Particle Rare Event Stochastic Simulation

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Outline

Some typical rare events

- Physical/biological/economical stochastic process : atomic/molecular configurations fluctuations, queueing evolutions, communication network, portfolio and financial assets, ...
- Potential function-Event restrictions : Energy/Hamiltonian potential functions, overflows levels, critical thresholds, epidemic propagations, radiation dispersion, ruin levels.

Objectives

- Compute rare event probabilities.
- Find the law of the whole random process trajectories evolving in a critical regime $\rightsquigarrow$ prediction $\oplus$ control.

$\rightsquigarrow$ Solution : Stochastic genealogical type tree fault model

$\sim$ Branching+interacting evolutionary particle model

(Branching on "more likely" gateways to critical regimes)

Event restrictions

Event restrictions

- X r.v. $\in (E, \mathcal{E})$ with $\mu = \mathrm{Law}(X)$
- $A \in \mathcal{E}$ with $0 < \mu(A) = \mathbb{P}(X \in A) \simeq 10^{-p}$ and $p >> 1$.

$$\eta(dx) \;=\; \frac{1}{\mu(A)}\, 1_A(x)\; \mu(dx) = \mathbb{P}(X \in dx \mid X \in A)$$

Examples

$$\begin{aligned} E &= \mathbb{R},\; \mathbb{R}^d,\; \mathbb{R}^{\{-n,\ldots,n\}^2},\; \cup_{n\geq 0} (\mathbb{R}^d)^{\{0,\ldots,n\}}, \ldots \\ A &= [a,\infty[,\; V^{-1}([a,\infty[), \{\text{an excursion hits B before C}\} \ldots \\ \mu &= \text{uniform on } E \text{ finite } \rightsquigarrow \text{combinatorial counting pb} \end{aligned}$$

First heuristic $A_n \downarrow A$

$\rightsquigarrow$ A_{n+1}-interacting MCMC with local targets $\propto 1_{A_n}(x)\; \mu(dx)$

A pair of more precise examples

- Non intersecting random walks/connectivity constants :

$$
\begin{aligned}
X &= (X'_0, \ldots, X'_n) \in E := (\mathbb{Z}^d \times \ldots \times \mathbb{Z}^d) \\
A &= \{(x'_0, \ldots, x'_n) : \forall 0 \leq p < q \leq n \;\; x'_p \neq x'_q\}
\end{aligned}
$$

$$
\begin{aligned}
\Rightarrow \mu(A) &= \frac{1}{(2d)^n} \times \#\{\text{not} \cap \text{ walks with length n}\} \\
&\simeq \exp(c \;\, n) \\
\Rightarrow \quad \eta &= \mathrm{Law}((X'_0, \ldots, X'_n) \mid \forall p < q \leq n \quad X'_p \neq X'_q)
\end{aligned}
$$

Second heuristic $\sim$ multiplicative structure :

$\rightsquigarrow$ Accept-Reject interacting X'-motions

- Random walk confinements/Lyap. exp. and top eigenval. :

$$A = \left\{ (x'_0, \ldots, x'_n) \in (\mathbb{Z}^d \times \ldots \times \mathbb{Z}^d) : \forall 0 \leq p \leq n \;\; x'_p \in A' \right\}$$

$$\Rightarrow \mu(A) = \mathbb{P}(\forall 0 \leq p \leq n \;\; X'_p \in A') \simeq e^{-\lambda(A')\; n}$$

and

$$\Rightarrow \eta = \mathrm{Law}((X'_0, \ldots, X'_n) \mid \forall 0 \leq p \leq n \quad X'_p \in A')$$

Same heuristic $\sim$ multiplicative structure :

$\rightsquigarrow$ Accept-Reject interacting X'-motions

More examples of stochastic rare event models

- $\mathbb{P}(\cap_{0\leq p\leq n}\{X_p \in A_p\})$, $\mathrm{Law}((X_p)_{0\leq p\leq n} \mid \cap_{0\leq p\leq n}\{X_p \in A_p\})$
  - Ex. : $\mathrm{Law}((X'_0,\ldots,X'_n) \mid \cap_{0\leq p<q\leq n}\{\|X'_p - X'_q\| \geq \epsilon)$
  - Soft penalization : $1_{A_n} \rightsquigarrow \exp\left(-\beta 1_{\notin A_n}\right)$
  - Terminal level set conditioning :

$$\mathbb{P}(V_n(X_n) \geq a) \quad \& \quad \mathrm{Law}((X_0,\ldots,X_n) \mid V_n(X_n) \geq a)$$

  - Fixed terminal value : $\mathrm{Law}_\pi((X_0,\ldots,X_n) \mid X_n = x_n)$.
- Critical excursion behavior : $\cup$ in excursion space
  $\mathbb{P}(X \text{ hits } B \text{ before } C) \quad \& \quad \mathrm{Law}(X \mid X \text{ hits } B \text{ before } C)$

Last heuristic :

$\rightsquigarrow$ Interacting X-excursions on gateways levels $\rightsquigarrow B$.
$\rightsquigarrow$ interacting X-transitions increasing the potential V_n.

A single (sequential) Feynman-Kac/Boltzmann-Gibbs formulation:

$$
\begin{aligned}
d\eta_n &= \frac{1}{\mathcal{Z}_n}\left\{\prod_{0\le p<n} G_p(X_p)\right\} d\mathbb{P}_n^X \\
&\overset{G_n=1_{A_n}}{=} \mathrm{Law}((X_0,\ldots,X_n) \mid X_0\in A_0,\ldots,X_n\in A_n) \\
\text{and } \mathcal{Z}_n &= \mathbb{P}(X_0\in A_0,\ldots,X_n\in A_n)
\end{aligned}
$$

Observation : $\eta_n =$ "complex nonlinear" transformation of η_{n-1}

$$
\left\{\prod_{0\le p\le n} G_p(X_p)\right\} = \left\{\prod_{0\le p\le (n-1)} G_p(X_p)\right\} G_n(X_n)
$$

Same heuristic $\sim$ multiplicative structure :

$\rightsquigarrow$ (Accept-Reject) G-interacting X-motions [and inversely!]

Stochastic modeling

- Rare event = cascade of intermediate (less) rare events (increasing energies, critical levels, multilevel gateways).
- η_n=Law(process | a series of n intermediate $\downarrow$ events) =nonlinear distribution flow with $\uparrow$ level of complexity.

$$\eta_0 \to \eta_1 \to \ldots \to \eta_{n-1} \to \eta_n(dx) = \frac{1}{\gamma_n(1)} \gamma_n(dx) \to \ldots$$

- Rare event probabilities = normalizing constants $\gamma_n(1) = \mathcal{Z}_n$.

Interacting stochastic sampling strategy

- Interacting stoch. algo. = sampling w.r.t. a flow of meas.
  - **Mean field particle models** *(sequential Monte Carlo, population Monte Carlo, particle filters, pruning, spawning, reconfiguration, quantum Monte carlo, go with the winner).*
  - **Interacting MCMC models (new i-MCMC technology)**.

Nonlinear distribution flows

- $\eta_n \in \mathcal{P}(E_n)$ probability measures on $(E_n, \mathcal{E}_n)$ ($\uparrow$ complexity).

$$\eta_n = \Phi_n(\eta_{n-1}) \quad \text{with} \quad \Phi_n : \mathcal{P}(E_{n-1}) \mapsto \mathcal{P}(E_n)$$

Two important transformations

- Markov transport eq. : $M_n(x_{n-1}, dx_n)$ from E_{n-1} into E_n

$$(\eta_{n-1}M_n)(dx_n) := \int_{E_{n-1}} \eta_{n-1}(dx_{n-1})\ M_n(x_{n-1}, dx_n)$$

- Boltzmann-Gibbs transformation : $G_n : E_n \rightarrow \mathbb{R}_+$

$$\Psi_{G_n}(\eta_n)(dx_n) := \frac{1}{\eta_n(G_n)}\ G_n(x_n)\ \eta_n(dx_n)$$

Feynman-Kac distribution flows

(Prédiction,Correction)=(Exploration,Selection)=(G_n, M_n)

Heuristics $\rightsquigarrow$ particle occupation measures
(ξ_n^i=i-th walker/individual/particle time=n)

$$\eta_n^N := \frac{1}{N}\sum_{i=1}^N \delta_{\xi_n^i} \simeq_{N\uparrow\infty} \eta_n = \Phi_n(\eta_{n-1}) := \Psi_{G_{n-1}}(\eta_{n-1})M_n$$

Solution : X_n Markov $\sim$ transitions M_n

$$\eta_n(f_n) \quad = \quad \frac{\gamma_n(f_n)}{\gamma_n(1)} \quad \text{with} \quad \gamma_n(f_n) = \mathbb{E}\left(f_n(X_n)\prod_{0\le p<n} G_p(X_p)\right)$$

Multiplicative formula $\rightsquigarrow$ Unbias estimation

$$\mathbb{E}\left(\prod_{0\le p<n} G_p(X_p)\right) = \prod_{0\le p<n}\eta_p(G_p) \simeq_{N\uparrow\infty} \prod_{0\le p<n}\eta_p^{\mathrm{N}}(G_p)$$

Running example

Confinement potential

Running example : $G_n = 1_A$ (or 1_{A_n}) :

$$\begin{aligned} \Rightarrow \gamma_n(1) &= \mathbb{P}(\forall 0 \leq p < n \quad X_p \in A) \\ \eta_n &= \mathbb{P}(X_n \in dx_n \mid \forall 0 \leq p < n \quad X_p \in A) \end{aligned}$$

Key multiplicative formula

$$\gamma_n(1) = \prod_{0 \leq p < n} \eta_p(G_p) = \prod_{0 \leq p < n} \mathbb{P}(X_p \in A \mid \forall 0 \leq q < p \quad X_q \in A)$$

Note :

$\eta_n \neq$ Law of a Markov process with local restrictions to A.

Structural stability properties

State space enlargements $\rightsquigarrow$ same model!

$$X_n = (X'_{n-1}, X'_n) \quad \text{or} \quad X_n = (X'_0, \ldots, X'_n) \quad \text{or} \quad \text{excursions}$$

Ex.: $X_n = (X'_0, \ldots, X'_n)$

$$\Rightarrow \eta_n(f_n) \propto \mathbb{E}\left(f_n(X'_0, \ldots, X'_n) \prod_{0 \leq p < n} G_p(X'_0, \ldots, X'_p) \right)$$

Boltzmann-Gibbs' formulation :

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

Structural stability properties

Importance sampling distributions $\rightsquigarrow$ same model!

- Change of proba. : $X_n = (X'_{n-1}, X'_n) \rightsquigarrow Y_n = (Y'_{n-1}, Y'_n)$

$$\mathbb{E}\left(f_n(X_n)\prod_{0\leq p<n} G_p(X_p)\right) \propto \mathbb{E}\left(f_n(Y_n)\prod_{0\leq p<n} H_p(Y_p)\right)$$

- Related weighted meas. $G_n = G_n^{\epsilon_n} \times G_n^{1-\epsilon_n} = G_n^{(1)} \times G_n^{(2)} = \ldots$

Complexity and Sampling problems

- Path integration formulae, infinite dimensional state spaces
- Nonlinear-Nongaussian models
- Complex probability mass variations

Some "Wrong" approximation ideas

- "Pure" weighted Monte Carlo methods : X^i iid copies of X

$$\frac{1}{N}\sum_{i=1}^{N} f_n(X_n^i)\left\{\prod_{0\leq p<n} G_p(X_p^i)\right\} \simeq \mathbb{E}\left(f_n(X_n)\prod_{0\leq p<n} G_p(X_p)\right)$$

$\rightsquigarrow$ bad grids X^i $\oplus$ degenerate weights (running ex $G_n = 1_A$).

- Uncorrelated MCMC for each target measure η_n ($\uparrow$ complex.).
- "Pure" branching interpretations $\rightsquigarrow$ random population sizes

$$G_n(x) = \mathbb{E}(g_n(x)) \quad \text{with} \quad g_n(x) \text{ r.v. } \in \mathbb{N}$$

- Harmonic/(Gaussian+linearisation) approximations.
- $G.M(H) \propto H \rightsquigarrow G \propto H/M(H) \rightsquigarrow H$-process X^H (unknown).

Nonlinear distribution flows

- **Nonlinear Markov models :** always $\exists K_{n,\eta}(x, dy)$ Markov s.t.

$$\eta_n = \Phi_n(\eta_{n-1}) = \eta_{n-1} K_{n,\eta_{n-1}} = \mathrm{Law}\left(\overline{X}_n\right)$$

i.e. :

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

Mean field particle interpretation

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

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

- Particle approximation transitions ($\forall 1 \leq i \leq N$)

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

Discrete generation mean field particle model

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 :

$$
\begin{aligned}
\eta_n^N \simeq_{N\uparrow\infty} \eta_n \quad & \Longrightarrow \quad K_{n+1,\eta_n^N} \simeq_{N\uparrow\infty} K_{n+1,\eta_n} \\
& \Longrightarrow \quad \xi_n^i \text{ almost iid copies of } \overline{X}_n
\end{aligned}
$$

Advantages

- Mean field model=Stoch. linearization/perturbation tech. :

$$\eta_n^N = \Phi_n(\eta_{n-1}^N) + \frac{1}{\sqrt{N}}\ W_n^N$$

  with $W_n^N \simeq W_n$ independent and centered Gauss field.

- $\eta_n = \Phi_n(\eta_{n-1})$ stable $\Rightarrow$ local errors do not propagate

$$\Longrightarrow \text{uniform control of errors w.r.t. the time parameter}$$

- "No need" to study the cv of equilibrium of MCMC models.
- Adaptive stochastic grid approximations
- Take advantage of the nonlinearity of the system to define beneficial interactions. Non intrusive methods.
- Natural and easy to implement, etc.

"Intuitive picture" $\rightsquigarrow$ nonlinear sg : $\eta_n = \Phi_n(\eta_{n-1}) = \Phi_{p,n}(\eta_p) = \eta_n$

Local errors

$$W_n^N := \sqrt{N}\,\left[\eta_n^N - \Phi_n\left(\eta_{n-1}^N\right)\right] \simeq W_n \;\perp\; \text{Gaussian field}$$

Local transport formulation :

$$\begin{array}{ccccccccc}
\eta_0 & \rightarrow & \eta_1 = \Phi_1(\eta_0) & \rightarrow & \eta_2 = \Phi_{0,2}(\eta_0) & \rightarrow & \cdots & \rightarrow & \Phi_{0,n}(\eta_0) \\
\Downarrow & & & & & & & & \\
\eta_0^N & \rightarrow & \Phi_1(\eta_0^N) & \rightarrow & \Phi_{0,2}(\eta_0^N) & \rightarrow & \cdots & \rightarrow & \Phi_{0,n}(\eta_0^N) \\
 & & \Downarrow & & & & & & \\
 & & \eta_1^N & \rightarrow & \Phi_2(\eta_1^N) & \rightarrow & \cdots & \rightarrow & \Phi_{1,n}(\eta_1^N) \\
 & & & & \Downarrow & & & & \\
 & & & & \eta_2^N & \rightarrow & \cdots & \rightarrow & \Phi_{2,n}(\eta_2^N) \\
 & & & & & & & & \vdots \\
 & & & & & & \Downarrow & & \\
 & & & & & & \eta_{n-1}^N & \rightarrow & \Phi_n(\eta_{n-1}^N) \\
 & & & & & & & & \Downarrow \\
 & & & & & & & & \eta_n^N
\end{array}$$

$\rightsquigarrow$ **Key decomposition formula**

$$\begin{aligned}
\eta_n^N - \eta_n &= \sum_{q=0}^{n} [\Phi_{q,n}(\eta_q^N) - \Phi_{q,n}(\Phi_q(\eta_{q-1}^N))] \\
&\simeq \frac{1}{\sqrt{N}} \sum_{q=0}^{n} W_q^N D_{q,n} \quad \text{first order decomp. } \Phi_{p,n}(\eta) - \Phi_{p,n}(\mu) \simeq (\eta-\mu)D_{p,n} + (\eta-\mu)^{\otimes 2}\ldots
\end{aligned}$$

$$\Rightarrow \quad \text{Example CLT :} \quad \sqrt{N}\left[\eta_n^N - \eta_n\right] \simeq \sum_{q=0}^{n} W_q D_{q,n}$$

Some Theoretical results : TCL,PGD, PDM,...(n,N) :

- McKean particle measure

$$\frac{1}{N}\sum_{i=1}^{N}\delta_{(\xi_0^i,\ldots,\xi_n^i)} \simeq_N \mathrm{Law}(\overline{X}_0,\ldots,\overline{X}_n) \;\&\; \eta_n^N = \frac{1}{N}\sum_{i=1}^{N}\delta_{\xi_n^i} \simeq_N \eta_n$$

- Empirical Processes : $\sup_{n\geq 0}\sup_{N\geq 1}\sqrt{N}\,\mathbb{E}(\|\eta_n^N-\eta_n\|_{\mathcal{F}_n}^p)<\infty$
- Uniform concentration inequalities :

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

- Propagations of chaos : $\mathbb{P}_{n,q}^N := \mathrm{Law}(\xi_n^1,\ldots,\xi_n^q)$

$$\mathbb{P}_{n,q}^N \simeq \eta_n^{\otimes q} + \frac{1}{N}\,\partial^1\mathbb{P}_{n,q} + \ldots + \frac{1}{N^k}\,\partial^k\mathbb{P}_{n,q} + \frac{1}{N^{k+1}}\,\partial^{k+1}\mathbb{P}_{n,q}^N$$

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

Ex.: Feynman-Kac distribution flows

- FK-Nonlinear Markov models :

  $\epsilon_n = \epsilon_n(\eta_n) \geq 0$ s.t. η_n-a.e. $\epsilon_n G_n \in [0,1]$ ($\epsilon_n = 0$ not excluded)

$$K_{n+1,\eta_n}(x,dz) = \int S_{n,\eta_n}(x,dy)\ M_{n+1}(y,dz)$$

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

- Mean field genetic type particle model :

$$\xi_n^i \in E_n \xrightarrow{\text{accept/reject/selection}} \widehat{\xi}_n^i \in E_n \xrightarrow{\text{proposal/mutation}} \xi_{n+1}^i \in E_{n+1}$$

- Running ex. : $G_n = 1_A \rightsquigarrow$ killing with uniform replacement.

Mean field genetic type particle model :

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

Accept/Reject/Selection transition :

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

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

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

Path space models

- $X_n = (X'_0, \ldots, X'_n) \rightsquigarrow$ genealogical tree/ancestral lines

$$\eta_n^N := \frac{1}{N} \sum_{1 \le i \le N} \delta_{\xi_n^i} = \frac{1}{N} \sum_{1 \le i \le N} \delta_{(\xi_{0,n}^i, \xi_{1,n}^i, \ldots, \xi_{n,n}^i)} \simeq_{N \uparrow \infty} \eta_n$$

- **Unbias particle approximations :**

$$\gamma_n^N(1) = \prod_{0 \le p < n} \eta_p^N(G_p) \simeq_{N \uparrow \infty} \gamma_n(1) = \prod_{0 \le p < n} \eta_p(G_p)$$

- Running ex. $G_n = 1_A$:

$$\Rightarrow \gamma_n^N(1) = \prod_{0 \le p < n} (\text{success \% at p})$$

Objective

- Find a series of MCMC models $X^{(n)} := (X_k^{(n)})_{k\geq 0}$ s.t.

$$\begin{aligned} \eta_k^{(n)} &= \frac{1}{k+1}\sum_{0\leq l\leq k}\delta_{X_l^{(n)}} \\ &\simeq_{k\uparrow\infty} \eta_n \\ &\Rightarrow \text{Use } \eta_k^{(n)} \simeq \eta_n \text{ to define } X^{(n+1)} \text{ with target } \eta_{n+1} \end{aligned}$$

Advantages

- Using η_n the sampling η_{n+1} is often easier.
- Improve the proposition step in any Metropolis type model with target η_{n+1} ($\rightsquigarrow$ enters the stability prop. of the flow η_n)
- Increases the precision at every time step.

  But CLT variance often $\geq$ CLT variance mean field models.
- Easy to combine with mean field stochastic algorithms.

Interacting Markov chain Monte Carlo models

- Find M_0 and a collection of transitions $M_{n,\mu}$ s.t.

$$\eta_0 = \eta_0 M_0 \quad \text{and} \quad \Phi_n(\mu) = \Phi_n(\mu) M_{n,\mu}$$

- $(X_k^{(0)})_{k\geq 0}$ Markov chain $\sim M_0$.
- Given $X^{(n)}$, we let $X_k^{(n+1)}$ with Markov transtions $M_{n+1,\eta_k^{(n)}}$

Rationale :

$$\begin{aligned} \eta_k^{(n)} \simeq \eta_n \quad &\Longrightarrow \quad \Phi_{n+1}(\eta_k^{(n)}) \simeq \Phi_{n+1}(\eta_n) = \eta_{n+1} \\ &\Longrightarrow \quad M_{n+1,\eta_k^{(n)}} \simeq M_{n+1,\eta_n} \quad \text{fixed point } \eta_{n+1} \end{aligned}$$

i-MCMC

$$
\begin{array}{ccc}
((n-1)\text{-th chain}) & & (n\text{-th chain}) \\
X_0^{(n-1)} & & X_0^{(n)} \\
\downarrow & & \downarrow \\
X_1^{(n-1)} & & \vdots \\
\downarrow & & \vdots \\
\vdots & & \downarrow \\
\downarrow & & X_k^{(n)} \\
 & & \downarrow \\
X_k^{(n-1)} & \xrightarrow{\eta_k^{(n-1)} \simeq \eta_{n-1}} & M_{n,\eta_k^{(n-1)}} \simeq M_{n,\eta_{n-1}} \\
\downarrow & & \downarrow \\
\vdots & & X_{k+1}^{(n)}
\end{array}
$$

Feynman-Kac particle sampling recipes

Nonlinear Feynman-Kac type flow $\sim (G_n, M_n)$

$$\eta_n = \Phi_n(\eta_{n-1}) = \Psi_{G_{n-1}}(\eta_{n-1})M_n$$

$$\Updownarrow$$

- Interacting stochastic algorithm *(mean field or i-MCMC)*

$$\begin{array}{rcl} \text{acceptance/rejection/selection/branching} & \rightsquigarrow & G_n \\ \text{exploration/proposition/mutation/prediction} & \rightsquigarrow & M_n \end{array}$$

- Normalizing constants $\rightsquigarrow$ key multiplicative formula.
- Path space models $\rightsquigarrow$ path-particles=ancestral lines

Occupation meas. of genealogical trees $\simeq \eta_n \in \text{path-space}$

Boltzmann-Gibbs distribution flows

Boltzmann-Gibbs measures

- X r.v. $\in (E, \mathcal{E})$ with $\mu = \mathrm{Law}(X)$
- Target measures associated with $g_n : E \to \mathbb{R}_+$

$$\eta_n(dx) := \Psi_{g_n}(\mu)(dx) = \frac{1}{\mu(g_n)} \, g_n(x) \, \mu(dx)$$

Running examples :

$$\begin{array}{rcl} g_n = 1_{A_n} & \Rightarrow & \eta_n(dx) \propto 1_{A_n}(x) \, \mu(dx) \\ g_n = e^{-\beta_n V} & \Rightarrow & \eta_n(dx) \propto e^{-\beta_n V(x)} \, \mu(dx) \\ g_n = \prod_{0 \le p \le n} h_p & \Rightarrow & \eta_n(dx) \propto \left\{ \prod_{0 \le p \le n} h_p(x) \right\} \mu(dx) \end{array}$$

Applications : global optimization pb., tails distributions, hidden Markov chain models, etc.

Boltzmann-Gibbs distribution flows

Boltzmann-Gibbs distribution flows

- Target distribution flow : $\eta_n(dx) \propto g_n(x)\ \mu(dx)$
- Product hypothesis :

$$g_n = g_{n-1} \times G_{n-1} \Longrightarrow \eta_n = \Psi_{G_{n-1}}(\eta_{n-1})$$

Running Ex.:

$$\begin{array}{rcllcl} g_n & = & 1_{A_n} & \text{with } A_n \downarrow & \Rightarrow & G_{n-1} = 1_{A_n} \\ g_n & = & e^{-\beta_n V} & \text{with } \beta_n \uparrow & \Rightarrow & G_{n-1} = e^{-(\beta_n - \beta_{n-1})V} \\ g_n & = & \prod_{0 \leq p \leq n} h_p & & \Rightarrow & G_{n-1} = h_n \end{array}$$

- Problem : $\eta_n = \Psi_{G_{n-1}}(\eta_{n-1}) =$ unstable equation.

Feynman-Kac distribution flows

FK-stabilization

- Choose $M_n(x, dy)$ s.t. local fixed point eq. $\rightarrow \eta_n = \eta_n M_n$ (Metropolis, Gibbs,...)
- **Stable equation :**

$$g_n = g_{n-1} \times G_{n-1} \quad \Longrightarrow \quad \eta_n = \Psi_{G_{n-1}}(\eta_{n-1})$$
$$\Longrightarrow \quad \eta_n = \eta_n M_n = \Psi_{G_{n-1}}(\eta_{n-1}) M_n$$

- **Feynman-Kac "dynamical" formulation (X_n Markov M_n)**

$$\int f(x)\; g_n(x)\; \mu(dx) \propto \mathbb{E}\left(f(X_n) \prod_{0 \leq p < n} G_p(X_p) \right)$$

- $\rightsquigarrow$ Interacting Metropolis/Gibbs/... stochastic algorithms.

Objectives - Markov processes with fixed terminal values

- X_n Markov with transitions $L(x, dy)$ on E
- $\mathrm{Law}(X_0) = \pi$ only known up to a normalizing constant.
- For a given fixed terminal value x solve/sample inductively the following flow of measures

$$n \mapsto \mathrm{Law}_\pi((X_0, \ldots, X_n) \mid X_n = x)$$

FK-formulation - Markov processes with fixed terminal values

- π "target type" measure$+(K, L)$ pair Markov transitions

$$\text{Metropolis potential} \quad G(x_1, x_2) = \frac{\pi(dx_2)L(x_2, dx_1)}{\pi(dx_1)K(x_1, dx_2)}$$

- Theorem [Time reversal formula] :

$$\mathbb{E}_\pi^L(f_n(X_n, X_{n-1} \ldots, X_0) | X_n = x)$$

$$= \frac{\mathbb{E}_x^K(f_n(X_0, X_1, \ldots, X_n) \ \{\prod_{0 \leq p < n} G(X_p, X_{p+1})\})}{\mathbb{E}_x^K(\{\prod_{0 \leq p < n} G(X_p, X_{p+1})\})}$$

- $\rightsquigarrow$ time reversal genealogical tree simulation

Rare event excursions

- $(E = A \cup A^c)$, Y_n Markov, $C \subset A^c$ absorbing set

$$Y_0 \in A_0(\subset A) \;\rightsquigarrow\; A^c = (B \cup C)$$

- Objectives :

$$\mathbb{P}(Y \text{ hits } B \text{ before } C) \quad \text{and} \quad \mathrm{Law}(Y \mid Y \text{ hits } B \text{ before } C)$$

Multi-splitting rare events

- *Multi-level decomposition* $B_0 \supset B_1 \supset \ldots \supset B_m = B$ $(A_0 = B_1 - B_0,\ B_0 \cap C = \emptyset)$
- *Inter-level excursions* : $T_n = \inf\{p \geq T_{n-1} \ :\ Y_p \in B_n \cup C\}$

$$X_n = (Y_p\ ;\ T_{n-1} \leq p \leq T_n) \quad \text{and} \quad G_n(X_n) = 1_{B_n}(Y_{T_n})$$

Feynman-Kac formulations :

$$\begin{aligned}\mathbb{P}(Y \text{ hits } B \text{ before } C) &= \mathbb{E}\Big(\prod_{1\leq p\leq m} G_p(X_p)\Big)\\ \mathbb{E}(f(Y_0,\ldots,Y_{T_m})\ 1_{B_m}(Y_{T_m})) &= \mathbb{E}(f(X_0,\ldots,X_m) \prod_{1\leq p\leq m} G_p(X_p))\end{aligned}$$

$\rightsquigarrow$ genealogical tree in excursion space.

Fixed time level set entrances

Fixed time level set entrances

- X_n Markov $\in E_n$, $V_n : E_n \to \mathbb{R}_+$, $a \in \mathbb{R}$
- Objectives :

$$\mathbb{P}(V_n(X_n) \geq a) \quad \text{and} \quad \mathrm{Law}((X_0, \ldots, X_n) \mid V_n(X_n) \geq a)$$

Large deviation analysis

Large deviation analysis

$$\mathbb{P}(V_n(X_n) \geq a) \overset{\forall\lambda}{=} \mathbb{E}\left(1_{V_n(X_n)\geq a}\; e^{\lambda V_n(X_n)}\; e^{-\lambda V_n(X_n)}\right)$$

$$\leq \quad e^{-(\lambda a - \Lambda_n(\lambda))} \text{ with } \Lambda_n(\lambda) = \log \mathbb{E}(e^{\lambda V_n(X_n)})$$

$$\text{Ex.:} \quad V_n(X_n) = X_n \quad \text{and} \quad \Delta X_n = N(0,1) \Longrightarrow \lambda^\star = a/n$$

Twisted measure

$$\eta_n(dx_n) \propto e^{\lambda V_n(x_n)}\; \mathbb{P}(X_n \in dx_n) := \gamma_n(dx_n)$$

$$\Rightarrow \mathbb{P}(V_n(X_n) \geq a) \quad = \quad \eta_n(1_{V_n \geq a}\; e^{-\lambda V_n}) \;\times\; \gamma_n(1)$$

Feynman-Kac representation formula

Feynman-Kac twisted measures ($V_{-1} = 0$)

$$\mathbb{E}(f_n(X_n)\ e^{\lambda V_n(X_n)}) = \mathbb{E}\left(f_n(X_n)\ \prod_{0\leq p\leq n} e^{\lambda(V_p(X_p)-V_{p-1}(X_{p-1}))}\right)$$

and

$$\mathbb{E}(f_n(X_0,\ldots,X_n) \mid V_n(X_n) \geq a)$$
$$\propto$$
$$\mathbb{E}\left(T_n(f_n)(X_0,\ldots,X_n)\ \prod_{0\leq p\leq n} e^{\lambda(V_p(X_p)-V_{p-1}(X_{p-1}))}\right)$$

with

$$T_n(f_n)(X_0,\ldots,X_n) = f_n(X_0,\ldots,X_n)e^{-\lambda V_n(X_n)}1_{V_n(X_n)\geq a}$$

Particle absorption models

Sub-Markov $\rightsquigarrow$ Markov

- X_n Markov $\in (E_n, \mathcal{E}_n)$ with transitions M_n, and $G_n : E_n \to [0,1]$

$$Q_n(x, dy) = G_{n-1}(x)\ M_n(x, dy) \quad \text{sub-Markov operator}$$

- $\rightsquigarrow E_n^c = E_n \cup \{c\}$.

$$X_n^c \in E_n^c \xrightarrow{\text{absorption } \sim G_n} \widehat{X}_n^c \xrightarrow{\text{exploration } \sim M_n} X_{n+1}^c$$

- Absorption: $\widehat{X}_n^c = X_n^c$, with proba $G(X_n^c)$; otherwise $\widehat{X}_n^c = c$.
- Exploration: like $X_n \rightsquigarrow X_{n+1}$

Feynman-Kac formulation

Feynman-Kac integral model

- $T = \inf\{n : \widehat{X}_n^c = c\}$ **absorption time :** $\forall f_n \in \mathcal{B}_b(E_n)$

$$\begin{aligned}\mathbb{P}(T \geq n) &= \gamma_n(1) := \mathbb{E}\left(\prod_{0\leq p<n} G(X_p)\right)\\ \mathbb{E}(f_n(X_n^c)\ ;\ (T \geq n)) &= \gamma_n(f_n) := \mathbb{E}\left(f_n(X_n)\prod_{0\leq p<n} G_p(X_p)\right)\end{aligned}$$

- **Continuous time models :** Δ = time step

$$(M, G) = (Id + \Delta\ L, e^{-V\Delta})$$

$\rightsquigarrow$ L-motions $\oplus$ expo. clocks rate V $\oplus$ Uniform selection.

Ex.: Feynman-Kac-Shrdinger ground states energies

Spectral radius-Lyapunov exponents

- $Q(x, dy) = G(x)M(x, dy)$ sub-Markov operator on $\mathcal{B}_b(E)$
- Normalized FK-model : $\eta_n(f) = \gamma_n(f)/\gamma_n(1)$.

$$\mathbb{P}(T \geq n) = \mathbb{E}\left(\prod_{0 \leq p \leq n} G(X_p)\right) = \prod_{0 \leq p \leq n} \eta_p(G) \simeq e^{-\lambda n}$$

with $e^{-\lambda} \overset{M\ reg.}{=}$ Q-top eigenvalue or

$$\begin{aligned}\lambda &= -\mathrm{LogLyap}(Q) = \lim_{n \to \infty} -\frac{1}{n} \log \|Q^n\| \\ &= -\frac{1}{n} \log \mathbb{P}(T \geq n) = -\frac{1}{n} \sum_{0 \leq p \leq n} \log \eta_p(G) = -\log \eta_\infty(G)\end{aligned}$$

Ex.: Feynman-Kac-Shrdinger ground states energies

Limiting Feynman-Kac measures

$M \quad \mu - \text{reversible}:$

$$\Rightarrow \mathbb{E}(f(X_n^c) \mid T > n) \simeq \frac{\mu(H\ f)}{\mu(H)} \quad \text{with} \quad Q(H) = e^{-\lambda} H$$

Limiting FK-measures

$$\eta_n = \Phi(\eta_{n-1}) \rightarrow_{n\uparrow\infty} \eta_\infty \quad \text{with} \quad \frac{\eta_\infty(G\ f)}{\eta_\infty(G)} = \frac{\mu(H\ f)}{\mu(H)}$$

leadsto Particle approximations :

$$\lambda \ \simeq_{n,N\uparrow} \ \lambda_n^N := \frac{1}{n} \sum_{0\leq p\leq n} \log \eta_p^N(G) \quad \text{and} \quad \eta_\infty \ \simeq_{n,N\uparrow} \ \eta_n^N$$

$$\text{Law}((X_0^c, \ldots, X_n^c) \mid (T \geq n)) \simeq \text{Genealogical tree measures}$$

Distribution flows (nonlinear sg.)

- **(weak sense)** : infinitesimal generators $L_{t,\eta}$

$$\frac{d}{dt}\eta_t(f) = \eta_t L_{t,\eta_t}(f) := \int_E \eta_t(dx)\ L_{t,\eta_t}(f)(x)$$

- **Example FKS** : $X_t \simeq \left(L \overset{ex.}{=} \frac{1}{2}\Delta\right) - \text{process} \oplus$ potential V.

$$\eta_t(f) := \frac{\gamma_t(f)}{\gamma_t(1)} \quad \text{avec} \quad \gamma_t(f) = \mathbb{E}\left(f(X_t)\exp\left\{-\int_0^t V(X_s)ds\right\}\right)$$

$$\begin{aligned}
\frac{d}{dt}\gamma_t(f) &= \gamma_t(L^V(f)) \quad \text{Schrodinger op.} \quad L^V := L - V \\
\frac{d}{dt}\eta_t(f) &= \eta_t L_{\eta_t}(f) \\
&:= \int \eta_t(dx)\left\{L(f)(x) + V(x)\int (f(y) - f(x))\eta_t(dy)\right\}
\end{aligned}$$

Mean field particle interpretation

- **Markov process** $\xi_t = (\xi_t^i)_{1\leq i\leq N}$ with infinitesimal generator

$$\mathcal{L}_t(F)(x^1,\ldots,x^N) := \sum_{i=1}^{N} L^{(i)}_{t,\frac{1}{N}\sum_{i=1}^{N}\delta_{x^i}} F(x^1,\ldots,x^i,\ldots,x^N)$$

- Occupation measures evolution $\eta_t^N := \frac{1}{N}\sum_{i=1}^{N}\delta_{\xi_t^i}$

$$d\eta_t^N(f) = \eta_t^N L_{t,\eta_t^N}(f)dt + \frac{1}{\sqrt{N}}\, dM_t^N(f)$$

with

$$\langle M^N(f)\rangle_t = \int_0^t \eta_s^N \Gamma_{L_{s,\eta_s^N}}(f,f)\, ds$$

Example : FKS model $\rightsquigarrow$ Moran type particle systems

- $(\xi_t^i)_{1\leq i\leq N}$ = L-explorations $\oplus$ interacting jumps (V-intensity)

$$\mathcal{L}_t(F)(x^1,\ldots,x^N)$$

$$= \sum_{i=1}^N L^{(i)}F(x^1,\ldots,x^i,\ldots,x^N) + \sum_{i=1}^N V(x^i)$$

$$\times \int \left(F(x^1,\ldots,y^i,\ldots,x^N) - F(x^1,\ldots,x^i,\ldots,x^N)\right) m(x)(dy^i)$$

with $m(x) = N^{-1}\sum_{i=1}^N \delta_{x^i}$.

- Asymptotic theory "$\sim$" discrete time models

Geometric clocks $\rightsquigarrow$ Exponential clocks

Asymptotic theory

FKS-model ⊕ Moran type particle systems

- **Particle estimations**

$$\mathbb{E}\left(f(X_t)e^{\int_0^t V(X_s)ds}\right) = \eta_t(f)\ e^{-\int_0^t \eta_s(V)ds}$$

$$\simeq_N \eta_t^N(f)\ e^{-\int_0^t \eta_s^N(V)ds} \quad \text{(unbias)}$$

- Ground states of Schrodinger op. : ($\supset$ DMC, QMC)
(v.p. λ ⊕ ground state h (L μ-reversible))

$$\lim_{N,t\to\infty} \eta_t^N(dx) \propto h(x)\ \mu(dx) \qquad \text{et} \quad e^{-\int_0^t \eta_s^N(V)ds} \simeq e^{-\lambda t}$$

- **Asymptotic theory "$\sim$" discrete time models.**

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