

# Particle Rare Event Stochastic Simulation

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## Some typical rare events

- **Physical/biological/economical stochastic process** : electronic 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  
 ~ 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  $\mu = \text{Law}(X)$
- $A \in \mathcal{E}$  with  $0 < \mu(A) = \mathbb{P}(X \in A) \simeq 10^{-p}$  and  $p \gg 1$ .

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

### Examples

$$E = \mathbb{R}, \mathbb{R}^d, \mathbb{R}^{\{-n, \dots, n\}^2}, \cup_{n \geq 0} (\mathbb{R}^d)^{\{0, \dots, n\}}, \dots$$

$$A = [a, \infty[, V^{-1}([a, \infty[), \{\text{an excursion hits B before C}\} \dots$$

### 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** :

$$X = (X'_0, \dots, X'_n) \in E := (\mathbb{Z}^d \times \dots \times \mathbb{Z}^d)$$

$$A = \{(x'_0, \dots, x'_n) : \forall 0 \leq p < q \leq n \quad x'_p \neq x'_q\}$$

$$\Rightarrow \mu(A) = \frac{1}{(2d)^n} \times \#\{\text{not } \cap \text{ walks with length } n\}$$

$$\simeq \exp(\mathbf{c} \, n)$$

$$\Rightarrow \eta = \text{Law}((X'_0, \dots, X'_n) \mid \forall p < q \leq n \quad X'_p \neq X'_q)$$

## Second heuristic $\sim$ multiplicative structure :

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

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

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

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

and

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

**Same heuristic ~ multiplicative structure :**

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

## More examples of stochastic rare event models

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

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

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

## 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:

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

$$\stackrel{G_n=1_{A_n}}{=} \text{Law}((X_0, \dots, X_n) \mid X_0 \in A_0, \dots, X_n \in A_n)$$

and  $\mathcal{Z}_n = \mathbb{P}(X_0 \in A_0, \dots, X_n \in A_n)$

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

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

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).
- $\eta_n = \text{Law}(\text{process} \mid \text{a series of } n \text{ intermediate } \downarrow \text{ events})$   
= **nonlinear distribution flow** with  $\uparrow$  level of complexity.

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

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

## 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

### Updating/Prediction transformations

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

**Integral functional solution :**  $X_n$  Markov transitions  $M_n$

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

### Key multiplicative formula

$$\gamma_n(\mathbf{1}) = \mathbb{E} \left( \prod_{0 \leq p < n} G_p(X_p) \right) = \prod_{0 \leq p < n} \eta_p(G_p)$$

## Running example

### Confinement potential

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

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

Key multiplicative formula

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

Note :

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

## Structural stability properties

State space enlargements  $\rightsquigarrow$  **same model!**

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

$$\text{Ex.: } X_n = (X'_0, \dots, X'_n)$$

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

**Boltzmann-Gibbs' formulation :**

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

## 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.

$$G_n = G_n^{\epsilon_n} \times G_n^{1-\epsilon_n} = G_n^{(1)} \times G_n^{(2)} = \dots$$

## 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  $\eta_n$  ( $\uparrow$  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.

$$\eta_n = \Phi_n(\eta_{n-1}) = \eta_{n-1} K_{n,\eta_{n-1}} = \text{Law}(\bar{X}_n)$$

i.e. :

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

## Mean field particle interpretation

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

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

- 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 :

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

## 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

$\Rightarrow$  **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.

## Asymptotic theory CLT, LDP, ... (n, N). Some examples :

- Empirical processes cv :

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

- Uniform concentration inequalities :

$$\sup_{n \geq 0} \mathbb{P}(|\eta_n^N(f_n) - \eta_n(f_n)| > \epsilon) \leq (1 + \epsilon \sqrt{N/2}) \exp - \frac{N\epsilon^2}{\sigma^2}$$

- Propagation-of-chaos estimates

$$\text{Law}(\xi_n^1, \dots, \xi_n^q) \simeq \eta_n^{\otimes q} + \frac{1}{N} \partial^1 \mathbb{P}_{n,q} \text{ with } \|\partial^1 \mathbb{P}_{n,q}\|_{\text{tv}} \leq c q^2$$

## Ex.: Feynman-Kac distribution flows

- **FK-Nonlinear Markov models :**

$\epsilon_n = \epsilon_n(\eta_n) \geq 0$  s.t.  $\epsilon_n G_n \in [0, 1]$  ( $\epsilon_n = 0$  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 :

$$\begin{array}{c} \xi_n^1 \\ \vdots \\ \xi_n^i \\ \vdots \\ \xi_n^N \end{array} \Bigg] \xrightarrow{S_{n,\eta_n^N}} \begin{array}{c} \widehat{\xi}_n^1 \\ \vdots \\ \widehat{\xi}_n^i \\ \vdots \\ \widehat{\xi}_n^N \end{array} \begin{array}{c} \xrightarrow{M_{n+1}} \\ \xrightarrow{\quad\quad\quad} \\ \xrightarrow{\quad\quad\quad} \\ \xrightarrow{\quad\quad\quad} \end{array} \begin{array}{c} \xi_{n+1}^1 \\ \vdots \\ \xi_{n+1}^i \\ \vdots \\ \xi_{n+1}^N \end{array} \Bigg]$$

Accept/Reject/Selection transition :

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

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

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

## Path space models

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

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

- **Unbias particle approximations :**

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

- **Running ex.  $G_n = 1_A$  :**

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

## Objective

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

$$\eta_k^{(n)} = \frac{1}{k+1} \sum_{0 \leq l \leq k} \delta_{X_l^{(n)}}$$

$$\simeq_{k \uparrow \infty} \eta_n$$

$\Rightarrow$  Use  $\eta_k^{(n)} \simeq \eta_n$  to define  $X^{(n+1)}$  with target  $\eta_{n+1}$

## Advantages

- Using  $\eta_n$  the sampling  $\eta_{n+1}$  is often easier.
- Improve the proposition step in a Metropolis model.
- In contrast to mean field techniques i-MCMC algo. Increases the precision at every time step.
- 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 transitions  $M_{n+1, \eta_k^{(n)}}$

Rationale :

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



## i-MCMC

(( $n - 1$ )-th chain) $X_0^{(n-1)}$ 

↓

 $X_1^{(n-1)}$ 

↓

⋮

↓

 $X_k^{(n-1)}$ 

↓

⋮

 $\xrightarrow{\eta_k^{(n-1)} \simeq \eta_{n-1}}$ ( $n$ -th chain) $X_0^{(n)}$ 

↓

⋮

⋮

↓

 $X_k^{(n)}$ 

↓

 $M_{n, \eta_k^{(n-1)}} \simeq M_{n, \eta_{n-1}}$ 

↓

 $X_{k+1}^{(n)}$

## Feynman-Kac particle sampling recipes

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

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



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

acceptance/rejection/selection/branching  $\rightsquigarrow G_n$

exploration/proposition/mutation/prediction  $\rightsquigarrow M_n$

- 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

# Boltzmann-Gibbs distribution flows

## Boltzmann-Gibbs measures

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

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

### Examples :

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

**Applications** : global optimization pb., tails distributions, etc.

## Boltzmann-Gibbs distribution flows

### Boltzmann-Gibbs distribution flows

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

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

Running Ex.:

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

- **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 :

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

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

- 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  $E$
- $\text{Law}(X_0) = \pi$  only known up to a normalizing constant.
- For a given fixed **terminal value**  $x$  solve/sample inductively the following flow of measures

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

## FK-formulation - Markov processes with fixed terminal values

- $\pi$  "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] :

$$\begin{aligned} & \mathbb{E}_{\pi}^L(f_n(X_n, X_{n-1}, \dots, X_0) | X_n = x) \\ &= \frac{\mathbb{E}_x^K(f_n(X_0, X_1, \dots, X_n) \{\prod_{0 \leq p < n} G(X_p, X_{p+1})\})}{\mathbb{E}_x^K(\{\prod_{0 \leq p < n} G(X_p, X_{p+1})\})} \end{aligned}$$

- $\rightsquigarrow$  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 :

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



## Multi-splitting rare events

- *Multi-level decomposition*  $B_0 \supset B_1 \supset \dots \supset B_m = B$   
( $A_0 = B_1 - B_0$ ,  $B_0 \cap C = \emptyset$ )
- *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 :

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

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

$\rightsquigarrow$  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 :

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

# Large deviation analysis

## Large deviation analysis

$$\begin{aligned} \mathbb{P}(V_n(X_n) \geq a) &\stackrel{\forall \lambda}{=} \mathbb{E} \left( \mathbf{1}_{V_n(X_n) \geq a} e^{\lambda V_n(X_n)} e^{-\lambda V_n(X_n)} \right) \\ &\leq e^{-(\lambda a - \Lambda_n(\lambda))} \text{ with } \Lambda_n(\lambda) = \log \mathbb{E}(e^{\lambda V_n(X_n)}) \end{aligned}$$

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

## Twisted measure

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

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

## 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

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

with

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

## Particle absorption models

### Sub-Markov $\rightsquigarrow$ Markov

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

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

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

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

- **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** :  $\forall f_n \in \mathcal{B}_b(E_n)$

$$\mathbb{P}(T \geq n) = \gamma_n(1) := \mathbb{E} \left( \prod_{0 \leq p < n} G(X_p) \right)$$

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

- **Continuous time models** :  $\Delta =$  time step

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

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

## Ex.: Feynman-Kac-Schrödinger 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  $e^{-\lambda} \stackrel{M}{=} \text{reg. Q-top eigenvalue}$  or

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

## Ex.: Feynman-Kac-Schrödinger ground states energies

### Limiting Feynman-Kac measures

$M$   $\mu$  – 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

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

**leadsto** Particle approximations :

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

Law $((X_0^c, \dots, X_n^c) \mid (T \geq n)) \simeq$  Genealogical tree measures



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