarrow \eta_n = \text{Law}(\text{process} \mid \text{series of } n \text{ intermediate events})$$

- Rare event probabilities= Normalizing constants.

Particle methods

(Sampling a genealogical type default tree model $\oplus$ % success or default)

- Explorations/Local search propositions of the solution space.
- Branching-Selection individuals $\in \uparrow$ critical regimes.

5 Examples of flow of target measures

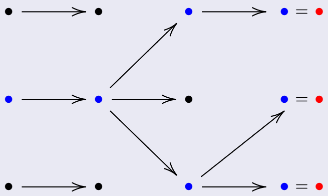
1. $\eta_n = \mathrm{Law}((X_0, \ldots, X_n) \mid \forall 0 \leq p \leq n \quad X_p \in A_p)$
2. $\eta_n(dx) \propto e^{-\beta_n V(x)}\ \lambda(dx)$ with $\beta_n \uparrow$
3. $\eta_n(dx) \propto 1_{A_n}(x)\ \lambda(dx)$ with $A_n \downarrow$
4. $\eta_n = \mathrm{Law}^K_\pi((X_0, \ldots, X_n) \mid X_n = x_n)$.
5. $\eta_n = \mathrm{Law}(\ X \text{ hits } B_n \mid X \text{ hits } B_n \text{ before } A)$

5 particle heuristics :

1. M_n-local moves $\oplus$ individual selections $\in A_n$ i.e. $\sim G_n = 1_{A_n}$
2. MCMC local moves $\eta_n = \eta_n M_n$ $\oplus$ individual selections $\propto G_n = e^{-(\beta_{n+1}-\beta_n)V}$
3. MCMC local moves $\eta_n = \eta_n M_n$ $\oplus$ individual selections $\propto G_n = 1_{A_{n+1}}$
4. M-local moves $\oplus$ Selection $G(x_1, x_2) = \frac{\pi(dx_2)K(x_2,dx_1)}{\pi(dx_1)M(x_1,dx_2)}$
5. M_n-local moves $\oplus$ Selection-branching on upper/lower levels B_n.

Interaction/branch. process $\hookrightarrow$ 3 types of occupation measures

$(N = 3)$



- Current population $\hookrightarrow \frac{1}{N}\sum_{i=1}^{N} \delta_{\xi_n^i}$ ← i-th individual at time n

- Genealogical tree model $\hookrightarrow \frac{1}{N}\sum_{i=1}^{N} \delta_{(\xi_{0,n}^i,\xi_{1,n}^i,\ldots,\xi_{n,n}^i)}$ ← i-th ancestral line

- **Complete genealogical tree model** $\hookrightarrow \frac{1}{N}\sum_{i=1}^{N} \delta_{(\xi_0^i,\xi_1^i,\ldots,\xi_n^i)}$

- $\oplus$ *Empirical mean potentials [success % ($G_n = 1_A$)]* $\hookrightarrow \frac{1}{N}\sum_{i=1}^{N} G_n(\xi_n^i)$

Equivalent Stochastic Algorithms :

- Genetic and evolutionary type algorithms.
- Spatial branching models, subset splitting techniques.
- Sequential Monte Carlo methods, population Monte Carlo models.
- Diffusion Monte Carlo (DMC), Quantum Monte Carlo (QMC), ...
- Some botanical names $\sim \neq$ application domain areas :

  bootsrapping, selection, pruning-enrichment, reconfiguration, cloning, go with the winner, spawning, condensation, grouping, rejuvenations, harmony searches, biomimetics, splitting, ...

$$\Updownarrow$$

1950 $\leq$ [(Meta)Heuristics] $\leq$ 1996 $\leq$ Feynman-Kac mean field particle model

Summary

Notation

E measurable state space, $\mathcal{P}(E)$ proba. on E, $\mathcal{B}(E)$ bounded meas. functions

- $(\mu, f) \in \mathcal{P}(E) \times \mathcal{B}(E) \quad \longrightarrow \quad \mu(f) = \int \mu(dx)\ f(x)$
- $M(x, dy)$ **integral operator over E**

$$\begin{aligned} M(f)(x) &= \int M(x, dy) f(y) \\ [\mu M](dy) &= \int \mu(dx) M(x, dy) \qquad (\Longrightarrow [\mu M](f) = \mu[M(f)]\ ) \end{aligned}$$

- **Bayes-Boltzmann-Gibbs transformation :** $G : E \to [0, \infty[$ with $\mu(G) > 0$

$$\Psi_G(\mu)(dx) = \frac{1}{\mu(G)}\ G(x)\ \mu(dx)$$

E finite $\Longleftrightarrow$ Matrix notations $\mu = [\mu(1), \ldots, \mu(d)]$ and $f = [f(1), \ldots, f(d)]'$

Infinite Population $N \uparrow \infty$ "=" Feynman-Kac measures $\simeq (G_n, M_n)$

- **Current population:**

$$\eta_n^N(f) := \frac{1}{N} \sum_{i=1}^{N} f(\xi_n^i) \longrightarrow_{N\uparrow\infty} \eta_n(f) := \frac{\gamma_n(f)}{\gamma_n(1)}$$

with [Potential functions G_n] & [X_n Markov chain $\sim$ transitions M_n]

$$\gamma_n(f) := \mathbb{E}\left(f_n(X_n) \prod_{0\leq p<n} G_p(X_p) \right)$$

- **Genealogical tree occupation measures:**

$$\frac{1}{N} \sum_{i=1}^{N} \delta_{(\xi_{0,n}^i, \xi_{1,n}^i, \ldots, \xi_{n,n}^i)} \longrightarrow_{N\uparrow\infty} d\mathbb{Q}_n := \frac{1}{\mathcal{Z}_n} \left\{ \prod_{0\leq p<n} G_p(X_p) \right\} d\mathbb{P}_n$$

- **Normalizing constants:** $\prod_{0\leq p<n} \eta_p^N(G_p) \longrightarrow_{N\uparrow\infty} \mathcal{Z}_n = \gamma_n(1)$

Feynman-Kac models $\supset$ ALL of the above heuristics

Example : $G_n = 1_{A_n}$ and X_n Markov chain

- Normalizing constants:

$$\gamma_n(1) = \mathbb{P}\left(n\text{-th rare event}\right) = \mathbb{P}(X_p \in A_p,\ 0 \leq p < n)$$

- n-th time marginals:

$$\eta_n = \mathrm{Law}(X_n \mid n\text{-th rare event}) = \mathrm{Law}(X_n \mid X_p \in A_p,\ 0 \leq p < n)$$

- Path space measures:

$$\mathbb{Q}_n = \mathrm{Law}((X_p)_{0\leq p\leq n} | n\text{-th rare event}) = \mathrm{Law}((X_p)_{0\leq p\leq n} |\ X_p \in A_p,\ p < n)$$

- Note : Including the n-th rare event level set

$$\rightsquigarrow \text{Updated measures } \widehat{\gamma}_n, \widehat{\eta}_n, , \widehat{\mathbb{Q}}_n \text{ with } \prod_{0\leq p\leq n}$$

Another "detailed" static example

Restriction of measures : $A_n \downarrow$ (Ex.: $A_n = [a_n, \infty[\rightsquigarrow$ tails probab.)

$$\eta_n(dx) = \frac{1}{Z_n} 1_{A_n}(x)\ \lambda(dx)$$

Feynman-Kac representation :

$$\eta_n(f) := \frac{\gamma_n(f)}{\gamma_n(1)} \quad \text{with} \quad \gamma_n(f) := \mathbb{E}\left(f_n(X_n) \prod_{0 \leq p < n} 1_{A_{p+1}}(X_p)\right)$$

and

$$\mathbb{P}\left(X_n \in dx_n \mid X_{n-1} = x_{n-1}\right) = M_n(x_{n-1}, dx_n) \quad \text{with} \quad \eta_n = \eta_n M_n$$

Note :

$$\begin{aligned} Z_n &= \lambda\left(A_n\right) \\ &= \underbrace{\frac{\lambda\left(1_{A_n}\ 1_{A_{n-1}}\right)}{\lambda\left(1_{A_{n-1}}\right)}}_{\eta_{n-1}(1_{A_n})} \times Z_{n-1} \overset{(A_0=E)}{=} \prod_{0 \leq p < n} \eta_p\left(1_{A_{p+1}}\right) \end{aligned}$$

Sensitivity analysis

$$\theta \mapsto \quad M_n(x_{n-1}, dx_n) = p_n^{\theta}(x_{n-1}, x_n)\ \lambda_n^X(dx_n) \quad \text{and} \quad G_n(x) = G_n^{\theta}(x)$$

$$\Downarrow$$

Parametric Feynman-Kac models : $(G_n, \mathbb{Q}_n, \gamma_n, \eta_n, \ldots) \rightsquigarrow (G_n^{\theta}, \mathbb{Q}_n^{\theta}, \gamma_n^{\theta}, \eta_n^{\theta}, \ldots)$

$$\frac{\partial}{\partial\theta} \log \widehat{\gamma}_n^{\theta}(1) = \widehat{\mathbb{Q}}_n^{\theta}(F_n^{\theta}) \quad \text{and} \quad \frac{\partial}{\partial\theta} \widehat{\mathbb{Q}}_n^{\theta}(\varphi_n) = \widehat{\mathbb{Q}}_n^{\theta}\left(F_n^{\theta}\ [\varphi_n - \widehat{\mathbb{Q}}_n^{\theta}(\varphi_n)]\right)$$

with the additive functional

$$F_n^{\theta}(x_0, \ldots, x_n) \quad := \quad \sum_{0 \le k \le n} f_k^{\theta}(x_{k-1}, x_k)$$

$$f_k^{\theta}(x_{k-1}, x_p) \quad := \quad \frac{\partial \log G_p^{\theta}(x_k)}{\partial\theta} + \frac{\partial \log p_k^{\theta}(x_{k-1}, x_k)}{\partial\theta}$$

Additive functionals *(with Doucet & Singh* `Hal-INRIA july 09`*)*

- Path space models $\mathbb{P}_n := \mathrm{Law}(X_0, \ldots, X_n)$

$$d\mathbb{Q}_n := \frac{1}{\mathcal{Z}_n} \left\{ \prod_{0 \leq p < n} G_p(X_p) \right\} d\mathbb{P}_n$$

- Hyp. : $M_n(x_{n-1}, dx_n) = H_n(x_{n-1}, x_n)\ \lambda_n(dx_n)$

$$\Rightarrow \mathbb{Q}_n(d(x_0, \ldots, x_n)) = \eta_n(dx_n)\ \mathcal{M}_{n,\eta_{n-1}}(x_n, dx_{n-1}) \ldots \mathcal{M}_{1,\eta_0}(x_1, dx_0)$$

with the backward transitions :

$$\mathcal{M}_{p+1,\eta}(x, dx') \propto G_p(x')\ H_{p+1}(x', x)\ \eta(dx')$$

- **Particle estimates** $\sim$ Ancestral tree or the complete genealogical tree :

$$\mathbb{Q}_n^N(d(x_0, \ldots, x_n)) = \eta_n^N(dx_n)\ \mathcal{M}_{n,\eta_{n-1}^N}(x_n, dx_{n-1}) \ldots \mathcal{M}_{1,\eta_0^N}(x_1, dx_0)$$

Summary

Flows of Feynman-Kac measures

- A two step correction prediction model

$$\eta_n \xrightarrow{\text{Updating-correction}} \widehat{\eta}_n = \Psi_{G_n}(\eta_n) \xrightarrow{\text{Prediction/Markov transport}} \eta_{n+1} = \widehat{\eta}_n M_{n+1}$$

- Selection nonlinear transport formulae

$$\Psi_{G_n}(\eta_n) = \eta_n S_{n,\eta_n}$$

with, for any $\epsilon_n = \epsilon_n(\eta_n) \in [0,1]$ s.t. $\epsilon_n G_n \leq 1$

$$S_{n,\eta_n}(x,.) := \epsilon_n G_n(x)\ \delta_x + (1 - \epsilon_n G_n(x))\ \Psi_{G_n}(\eta_n)$$

$$\Downarrow$$

$$\eta_{n+1} = \eta_n \left(S_{n,\eta_n} M_{n+1}\right) := \eta_n K_{n+1,\eta_n}$$

Nonlinear Markov chains $\eta_n = \mathrm{Law}(\overline{X}_n)$=Perfect sampling algorithm

- **Nonlinear transport formulae :**

$$\eta_{n+1} = \eta_n K_{n+1,\eta_n}$$

with the collection of Markov probability transitions :

$$K_{n+1,\eta_n} = S_{n,\eta_n} M_{n+1}$$

- **Local transitions :**

$$\mathbb{P}(\overline{X}_n \in dx_n \mid \overline{X}_{n-1}) = K_{n,\eta_{n-1}}(\overline{X}_{n-1}, dx_n) \quad \text{with} \quad \eta_{n-1} = \mathrm{Law}(\overline{X}_{n-1})$$

- **McKean measures (canonical process) :**

$$\mathbb{P}_n(d(x_0, \ldots, x_n)) = \eta_0(dx_0)\ K_{1,\eta_0}(x_0, dx_1) \ldots K_{n,\eta_{n-1}}(x_{n-1}, dx_n)$$

Sampling pb $\Rightarrow$ Mean field particle interpretations

- Markov Chain $\xi_n = (\xi_n^1, \ldots, \xi_n^N) \in E_n^N$ s.t.

$$\eta_n^N := \frac{1}{N} \sum_{1 \leq i \leq N} \delta_{\xi_n^i} \simeq_{N\uparrow\infty} \eta_n$$

- Approximated local transitions ($\forall 1 \leq i \leq N$)

$$\xi_{n-1}^i \rightsquigarrow \xi_n^i \sim K_{n,\eta_{n-1}^N}(\xi_{n-1}^i, dx_n)$$

Schematic picture : $\xi_n \in E_n^N \rightsquigarrow \xi_{n+1} \in E_{n+1}^N$

$$\begin{array}{ccc}
\xi_n^1 & \xrightarrow{K_{n+1,\eta_n^N}} & \xi_{n+1}^1 \\
\vdots & & \vdots \\
\xi_n^i & \longrightarrow & \xi_{n+1}^i \\
\vdots & & \vdots \\
\xi_n^N & \longrightarrow & \xi_{n+1}^N
\end{array}$$

Rationale :

$$\eta_n^N \simeq_{N\uparrow\infty} \eta_n \Longrightarrow K_{n+1,\eta_n^N} \simeq_{N\uparrow\infty} K_{n+1,\eta_n} \Longrightarrow \xi^i \sim \text{i.i.d. copies of } \overline{X}$$

$$\Downarrow$$

Particle McKean measures :

$$\frac{1}{N}\sum_{i=1}^{N} \delta_{(\xi_0^i,\ldots,\xi_n^i)} \longrightarrow_{N\uparrow\infty} \text{Law}(\overline{X}_0,\ldots,\overline{X}_n)$$

Feynman-Kac models $\Leftrightarrow$ Genetic type stochastic algo.

$$
\left.\begin{matrix} \xi_n^1 \\ \vdots \\ \xi_n^i \\ \vdots \\ \xi_n^N \end{matrix}\right] \xrightarrow{S_{n,\eta_n^N}} \left[\begin{matrix} \widehat{\xi}_n^1 & \xrightarrow{M_{n+1}} & \xi_{n+1}^1 \\ \vdots & & \vdots \\ \widehat{\xi}_n^i & \longrightarrow & \xi_{n+1}^i \\ \vdots & & \vdots \\ \widehat{\xi}_n^N & \longrightarrow & \xi_{n+1}^N \end{matrix}\right]
$$

Acceptance/Rejection-Selection : [Geometric type clocks]

$$
S_{n,\eta_n^N}(\xi_n^i, dx)
$$

$$
:= \epsilon_n G_n(\xi_n^i)\ \delta_{\xi_n^i}(dx) + \left(1 - \epsilon_n G_n(\xi_n^i)\right)\ \sum_{j=1}^N \frac{G_n(\xi_n^j)}{\sum_{k=1}^N G_n(\xi_n^k)} \delta_{\xi_n^j}(dx)
$$

Ex. : $G_n = 1_A \rightsquigarrow G_n(\xi_n^i) = 1_A(\xi_n^i)$

Some key advantages

- Mean field models=stochastic linearization/perturbation technique :

$$\eta_n^N = \eta_{n-1}^N K_{n,\eta_{n-1}^N} + \frac{1}{\sqrt{N}}\, W_n^N$$

with $W_n^N \simeq W_n$ Centered Gaussian Fields $\perp$.

- $\eta_n = \eta_{n-1} K_{n,\eta_{n-1}}$ stable $\Rightarrow$ No propagation of local sampling errors

$\Longrightarrow$ Uniform control w.r.t. the time horizon

- "No burning, no need to study the stability of MCMC models".
- Stochastic adaptive grid approximation
- Nonlinear system $\rightsquigarrow$ "positive-benefic interactions.
- Simple and natural sampling algorithm.

Summary

"Asympt." theo. TCL,PGD, PDM $\oplus$ (n,N) fixed $\rightsquigarrow$ some examples :

- Empirical processes :

$$\sup_{n\geq 0}\sup_{N\geq 1}\sqrt{N}\;\mathbb{E}(\|\eta_n^N-\eta_n\|_{\mathcal{F}_n}^p)<\infty$$

- Concentration inequalities uniform w.r.t. time :

$$\sup_{n\geq 0}\mathbb{P}(|\eta_n^N(f_n)-\eta_n(f_n)|>\epsilon)\leq c\;\exp-(N\epsilon^2)/(2\;\sigma^2)$$

$+$ *Guionnet* $\sup_{n\geq 0}$ (IHP 01) & *Ledoux* $\sup_{\mathcal{F}_n}$ (JTP 00) & *Rio* AAP 10

- Propagations of chaos exansions *(+Patras,Rubenthaler* (AAP 09)) :

$$\begin{aligned}\mathbb{P}_{n,q}^N &:= \mathrm{Law}(\xi_n^1,\ldots,\xi_n^q)\\ &\simeq \eta_n^{\otimes q}+\frac{1}{N}\;\partial^1\mathbb{P}_{n,q}+\ldots+\frac{1}{N^k}\;\partial^k\mathbb{P}_{n,q}+\frac{1}{N^{k+1}}\;\partial^{k+1}\mathbb{P}_{n,q}^N\end{aligned}$$

with $\sup_{N\geq 1}\|\partial^{k+1}\mathbb{P}_{n,q}^N\|_{\mathrm{tv}}<\infty$ & $\sup_{n\geq 0}\|\partial^1\mathbb{P}_{n,q}\|_{\mathrm{tv}}\leq c\;q^2$.

Unnormalized models

Un-bias particle approximation measures

$$\gamma_n^N(f_n) := \eta_n^N(f_n) \prod_{0\leq p<n} \eta_p^N(G_p)$$

- **Asymptotic theorms** : fluctuations & deviations
  + A. Guionnet (`AAP 99, SPA 98`*), + L. Miclo* `(SP 00)`, *+ D. Dawson (01)*
- Non asymptotic theory : bias and variance estimates
  1. Taylor type expansion *(+Patras & Rubenthaler* `(AAP 09)` :

  $$\mathbb{E}\left((\gamma_n^N)^{\otimes q}(F)\right) =: \mathbb{Q}_{n,q}^N(F) = \gamma_n^{\otimes q}(F) + \sum_{1\leq k\leq (q-1)(n+1)} \frac{1}{N^k}\, \partial^k \mathbb{Q}_{n,q}(F)$$

  2. *Variance estimates* (+Cerou & Guyader `Hal-INRIA 08` & IPH 2010) *:*

  $$\mathbb{E}\left(\left[\gamma_n^N(f_n) - \gamma_n(f_n)\right]^2\right) \leq \; c\,\frac{n}{N} \;\times\; \gamma_n(1)^2$$

Additive functionals

$$F_n(x_0,\ldots,x_n) = \frac{1}{n+1}\sum_{0\leq p\leq n} f_p(x_p)$$

- Bias estimate+uniform $\mathbb{L}_p$-bounds + variance $(1/N^2)$

$$N\ \mathbb{E}\left([(\mathbb{Q}_n^N-\mathbb{Q}_n)(F_n)]^2\right)\leq c\times\left(\underbrace{1/n}_{\text{bias term}}+1/N\right)$$

- Uniform exponential concentration

$$\frac{1}{N}\log\sup_{n\geq 0}\mathbb{P}\left(\left|[\mathbb{Q}_n^N-\mathbb{Q}_n](F_n)\right|\geq\frac{b}{\sqrt{N}}+\epsilon\right)\leq -\epsilon^2/(2b^2)$$

Summary

Particle methods & Sequential Monte Carlo

- Feynman-Kac formulae. Genealogical and interacting particle systems, Springer (2004) ⊕ Refs.
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Rare event analysis

- **Particle simulation of twisted measures**
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- **Branching processes**
  - (with P. Lezaud) Branching and interacting particle interpretation of rare event proba.. Stochastic Hybrid Systems : Theory and Safety Critical Applications, eds. H. Blom and J. Lygeros. Springer (2006).
  - (with F. Cerou, Le Gland F., Lezaud P.) Genealogical Models in Entrance Times Rare Event Analysis, *Alea*, Vol. I, (2006).
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  - (with F. Cerou, A. Guyader, F. LeGland, P. Lezaud et H. Topart) Some recent improvements to importance splitting

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- (with A. Doucet et A. Jasra) `On Adaptive Resampling Procedures for Sequential Monte Carlo Methods` (HAL-INRIA 2008).