Particle rare event simulation

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Credit Risk Workshop, Evry Univ., June 2008.

Outline

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.

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

- 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 tech.)** $\rightsquigarrow$ **Ref.**.

Notation

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

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

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

- **Boltzmann-Gibbs transformation :** $G : E \to [0,1]$ with $\mu(G) > 0$

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

Updating-prediction transformations

Time parameter $n \in \mathbb{N}$, $M_n(x, dy)$ Markov transitions and $G_n : E \to [0, 1]$

$$\eta_{n+1} = \Phi_{n+1}(\eta_n) := \Psi_{G_n}(\eta_n) M_{n+1} \qquad (1)$$

Markov chain X_n with transitions M_n and initial condition $X_0 \simeq \eta_0$:

$$(1) \Longleftrightarrow \eta_n(f) \propto \gamma_n(f) = \mathbb{E}\left(f(X_n) \prod_{0 \leq p < n} G_p(X_p) \right)$$

Observations

- $G_n = 1 \Rightarrow \eta_n =Law(X_n)$.
- Path space models $X_n = (X'_0, \ldots, X'_n) \in E_n = (E'_0 \times \ldots \times E'_n)$
- Normalizing constants :
  $\gamma_n(1) = \mathbb{E}\left(\prod_{0 \leq p < n} G_p(X_p) \right) = \prod_{0 \leq p < n} \eta_p(G_p)$

Nonlinear distribution flows

- **Nonlinear Markov models :** $\eta_n = \eta_{n-1} K_{n,\eta_{n-1}} = \mathrm{Law}\left(\overline{X}_n\right)$

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

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

Mean field 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 ($\forall 1 \leq i \leq N$)

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

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 :

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

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

Path space models

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

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

- **Unbias particle approximations :**

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

Summary : 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 sampling algorithm

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

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

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

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

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 :

$$\begin{array}{ccc} g_n = 1_{A_n} & \Rightarrow & \eta_n(dx) \propto 1_{A_n}(x)\ \mu(dx) \\ g_n = e^{-\beta_n V} & \Rightarrow & \eta_n(dx) \propto e^{-\beta_n V(x)}\ \mu(dx) \end{array}$$

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.:

$$\begin{array}{lclcl} g_n & = & 1_{A_n} \text{ with } A_n \downarrow & \Rightarrow & G_{n-1} = 1_{A_n} \\ g_n & = & e^{-\beta_n V} \text{ with } \beta_n \uparrow & \Rightarrow & G_{n-1} = e^{-(\beta_n - \beta_{n-1})V} \end{array}$$

- 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] :

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

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

- $\rightsquigarrow$ 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 :

$$\mathbb{P}(Y \text{ hits } B \text{ before } C) = \mathbb{E}\Big(\prod_{1 \leq p \leq m} G_p(X_p)\Big)$$

$$\mathbb{E}(f(Y_0, \ldots, Y_{T_m})\, 1_{B_m}(Y_{T_m})) = \mathbb{E}(f(X_0, \ldots, X_m) \prod_{1 \leq p \leq m} G_p(X_p))$$

$\rightsquigarrow$ genealogical tree in excursion space.

Fixed time level set entrances

Fixed time level set entrances

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

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

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

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

Twisted measure

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

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

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

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

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Interacting stochastic simulation algorithms

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