# Some theoretical aspects of Particle/SMC Methods

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$\hookrightarrow \sim$ **Joint works :**
*D. Crisan, D. Dawson, A. Doucet, J. Jacod, A. Jasra, A. Guionnet, M. Ledoux, L. Miclo, F. Patras, T. Lyons, S. Rubenthaler,...*

*http-references :*

$\hookrightarrow$ `Feynman-Kac formulae. Genealogical and interacting particle systems, Springer (2004),` `+ References`

$\hookrightarrow$ `DM, Doucet, Jasra. SMC Samplers.` *JRSS B (2006).*

# Outline

# Summary

## Particle Interpretation models

- **Mathematical physics and molecular chemistry** ($\geq 1950's$) : Particle/microscopic interpretation models, particle absorption, macro-molecular chains, quantum and diffusion Monte Carlo.
- **Environmental studies and biology** ($\geq 1950's$): Population, gene evolutions, species genealogies, branching/birth and death models.
- **Evolutionary mathematics and engineering sciences** ($\geq 1970's$): Adaptive stochastic search method, evolutionary learning models, interacting stochastic grids approximations, genetic algorithms.
- **Applied Probability and Bayesian Statistics** ($\geq 1990's$): Approximating simulation technique (recursive acceptance-rejection model), Sequential Monte Carlo, `http-ref : interacting Monte Carlo Markov chains (Andrieu, Bercu, DM, Doucet, Jasra).`
- **Pure mathematics (**$\geq 1960's$ **for fluid models,** $\geq 1990's$ **for discrete time and interacting jump models)**: Stochastic linearization tech., mean field particle interpretations of nonlinear PDE and measure valued equations.

- **Central idea of particle/SMC in stochastic engineering :**

$$\left\{ \begin{array}{l} \textbf{Physical and Biological intuitions} \\ \textit{[learning, adaptation, optimization,...]} \end{array} \right\} \in \textbf{Engineering problems}$$

| | | |
|---|---|---|
| Sequential Monte Carlo | Sampling | Resampling |
| Particle Filters | Prediction | Updating |
| Genetic Algorithms | Mutation | Selection |
| Evolutionary Population | Exploration | Branching |
| Diffusion Monte Carlo | Free evolutions | Absorption |
| Quantum Monte Carlo | Walkers motions | Reconfiguration |
| Sampling Algorithms | Transition proposals | Acceptance-rejection |

*More botanical names :* spawning, cloning, pruning, enrichment, go with the winner, and many others.

- **Pure mathematical point of view :**
  **= Mean field particle interpretation of Feynman-Kac measures**

## Some application areas of Feynman-Kac formulae

- **Physics** :
  - Feynman-Kac-Schroedinger semigroups $\in$ nonlinear integro-differential equations ($\sim$ generalized Boltzmann models).
  - Spectral analysis of Schrödinger operators and large matrices with nonnegative entries.
  - Particle evolutions in disordered/absorbing media.
  - Multiplicative Dirichlet problems with boundary conditions.
  - Microscopic and macroscopic interacting particle interpretations.
- **Chemistry and Biology**:
  - Self-avoiding walks, macromolecular simulation, directed polymers.
  - Spatial branching and evolutionary population models.
  - Coalescent and Genealogical tree based evolutions.

# Some application areas of Feynman-Kac formulae

- **Rare events analysis**:
  - Multisplitting and branching particle models (Restart type methods).
  - Importance sampling and twisted probability measures.
  - Genealogical tree based simulations (default tree sampling models).
- **Advanced Signal processing**:
  - Optimal filtering, prediction, smoothing.
  - Open loop optimal control, optimal regulation.
  - Interacting Kalman-Bucy filters.
  - Stochastic and adaptative grid approximation-models
- **Statistics/Probability**:
  - Restricted Markov chains (w.r.t terminal values, visiting regions, constraints simulation problems,...)
  - Analysis of Boltzmann-Gibbs type distributions (simulation, partition functions, localization models...).
  - Random search evolutionary algorithms, interacting Metropolis/simulated annealing algo, combinatorial counting.

# Summary

## Standard notation

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

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

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

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

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

# Note

If $\quad \mu = \mathrm{Law}(X) \quad \text{and} \quad M(x, dy) := \mathbb{P}(Y \in dy \mid X = x)$

Then

- **Expectation operators**

$$\begin{aligned}
\mu(f) &= \int \mathbb{P}(X \in dx)\ f(x) = \mathbb{E}(f(X)) \\
M(f)(x) &= \int \mathbb{P}(Y \in dy \mid |X = x)\ f(y) = \mathbb{E}(f(Y) \mid X = x) \\
[\mu M](dy) &= \int \mathbb{P}(Y \in dy \mid X = x)\ \mathbb{P}(X \in dx) = \mathbb{P}(Y \in dy)
\end{aligned}$$

- **Bayes rule ($Y = y$ fixed observation) :**

$$\mu(dx) := p(x)\ dx \quad \text{and} \quad G(x) = p(y \mid x)$$

$$\Downarrow$$

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

## Only 3 Ingredients

- **A state space :**

  $E_n$ with $n =$ time/level index **[transitions, paths, excursions,...].**

  $$X_n := (X'_{n-1}, X'_n), \quad X'_{[0,n]}, \quad X'_{[t_{n-1},t_n]}, \quad X'_{[T_{n-1},T_n]}, \cdots$$

- **A Markov Proposal/Exploration/Mutation transition :**

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

- **A potential/likelihood/fitness/weight function on $E_n$ :**

  $$G_n \; : \; x_n \in E_n \longrightarrow G_n(x_n) \in [0, \infty[$$

**Running Examples :**

- [Confinement] $X_n$=Simple random walk (SRW) on $E_n = \mathbb{Z}$ and $G_n = 1_A$.
- [Filtering] $M_n$=signal transitions, $G_n$=Likelihood weight function.

## SMC/Genetic type branching particle model :

$$\begin{bmatrix} \xi_n^1 \\ \vdots \\ \xi_n^i \\ \vdots \\ \xi_n^N \end{bmatrix} \xrightarrow{\text{Updating/Branching}} \begin{bmatrix} \widehat{\xi}_n^1 \\ \vdots \\ \widehat{\xi}_n^i \\ \vdots \\ \widehat{\xi}_n^N \end{bmatrix} \begin{array}{c} \xrightarrow{M_{n+1}} \\ \vdots \\ \xrightarrow{\text{Prediction/Exploration}} \\ \vdots \\ \longrightarrow \end{array} \begin{bmatrix} \xi_{n+1}^1 \\ \vdots \\ \xi_{n+1}^i \\ \vdots \\ \xi_{n+1}^N \end{bmatrix}$$

**Selection/Branching :** $(\forall \epsilon_n \geq 0 \text{ s.t. } \epsilon_n(x^1, \ldots, x^N) \times G_n(x^i) \in [0,1])$

- **Acceptance probability:**

$$\widehat{\xi}_n^i = \xi_n^i \quad \text{with probability} \quad \epsilon_n(\xi_n^1, \ldots, \xi_n^N) \; G_n(\xi_n^i)$$

- **Otherwise :**

$$\widehat{\xi}_n^i = \xi_n^j \quad \text{with probability} \quad \frac{G_n(\xi_n^j)}{\sum_{k=1}^N G_n(\xi_n^k)}$$

*Running examples:* [Confinement & Filtering] = $[(G_n = 1_A)$ & $(G_n = \text{Likelihood})]$.

## Some remarks :

- $\epsilon_n = 0 \implies$ *Simple Mutation-Selection Genetic model.*
- $G_n = \exp\{-V_t \Delta t\}$ & $\epsilon_n = 1 \implies$ $V_t$*-expo-clocks* $\oplus$ uniform selection
- $G_n \in [0,1]$ & $\epsilon_n = 1 \Rightarrow$ *Interacting Acceptance-Rejection Sampling.*
- Better fitted individuals acceptance :

$$\text{For} \qquad \epsilon_n(x^1, \ldots, x^N) G_n(x^i) = G_n(x^i) / \sup_{1 \leq j \leq N} G_n(x^j)$$

- Related branching rules:

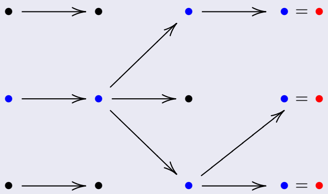
  [DM-Crisan-Lyons MPRF 99, DM 04] (Given $\xi_n = (\xi_n^i)_i$)

$$P_n^i := \text{Proportion of offsprings of the individual } \xi_n^i$$

  - Unbiasedness property : $\mathbb{E}\left(P_n^i\right) = G_n(\xi_n^j) / \sum_{k=1}^N G_n(\xi_n^k)$
  - Local mean error : $\mathbb{E}\left(\left[\sum_{i=1}^N \left[P_n^i - \mathbb{E}\left(P_n^i\right)\right] f(\xi_n^i)\right]^2\right) \leq \frac{Cte}{N}$

# Interacting-Branching proc. $\hookrightarrow$ 3 Particle/SMC occupation measures:

$(N = 3)$



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

- Historical/genealogical tree $\hookrightarrow \frac{1}{N}\sum_{i=1}^{N} \delta_{\left(\xi_{0,n}^i,\xi_{1,n}^i,\ldots,\xi_{n,n}^i\right)}$ $\leftarrow$ $i$-th ancestral line

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

- $\oplus$ *Mean potential values [Success proportions $(G_n = 1_A)$]* $\hookrightarrow \frac{1}{N}\sum_{i=1}^{N} G_n(\xi_n^i)$

## Limiting measures ("Test" functions $f : E_n \to \mathbb{R}$)

- **Occupation measures of the 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 the Feynman-Kac measures ($X_n$ Markov with transitions $M_n$):

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

- *Running examples :*
  - *Confinement $G_n = 1_A$ :*

$$\gamma_n(1) = \mathbb{P}\left(\forall 0 \leq p < n \quad X_p \in A\right) \quad \& \quad \eta_n = \mathrm{Law}\left(X_n \mid \forall 0 \leq p < n \quad X_p \in A\right)$$

  - *Filtering: $G_n$=Likelihood function :*

$$\gamma_n(1) = p_n(y_0, \ldots, y_{n-1}) \quad \& \quad \eta_n = \mathrm{Law}\left(X_n \mid Y_0 = y_0, \ldots, Y_{n-1} = y_{n-1}\right)$$

## Limiting measures
## ("Test" function on path space $f_n : E_n = (E'_0 \times \ldots \times E'_n) \to \mathbb{R}$)

- **Occupation measures of the historical/genealogical tree**

$$\eta_n^N(f_n) := \frac{1}{N}\sum_{i=1}^{N} f_n\left(\xi^i_{0,n}, \xi^i_{1,n}, \ldots, \xi^i_{n,n}\right) \longrightarrow_{N\uparrow\infty} \eta_n(f_n) := \frac{\gamma_n(f_n)}{\gamma_n(1)}$$

with the Feynman-Kac measures on path space :

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

- *Running examples :* $X_n = (X'_0, \ldots, X'_n)$ SRW & $G_n(X_n) = 1_A(X'_n)$

$$\begin{aligned}
\gamma_n(1) &= \mathbb{P}\left(\forall 0 \leq p < n \quad X'_p \in A\right) \\
\eta_n &= \mathrm{Law}\left((X'_0, \ldots, X'_n) \mid \forall 0 \leq p < n \quad X'_p \in A\right)
\end{aligned}$$

Filtering $\rightsquigarrow \eta_n = \mathrm{Law}\left((X'_0, \ldots, X'_n) \mid Y_0 = y_0, \ldots, Y_{n-1} = y_{n-1}\right)$

# Note

**Updated Feynman-Kac models**

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

$\Updownarrow$ **[Path space models]** $x_n = (x'_0,\ldots,x'_n)$

$$\begin{aligned}\widehat{\gamma}_n(dx_n) &= \left\{\eta'_0(dx'_0)\prod_{p=1}^{n} M'_p(x'_{p-1},dx'_p)\right\}\times\left\{\prod_{0\leq p\leq n} G_p(x'_0,\ldots,x'_p)\right\}\\ &= \widehat{\gamma}_{n-1}(dx_{n-1})\times M'_n(x'_{n-1},dx'_n)\times G_n(x_n)\end{aligned}$$

$$\Updownarrow$$

(SMC) Updating weight functions : $\quad G_n(x_n) = \dfrac{\widehat{\gamma}_n(dx_n)}{\widehat{\gamma}_{n-1}(dx_{n-1})\times M'_n(x'_{n-1},dx'_n)}$

Local explorations : $x_{n-1} \rightsquigarrow x_n = (x_{n-1},x'_n) \quad \text{with} \quad x'_n \sim M'_n(x'_{n-1},dx'_n)$

## Limiting measures
## ("Test" function on path space $F_n : (E_0 \times \ldots \times E_n) \to \mathbb{R}$)

- **Occupation measures of the complete genealogical tree ($\epsilon_n = 0$)**

$$\frac{1}{N}\sum_{i=1}^{N} F_n\left(\xi_0^i, \xi_1^i, \ldots, \xi_n^i\right) \longrightarrow_{N\uparrow\infty} (\eta_0 \otimes \ldots \otimes \eta_n)(F_n)$$

with the Feynman-Kac tensor product measures :

$$(\eta_0 \otimes \ldots \otimes \eta_n)(F_n) = \int_{E_0} \ldots \int_{E_n} \eta_0(dx_0) \ldots \eta_n(dx_n)\; F_n(x_0, \ldots, x_n)$$

- Acceptance parameter $\epsilon_n \neq 0 \rightsquigarrow$ Limiting McKean measures.

$$\eta_n = \mathrm{Law}(\overline{X}_n) \quad \text{with Markov transition} \quad \overline{X}_n \overset{\eta_n}{\rightsquigarrow} \overline{X}_{n+1}$$

Interacting-Branching model $=$ Mean-field interpretation of $\overline{X}_n$

# Limiting mean potential/success proportions ($G_n = 1_A$)

$$\eta_n^N(G_n) := \frac{1}{N}\sum_{i=1}^{N} G_n(\xi_n^i) \longrightarrow_{N\uparrow\infty} \eta_n(G_n) \stackrel{def.}{=} \frac{\gamma_n(G_n)}{\gamma_n(1)} = \frac{\gamma_{n+1}(1)}{\gamma_n(1)} \tag{1}$$

$\Rightarrow$**Unbiased estimate of the normalizing cts/partition functions :**

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

**with the key product formula :**

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

*Running ex. :* [$X_n$ SRW & $G_n = 1_A$]

$$\prod_{0\leq p<n} \textbf{(Success proportion time p)} \simeq \mathbb{P}\left(\forall 0 \leq p < n \quad X_p \in A\right)$$

## Summary-Conclusions

**SMC/Genetic type branching/particle model**

[$M_n$-**free exploration** $\oplus$ $G_n$-**weighted branchings/adaptation**]

$$\Downarrow \quad \& \quad \Uparrow$$

**Feynman-Kac measures**

[$M_n$-**free motion** $\oplus$ $G_n$-**potential functions**]

# Summary

## Some evolutionary sampling recipes

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

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

- $\rightsquigarrow$ **Interacting stochastic algorithm :**

$$\begin{array}{rcl} \text{accept/reject/select/branch/prune/clone/spawn/enrich} & \rightsquigarrow & G_n \\ \text{exploration/proposition/prediction/mutation/free evolution} & \rightsquigarrow & M_n \end{array}$$

**And Inversely !**

- 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

- **Tuning parameters:** $(G_n, M_n) \sim$ change of ref. measures, path/excursion spaces, selection periods, weights interpretations,...

# 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 $G_n = 1_A$)

$\oplus$ DM, Jacod J. : Interacting particle filtering with discrete-time observations: asymptotic behaviour in the Gaussian case. Stochastics in infinite dimensions, Trends in Mathematics, Birkhauser (2001).

- Uncorrelated MCMC for each target measure $\eta_n$ ($\uparrow$ complex.).
- "Pure" branching $\rightsquigarrow$ critical 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).

## A nonlinear approach $\sim$ **Feynman-Kac evolution equation**

[$\eta_n \in \mathcal{P}(E_n)$ probability measures $\uparrow$ complexity].

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

**With only 2 transformations:**

- Bayes-Boltzmann-Gibbs updating transformation :

$$\Psi_{G_n}(\eta_n)(dx) := \frac{1}{\eta_n(G_n)} \; G_n(x) \; \eta_n(dx)$$

- $X$-Free Markov transport/prediction eq. : [$X_n$ Markov $M_n$]

$$\mu(dx) \; \rightsquigarrow \; (\mu M_n)(dy) := \int \mu(dx) \; M_n(x, dy)$$

$$\Updownarrow$$

(**Updating**/**Prediction**)$\simeq$(**Select.**/**Mutation**)=(**Branching**/**Exploration**)

$$\eta_n \xrightarrow{\text{Updating}} \Psi_{G_n}(\eta_n) \xrightarrow{\text{Prediction}} \eta_{n+1} = \Psi_{G_n}(\eta_n) M_{n+1}$$

$$\Updownarrow$$

$$\xi_n = (\xi_n^i)_{1\leq i\leq N} \xrightarrow{\text{Branching/Selection}} \widehat{\xi}_n = (\widehat{\xi}_n^i)_{1\leq i\leq N} \xrightarrow{\text{Exploration/Mutation}} \xi_{n+1}$$

**2 Local sources of randomness with mean :**

$$\mathbb{E}\left(\eta_{n+1}^N(f) \mid \xi_n\right) = \sum_{i=1}^N \frac{G_n(\xi_n^i)}{\sum_{j=1}^N G_n(\xi_n^j)} M_{n+1}(f)(\xi_n^i) = \Phi_{n+1}\left(\eta_n^N\right)(f)$$

$$\Updownarrow$$

**The particle measures $\eta_n^N$ "almost" solve the updating/prediction system :**

$$\mathbb{E}\left( \left[\eta_{n+1}^N - \Phi_{n+1}\left(\eta_n^N\right)\right](f) \mid \xi_n\right) = 0 \longleftrightarrow \eta_{n+1} = \Phi_{n+1}(\eta_n)$$

**Up to the local fluctuation errors :**

$$\eta_{n+1}^N = \Phi_{n+1}\left(\eta_n^N\right) + \underbrace{\frac{1}{\sqrt{N}}}_{\text{Monte Carlo precision}} \times \underbrace{\left[\sqrt{N}\left(\eta_{n+1}^N - \Phi_{n+1}\left(\eta_n^N\right)\right)\right]}_{:=W_n^N \simeq \text{Gaussian Field}}$$

## Some key advantages

- $\rightsquigarrow$ Stochastic linearization/perturbation model :

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

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

- **If** $\eta_n = \Phi_n(\eta_{n-1})$ **stable dynamical system**

$$\Longrightarrow \quad \text{local errors do not propagate}$$

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

- "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.

## Summary

## Filtering models

- **Signal-Observation likelihood functions** $(X_n, G_n)$ :

$$\begin{array}{rcl} \eta_n & = & \mathrm{Law}((X_0,\ldots,X_n) \mid (Y_0,\ldots,Y_n)) \\ L_n & = & \dfrac{1}{n}\log\gamma_n(1) = \mathrm{Log\text{-}likelihood\ function} \end{array}$$

- **Example :**

$$Y_n = H_n(X_n) + V_n \quad \text{with} \quad \mathbb{P}(V_n \in dv_n) = g_n(v_n)\ dv_n$$

$$\Downarrow [Y_n = y_n]$$

$$G_n(x_n) = g_n(y_n - H_n(x_n))$$

- $\rightsquigarrow$ Particle filters, sampling/resampling alg., bootstrap filter, genetic filter,...

## Rare events analysis

- Confinements potentials: $G_n = 1_{A_n}$

$$\begin{aligned} \eta_n &= \mathrm{Law}((X_0, \ldots, X_n) \mid X_0 \in A_0, \ldots, X_n \in A_n) \\ \mathcal{Z}_n &= \mathbb{P}(X_0 \in A_0, \ldots, X_n \in A_n) \end{aligned}$$

$\rightsquigarrow$ Interacting acceptance/rejection stochastic simulation

- Twisted measures $\sim \mathbb{P}(V_n(X_n) \geq a)$?

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

$\rightsquigarrow$ Interacting particle simulation of twisted measures

# Hitting $B$ before $C$

- *Multi-level decomposition* $B_0 \supset B_1 \supset \ldots \supset B_m$, $B_0 \cap C = \emptyset$.
- *Inter-level excursions :*

$$T_n = \inf\{p \geq T_{n-1} \ : \ Y_p \in B_n \cup C\}$$

- *Level excursions and level detection potentials:*

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

$$\Updownarrow$$

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

$\rightsquigarrow$ Branching-multilevel splitting 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

- $\pi$ "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 ] :

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

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

- $\leadsto$ time reversal genealogical tree simulation

  $\leadsto$ Interacting Metropolis-Hastings algorithms

## Non intersecting random walks (& connectivity constants)

$$X_n := (X'_0, \ldots, X'_n) \quad \text{and} \quad G_n(X_n) = 1_{\not\in \{X'_p\ ,\ p<n\}}(X'_n)$$

$$\Downarrow$$

$$\eta_n = \mathrm{Law}((X'_0, \ldots, X'_n) \mid \forall p < q < n \quad X'_p \neq X'_q)$$

$\rightsquigarrow$ Dynamic Pruning-Enrichment Rosenbluth Monte Carlo model

## Molecular simulation $\sim$ Particle absorption models

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

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

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

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

With:

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

## Feynman-Kac integral model

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

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

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

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

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

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

## 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

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

# Feynman-Kac-Shroedinger ground states energies

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

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

Limiting FK-measures

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

$\rightsquigarrow$ Branching particle approximations :

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

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

$$\Updownarrow$$

Diffusion and quantum Monte Carlo models

## 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 :

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

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

## Boltzmann-Gibbs distribution flows

- 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 Examples:

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

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

## 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.

# Summary

# Non asymptotic results

- **Weak estimates $\leftrightarrow$ Bias estimates ($\leftrightarrow$ Propagations of chaos)**

**Law(q particles among N at time n) $\simeq_{N\uparrow\infty}$ Law(q iid r.v. w.r.t. $\eta_n$)**

1. Total variation $= \frac{q^2}{N} c(n)$, Boltzmann entropy $= \frac{q}{N} c(n)$.
2. Stable models: uniform estimates w.r.t. time $\sup_n c(n) < \infty$.
3. Path space and genealogical tree models $c(n) = c \times n$.
4. Explicit weak decompositions at any order $\frac{1}{N^k}$.

$\hookrightarrow$http-ref : DM-Patras-Rubenthaler, Coalescent tree based functional representations for some Feynman-Kac particle models, Hal-INRIA (2006).

- **$\mathbb{L}_p$-mean error bounds** [(2),(3) as above]

$$\sup_{N\geq 1} \sqrt{N}\, \mathbb{E}\left(\sup_{f_n\in\mathcal{F}_n} \left|\eta_n^N(f_n) - \eta_n(f_n)\right|^p\right) \leq b(p)\ c(n)$$

- **Exponential estimates** [(2) as above & empirical processes $\sim \mathcal{F}_n$]

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

**Feynman-Kac (nonlinear) dynamical semigroup :** $\boxed{\eta_p \rightsquigarrow \Phi_{p,n}(\eta_p) := \eta_n}$

**A local transport formulation** **(works $\forall$ approximation scheme $\eta_n^N \simeq \eta_n$!)**

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

$\rightsquigarrow$**Key decomposition formula**

$$
\eta_n^N - \eta_n = \sum_{q=0}^{n} \left[\Phi_{q,n}(\eta_q^N) - \Phi_{q,n}(\Phi_q(\eta_{q-1}^N))\right] \text{ "} \simeq \text{" } \sum_{q=0}^{n} \frac{1}{\sqrt{N}}\, e^{-\lambda\,(n-q)}
$$

## Some crude uniform estimates w.r.t. time

**Hypothesis :** (Time homogeneous models) $\exists(m,r)$ s.t. for any $(x,y)$

$$M^m(x,.)\ \geq\ \epsilon\, M^m(y,.)\quad \text{and}\quad G_n(x)\ \leq\ r\ G_n(y)$$

- **Limiting system stability properties :**

$$\|\Phi_{p,p+nm}(\eta)-\Phi_{p,p+nm}(\mu)\|_{tv}\ \leq\ (1-\epsilon^2/r^{m-1})^n$$

  **and w.r.t. Csiszár's *H*-entropy criteria**

$$H(\Phi_{p,p+nm}(\mu),\Phi_{p,p+nm}(\eta))\ \leq\ \alpha_H(r^m/\epsilon)\ (1-\epsilon^2/r^{m-1})^n\ H(\mu,\eta)$$

- **Examples :**

  $\alpha_H(t)=t$ (tv norm & Boltzmann entropy), $\alpha_H(t)=t^{1+p}$ (Havrda-Charvat & Kakutani-Hellinger $p$-integrals, $\alpha_H(t)=t^3$ ($\mathbb{L}_2$-norm),...

## Some crude uniform estimates w.r.t. time

**Hypothesis :** (Time homogeneous models) $\exists(m,r)$ s.t. for any $(x,y)$

$$M^m(x,.) \geq \epsilon\, M^m(y,.) \quad \text{and} \quad G_n(x) \leq r\, G_n(y)$$

- $\mathbb{L}_p$**-mean error bounds**

$$\sup_{n\geq 0}\ \sup_{N\geq 1} \sqrt{N}\, \mathbb{E}\left(\left|\left[\eta_n^N-\eta_n\right](f)\right|^p\right)^{\frac{1}{p}} \leq 2\ b(p)\ m\ r^{2m-1}/\epsilon^3$$

with $\quad b(2p)^{2p}=(2p)_p\, 2^{-p} \quad$ and $\quad b(2p+1)^{2p+1}=\dfrac{(2p+1)_{(p+1)}}{\sqrt{p+1/2}}\, 2^{-(p+1/2)}$

- **Uniform concentration estimates :**

$$\sup_{n\geq 0} \mathbb{P}\left(\left|\left[\eta_n^N-\eta_n\right](f)\right| \geq \delta\right) \leq 6\ \exp\left(-N\, \delta^2\, \epsilon^5/(32 m r^{4m-1})\right)$$

- **Extensions to Zolotarev's seminorms** $\|\eta_n^N-\eta_n\|_{\mathcal{F}}=\sup_{f\in\mathcal{F}}|[\eta_n^N-\eta_n](f)|$

# Fluctuations and large deviations

- **Central Limit Theorems** [Sharp $\mathbb{L}_p$ estimates]

{http-ref : 1999⇝2004 : DM, Guionnet, Jacod, Ledoux, Tindel}

$$V_n^N(f) := \sqrt{N}\ \left[\eta_n^N(f) - \eta_n(f)\right] \Longrightarrow V_n(f) = \text{Centered Gaussian r.v.}$$

1. **Functional Central Limit Theorems.** [$\forall d,\ \forall (f^i)_{1\leq i\leq d}$]

$$(V_n^N(f^1), \ldots, V_n^N(f^d)) \Longrightarrow \left(V_n(f^1), \ldots, V_n(f^d)\right)$$

2. Empirical processes $\rightsquigarrow$ Donsker type theorems.
3. Convergence rates $\rightsquigarrow$ Berry Esseen type theorems.
4. Path space models (Complete tree and genealogical tree).

- **Large deviations principles** [Sharp asymptotic expo estimates]

$$\lim_{N\to\infty} \frac{1}{N} \log \mathbb{P}\left(\eta_n^N \not\in \mathcal{V}(\eta_n)\right)$$

*Example* : $\mathcal{V}(\eta_n) = \{\mu\ :\ |\eta_n^N(f) - \eta_n(f)| \leq \epsilon\}$ (weak and strong $\tau$-topo).

{http-ref 1998⇝2004 : DM, Dawson, Guionnet, Zajic}

**Feynman-Kac (nonlinear) semigroup** $\eta_p \longrightarrow \Phi_{p,n}(\eta_p) := \eta_n$

**LOCAL FLUCTUATION THEOREM :** $W_n^N := \sqrt{N}\left[\eta_n^N - \Phi_n\left(\eta_{n-1}^N\right)\right] \simeq W_n$ **Centered and Independent 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 entering the stability of the limiting system:**

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

$\Rightarrow$ **Two lines proof of a Functional CLT :** $\sqrt{N}\left[\eta_n^N - \eta_n\right] \simeq \sum_{q=0}^{n} W_q D_{q,n}$