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 and default probabilities, financial crashes, economic 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.

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

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 $\mathbb{Q}$

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

$$\text{Variance} \simeq \int \frac{d\mathbb{P}}{d\mathbb{Q}}(x)\ 1_A(x)\ \mathbb{P}(dx)$$

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 $X = (X_0, \ldots, X_n)$

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

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

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

- 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

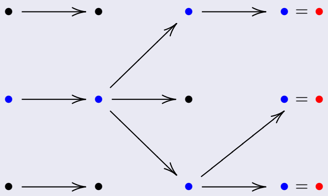
1. $\eta_n = \text{Loi}((X_0, \ldots, X_n) \mid \forall 0 \leq p \leq n \quad X_p \in A_p)$
2. $\eta_n(dx) \propto e^{-\beta_n V(x)}\ \lambda(dx)$ with $\beta_n \uparrow$
3. $\eta_n(dx) \propto 1_{A_n}(x)\ \lambda(dx)$ with $A_n \downarrow$
4. $\eta_n = \text{Loi}_\pi^K((X_0, \ldots, X_n) \mid X_n =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

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.
- 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, ...

$$\Updownarrow$$

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

Summary

Some 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**

$$M(f)(x) = \int M(x, dy) f(y)$$

$$[\mu M](dy) = \int \mu(dx) M(x, dy) \qquad (\Longrightarrow [\mu M](f) = \mu[M(f)]\ )$$

- **Bayes-Boltzmann-Gibbs transformation :** $G : E \rightarrow [0, \infty[$ 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 $\simeq (G_n, M_n)$

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

with the un-normalized measures :

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

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

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

- $G_n = 1_{A_n}$, $G_n = e^{-(\beta_n-\beta_{n-1})V}$ or more generally $G_n = e^{(V_{n+1}-V_n)}$.
- Metropolis potential ratio, level crossing detections.
- Importance-(LDP)Twisted distributions $\propto e^{\lambda V(X_n)}\,\mathbb{P}(X_n \in .) \rightsquigarrow G_n(X_{n-1}, X_n) = e^{\lambda[V(X_n)-V(X_{n-1})]}$
- X_n-particle absorption with rate $G_n \rightsquigarrow$ Survival probab at time $n = \gamma_n(1)$

A first "detailed" example

Boltzmann-Gibbs Measures :

$$\eta_n(dx) = \frac{1}{Z_n} e^{-\beta_n V(x)}\ \lambda(dx)$$

Feynman-Kac representation :

$$\eta_n(f) := \frac{\gamma_n(f)}{\gamma_n(1)} \quad \text{with} \quad \gamma_n(f) := \mathbb{E}\left(f_n(X_n) \prod_{0 \leq p < n} e^{-(\beta_{p+1}-\beta_p)V(X_p)} \right)$$

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 :

$$\begin{aligned} Z_n &= \lambda\left(e^{-\beta_n V}\right) \\ &= \underbrace{\frac{\lambda\left(e^{-(\beta_n-\beta_{n-1})V}\ e^{-\beta_{n-1}V}\right)}{\lambda\left(e^{-\beta_{n-1}V}\right)}}_{\eta_{n-1}\left(e^{-(\beta_n-\beta_{n-1})V}\right)} \times Z_{n-1} \overset{(\beta_0=0)}{=} \prod_{0 \leq p < n} \eta_p\left(e^{-(\beta_{p+1}-\beta_p)V}\right) \end{aligned}$$

A second "detailed" 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 :

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

Path space measures= *Same math. models*

Historical process : $X_n := (X'_0, \ldots, X'_n) \in E_n = (E'_0 \times \ldots \times E'_n)$

$$\Downarrow$$

Path space particles : $\xi^i_n := \left(\xi^i_{0,n}, \xi^i_{1,n}, \ldots, \xi^i_{n,n}\right) \in E_n = (E'_0 \times \ldots \times E'_n)$

$$\Downarrow$$

$$\eta^N_n(f) := \frac{1}{N} \sum_{i=1}^{N} f_n(\xi^i_n) \longrightarrow_{N\uparrow\infty} \eta_n(f_n) := \frac{\gamma_n(f_n)}{\gamma_n(1)}$$

with the un-normalized Feynman-Kac meas. on paths spaces :

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

Example $\hookrightarrow \eta_n = \mathrm{Law}((X'_0, \ldots, X'_n) \mid \mathrm{without\ intersections})$

$$X' = \mathrm{Random\ walk} \in \mathbb{Z}^d \quad \& \quad G_n\left(X'_0, \ldots, X'_n\right) = 1_{\{X'_0, \ldots, X'_{n-1}\}}(X'_n)$$

Flows of Feynman-Kac measures

$$\eta_n \xrightarrow{\text{Correction/mise à jour}} \widehat{\eta}_n = \Psi_{G_n}(\eta_n) \xrightarrow{\text{Prédiction/exploration}} \eta_{n+1} = \widehat{\eta}_n M_{n+1}$$

Nonlinear transport formulae

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

with

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

$$\Downarrow$$

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

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 :**

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

- **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 :

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

$$
\Downarrow
$$

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 :

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

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

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

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

- "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.

"Asymptotic" theory: TCL,PGD, PDM,...(n,N). 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* `hal-09`

- Propagations of chaos *(+Patras,Rubenthaler* `(AAP 09-10)` :

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

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

Summary

Problem : Un-normalized measures estimation

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

Key observation :

$$\eta_n(G_n)\ \gamma_n(1) = \gamma_n(G_n) = \gamma_{n+1}(1)$$

$\Longrightarrow$ Multiplicative formula $\rightsquigarrow$ unbias particle estimates

$$\begin{array}{rcl} \gamma_n(1) & = & \displaystyle\prod_{0\leq p<n} \eta_p(G_p) \longleftarrow_{N\uparrow\infty} \gamma_n^N(1) := \prod_{0\leq p<n} \eta_p^N(G_p) \\ & \Downarrow & \\ \gamma_n(f) & := & \gamma_n(1) \times \eta_n(f) \longleftarrow_{N\uparrow\infty} \gamma_n^N(f) := \gamma_n^N(1) \times \eta_n^N(f) \end{array}$$

Note. : If G_n takes null values (ex. $G_n = 1_A$) $\Rightarrow$ convention = we estimate by 0.

2 Examples : Feynman-Kac models

- **Tube confinement :**

$$\gamma_n(1) \stackrel{G_n=1_A}{=} \mathbb{P}\left(\cap_{0\leq p<n} X_p \in A\right) \simeq_{N\uparrow\infty} \gamma_n^N(1) := \prod_{0\leq p<n} \eta_p^N(A)$$

- **Self avoiding walks :**

$$\gamma_{n+1}(1) = \mathbb{P}\left(\forall p < q \leq n \;\; X_p \neq X_q\right) = \frac{1}{(2d)^n} \text{Card}\left\{\text{s.a.w. with length =n}\right\}$$

$$\simeq_{N\uparrow\infty}$$

$$\gamma_{n+1}^N(1) := \prod_{0\leq p\leq n} \text{empirical mean potential at time } p$$

Several strategies :

1. Path evolutions with G-intersection detection
2. Local transitions without intersections with $\widehat{G}$-future proba. of intersection.
3. ...

+2 Examples : Boltzmann-Gibbs static measures

- **Partition functions:** $\left(G_n = e^{-(\beta_{n+1}-\beta_n)V}\right)$ et $(\eta_n M_n = \eta_n) \Rightarrow$ $d\eta_n \propto e^{-\beta_n V}\ d\lambda$

$$\left(\rightsquigarrow\ \ \textit{Note :}\quad \lambda\left(e^{-\beta_n V}\right) = \lambda\left(G_n \times e^{-\beta_{n-1} V}\right) = \eta_n\left(G_n\right)\ \lambda\left(e^{-\beta_{n-1} V}\right)\right)$$

$$\Downarrow$$

$$\lambda\left(e^{-\beta_n V}\right) = \gamma_n(1)\ \simeq_{N\uparrow\infty}\ \gamma_n^N(1) := \prod_{0\leq p<n} \eta_p^N\left(e^{-(\beta_{p+1}-\beta_p)V}\right)$$

- **Volumes and Cardinals :**

$$\left(G_n = 1_{A_{n+1}}\right)\quad \text{and}\quad \left(\eta_n M_n = \eta_n\right) \Longrightarrow \eta_n(dx) \propto 1_{A_{n+1}}\ \lambda(dx)$$

$$\Downarrow$$

$$\lambda\left(A_n\right) = \gamma_n(1)\ \simeq_{N\uparrow\infty}\ \gamma_n^N(1) := \prod_{0\leq p\leq n} \eta_p^N\left(A_{p+1}\right)$$

Convergence analysis

- Asymptotic theory : fluctuations & deviations
  + *A. Guionnet* (AAP 99, SPA 98), + *L. Miclo* (SP 2000), + *D. Dawson*
- Non asymptotic theory : bias and variance estimates
  1. Taylor type expansion (+*Patras & Rubenthaler* (AAP 09) :

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

[Hyp.$\sim$ simple genetic algo. $\epsilon_n = 0$ & potentiel > 0]

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

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

Hyp. + weak conditions $\supset$:

- Mean field models with acceptance rate $\forall \epsilon_n \geq 0$.
- Potential functions ≥ 0 ($\supset$ indicator functions).
- Path space models $X_n = (X'_0, \ldots, X'_n)$, with X' " mixing".

Particle methods & Sequential Monte Carlo

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