

# Mean field simulation of (quasi-)invariant measures and related topics

P. Del Moral

INRIA Bordeaux - Sud Ouest

Genetic Models and Quasi-stationarity, CIRM Luminy, March 2013

## Some hyper-references

- ▶ Branching and interacting particle systems. (with L. Miclo) Sémin. Proba. de Strasbourg (2000).
- ▶ A Moran particle system approximation of Feynman-Kac formulae. (with L. Miclo) SPA (2000).
- ▶ On the stability of interacting processes (with A. Guionnet) IHP (2001).
- ▶ On the Stability of Feynman-Kac sg. (with L. Miclo) Annales de la Fac. Sci. Toulouse (2002)
- ▶ Particle Lyapunov exponents connected to Schrödinger op. (with L. Miclo) ESAIM PS (2003).
- ▶ Particle Motions in Absorbing Medium with Hard and Soft Obst. (with A. Doucet) SAA (2004).

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- ▶ Feynman-Kac formulae, Genealogical & Interacting Particle Systems, Springer (2004).
- ▶ On the concentration of interacting processes. FTML (with P. Hu & L. Wu) (2012)
- ▶ Mean field simulation for Monte Carlo integration. Chapman & Hall CRC Press (2013)

Introduction

Absorption models

Extended path integration models

Feynman-Kac models

Stochastic analysis

How & Why it works

Continuous time models

## Introduction

Some basic notation

Boltzmann-Gibbs transformation

Nonlinear transport models

Absorption models

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# Basic notation

- ▶ **Lebesgue integral** Measures  $\mu$ , functions  $f$  on  $E$

$$\mu(f) = \int \mu(dx) f(x)$$

- ▶ **Integral operators**  $Q(x_1, dx_2)$ ,  $x_1 \in E_1 \rightsquigarrow x_2 \in E_2$

$$Q(f)(x_1) = \int Q(x_1, dx_2) f(x_2)$$

$$[\mu Q](dx_2) = \int \mu(dx_1) Q(x_1, dx_2) \quad (\implies [\mu Q](f) = \mu[Q(f)])$$

- ▶ **Composition**

$$(Q_1 Q_2)(x_1, dx_3) = \int Q_1(x_1, dx_2) Q_2(x_2, dx_3)$$

- ▶ **Semigroups**

$$Q_{p,n} = Q_{p+1} Q_{p+1} \dots Q_n$$

# Boltzmann-Gibbs transformation

**Boltzmann-Gibbs transformation :**

- ▶  $G$  positive and bounded potential function on  $E$
- ▶  $\mu$  positive bounded measure on  $E$

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

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**Important observation :**  $\exists$  a (nonlinear) Markov transport eq.

$$\Psi_G(\mu) = \mu S_\mu \quad \left( \Leftrightarrow \int \mu(dx) S_\mu(x, dy) = \Psi_G(\mu)(dy) \right)$$

for some (non unique) collection Markov transition  $S_\mu$  from  $E$  into itself.

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**Later**  $\mu \simeq \mu^N := \frac{1}{N} \sum_{1 \leq i \leq N} \delta_{X^i} \rightsquigarrow$  **Mean field selection transition**

$$X^i \rightsquigarrow \widehat{X}^i \text{ with law } S_{\mu^N}(X^i, dx)$$

**Example 1** :  $\forall \epsilon$  s.t.  $\epsilon G \leq 1$

$$S_\mu(x, dy) = \epsilon G(x) \delta_x(dy) + (1 - \epsilon G(x)) \Psi_G(\mu)(dy)$$

Some choices :

$$\begin{aligned}\epsilon^{-1} &= \mu - \text{ess-sup } G & \epsilon^{-1} &= \|G\| \\ \epsilon &= 0, \quad \text{or} \quad \epsilon = 1 \quad \text{when} \quad G \leq 1\end{aligned}$$

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**Example 3** :  $\forall G$

$$S_\mu(x, dy) = \alpha(x) \delta_x(dy) + (1 - \alpha(x)) \Psi_{(G-G(x))_+}(\mu)(dy)$$

with the acceptance rate

$$\alpha(x) = \mu(G \wedge G(x))/\mu(G)$$

Introduction

## Absorption models

Hard obstacles

Soft obstacles

A brief review on genetic type models

MCMC absorption models

Extended path integration models

Feynman-Kac models

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# Absorption models

**Example 1** : Markov chain models  $\mathbf{X}_n \in \mathbf{E}_n$  restricted to subsets  $A_n$

$$\mathbf{X} = (X_0, \dots, X_n) \in \mathbf{A} = (A_0 \times \dots \times A_n)$$



## Non absorption conditional distributions

$$\text{Law}(\mathbf{X} \mid \mathbf{X} \in \mathbf{A}) = \text{Law}((X_0, \dots, X_n) \mid X_p \in A_p, \quad p < n) = \mathbb{Q}_n$$

and

$$\text{Proba}(X_p \in A_p, \quad p < n) = \mathcal{Z}_n$$

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

with

$$\mathbb{P}_n = \text{Law}(X_0, \dots, X_n) \quad \text{and} \quad G_p = 1_{A_p}, \quad p < n$$

# Particle absorption models

**N-Particle system  $(\xi_n^i)_{1 \leq i \leq N}$  with selection-mutation transitions**

- ▶  $N$  iid  $(\xi_0^i)_{1 \leq i \leq N}$  copies of  $X_0$ , and set  $P_0^N = \frac{1}{N} \sum_{1 \leq i \leq N} 1_{A_0}(\xi_0^i)$ .

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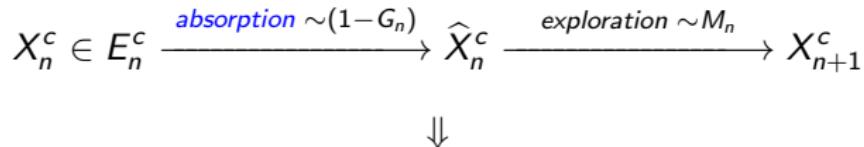
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## Absorption models $G_n \leq 1$

**Example 2** : Absorbed Markov chain with rate  $(1 - G_n)$  on  $E_n$



### Non absorption conditional distributions

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

$\Downarrow$

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n-th time marginals:

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

$$\gamma_n(1) = \mathbb{E} \left( \prod_{0 \leq p < n} G_p(X_p) \right) = \mathbb{P}(T^{\text{absorption}} \geq n)$$

and

$$\eta_n(f) = \mathbb{E} (f(X_n^c) \mid T^{\text{absorption}} \geq n)$$

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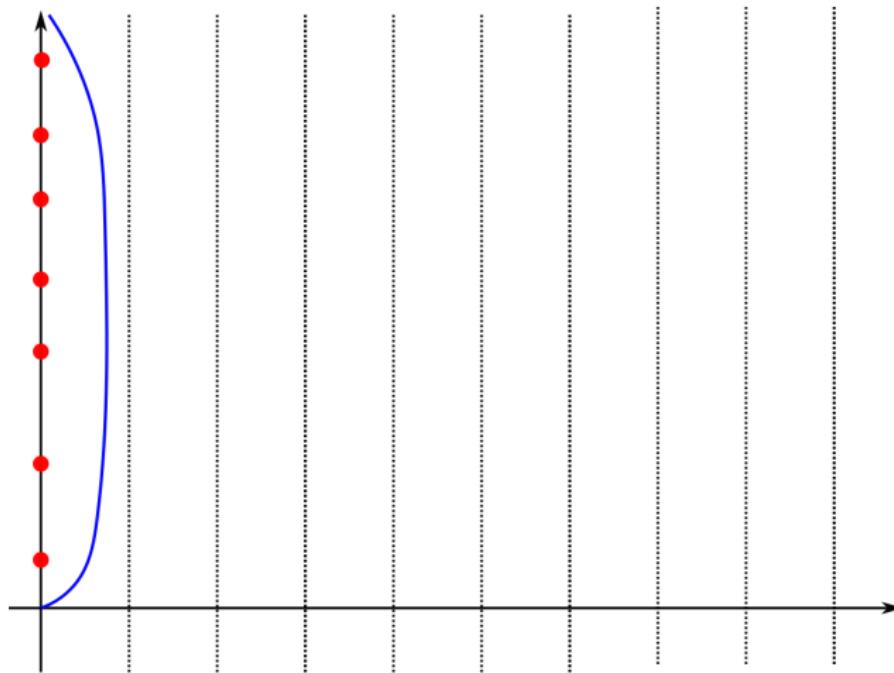
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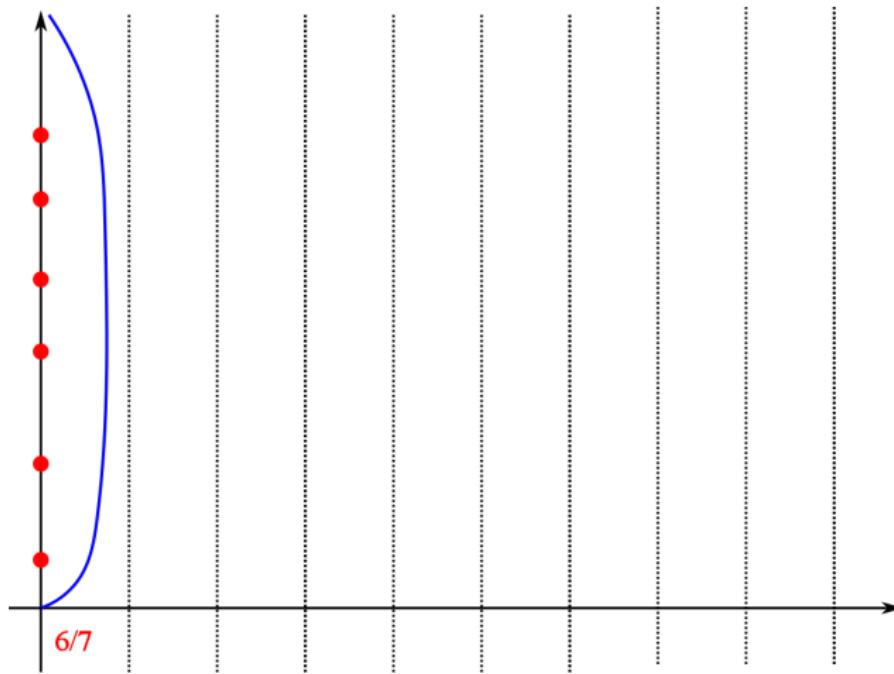
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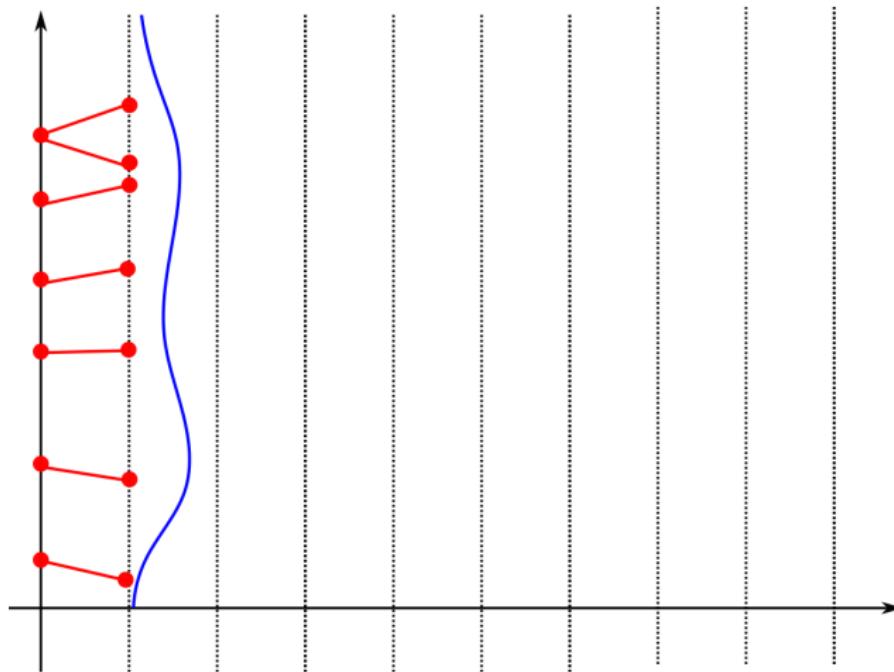
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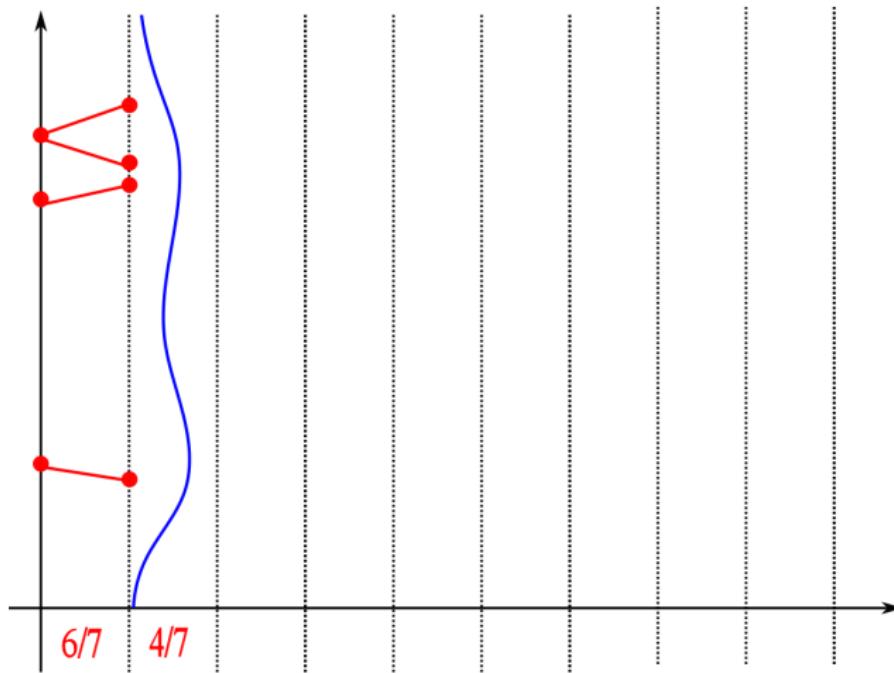
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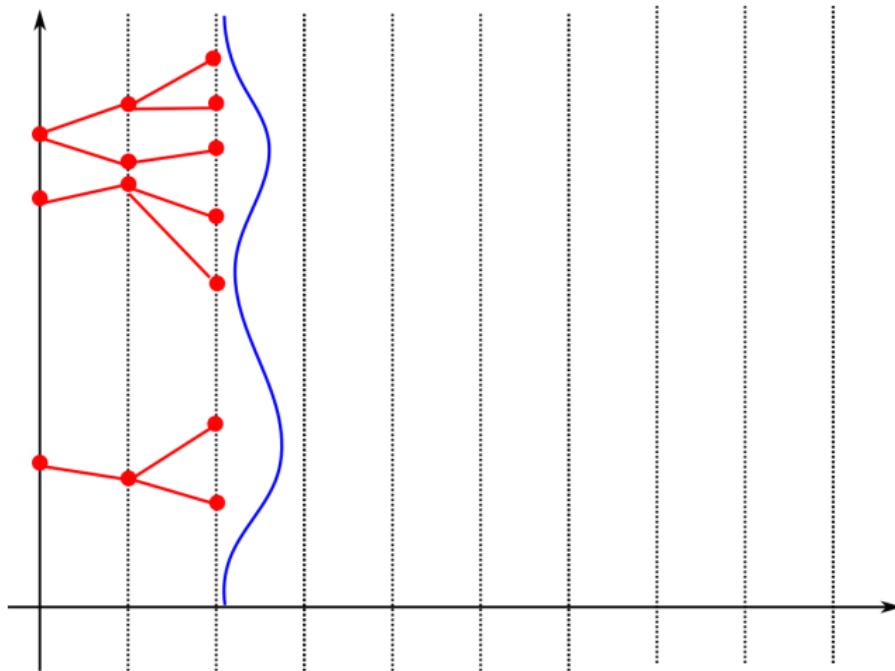
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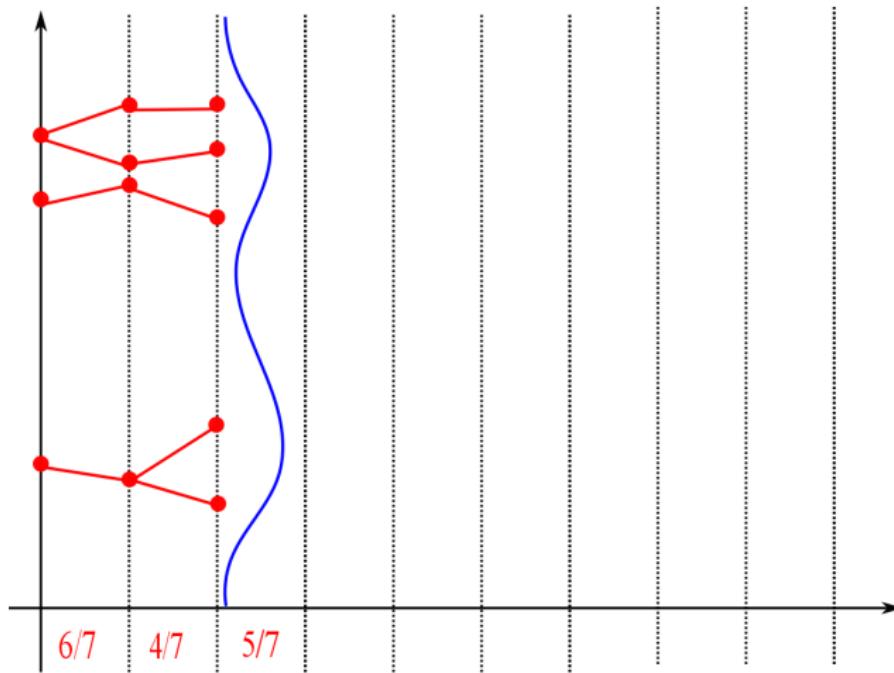
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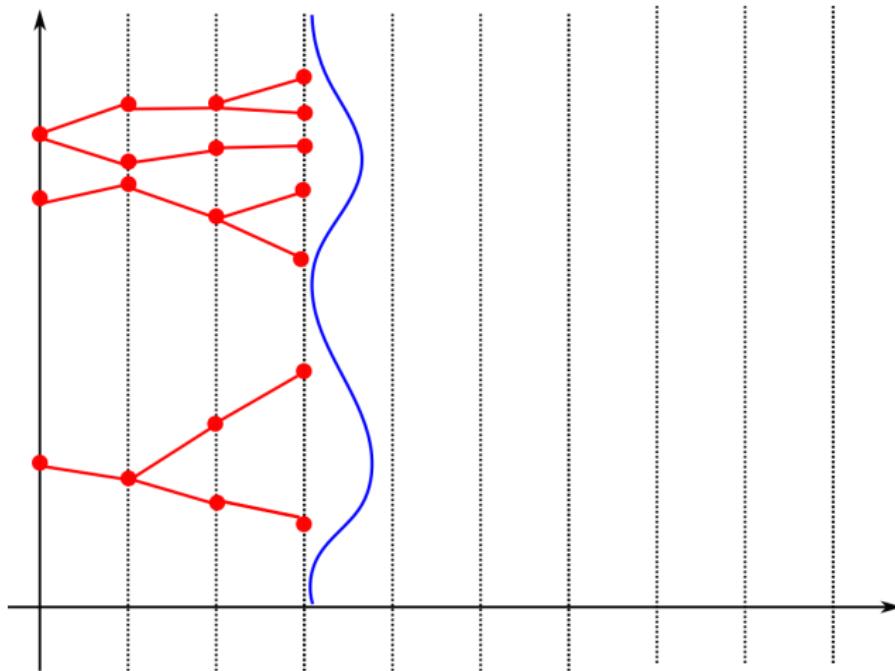
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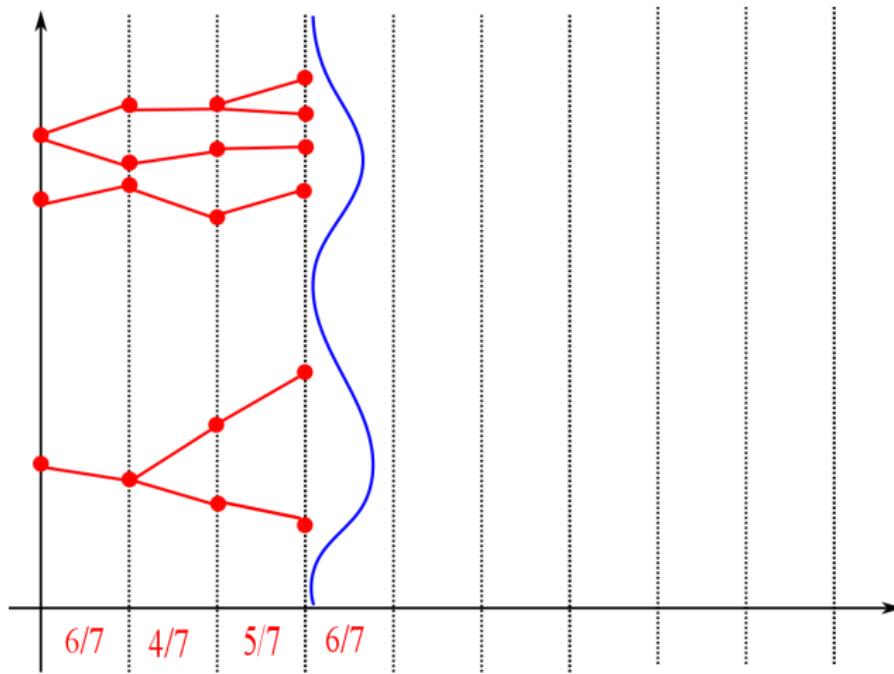
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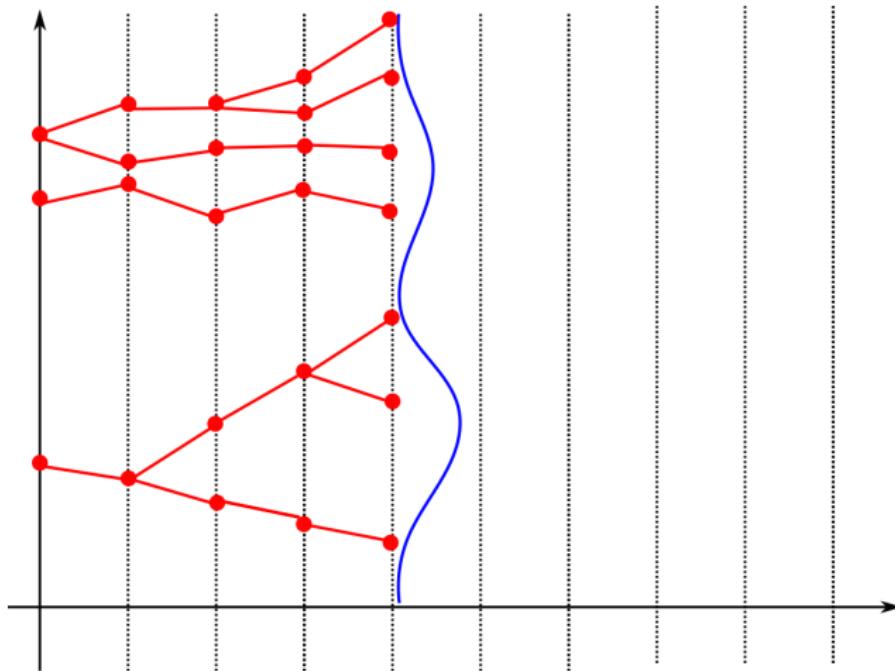
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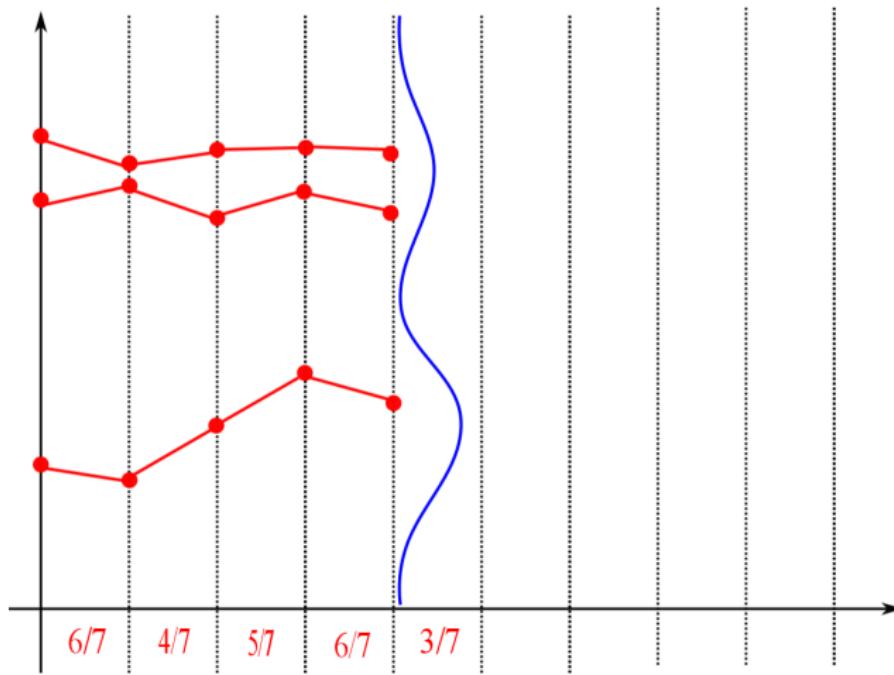
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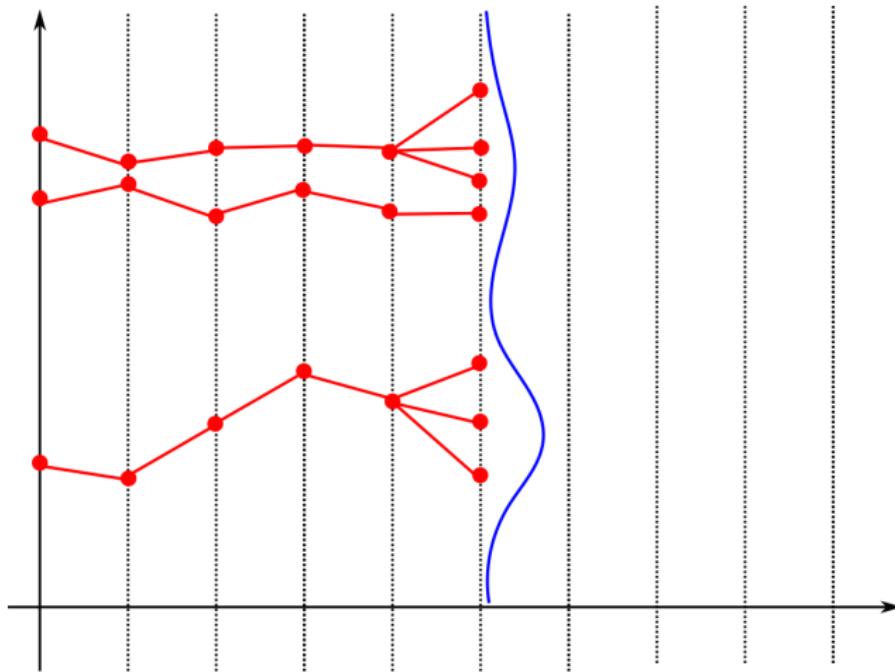
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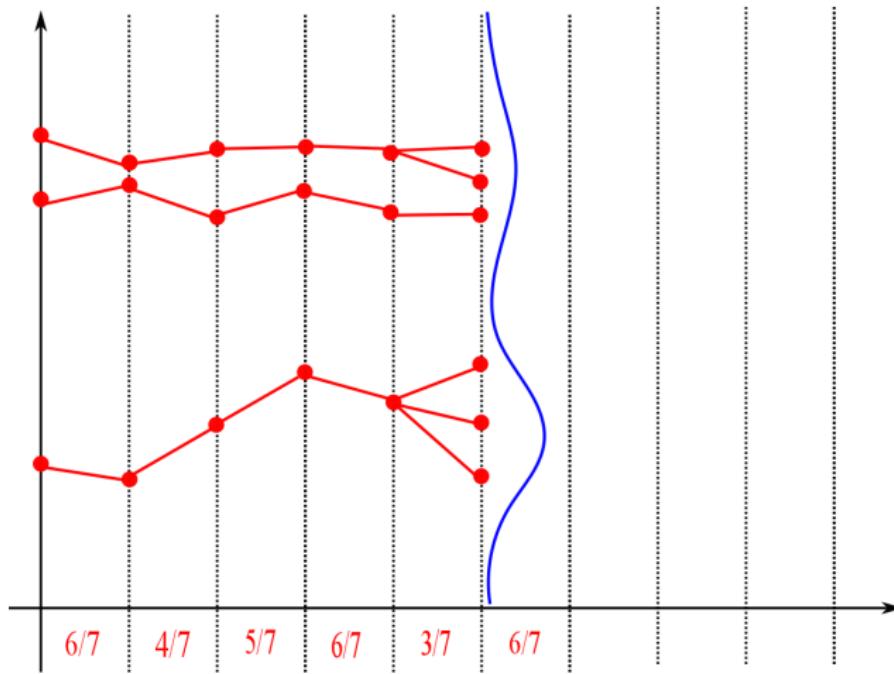
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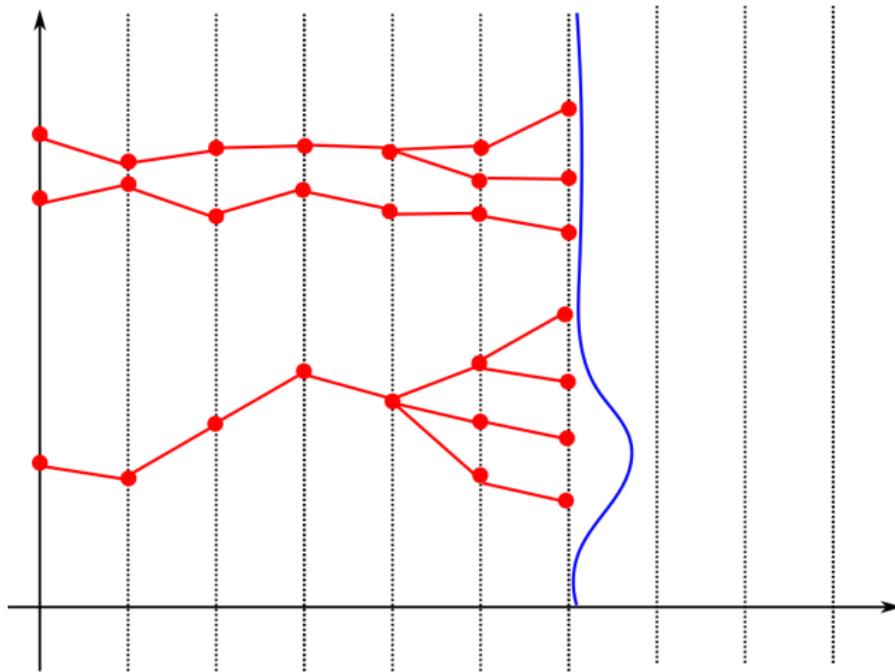
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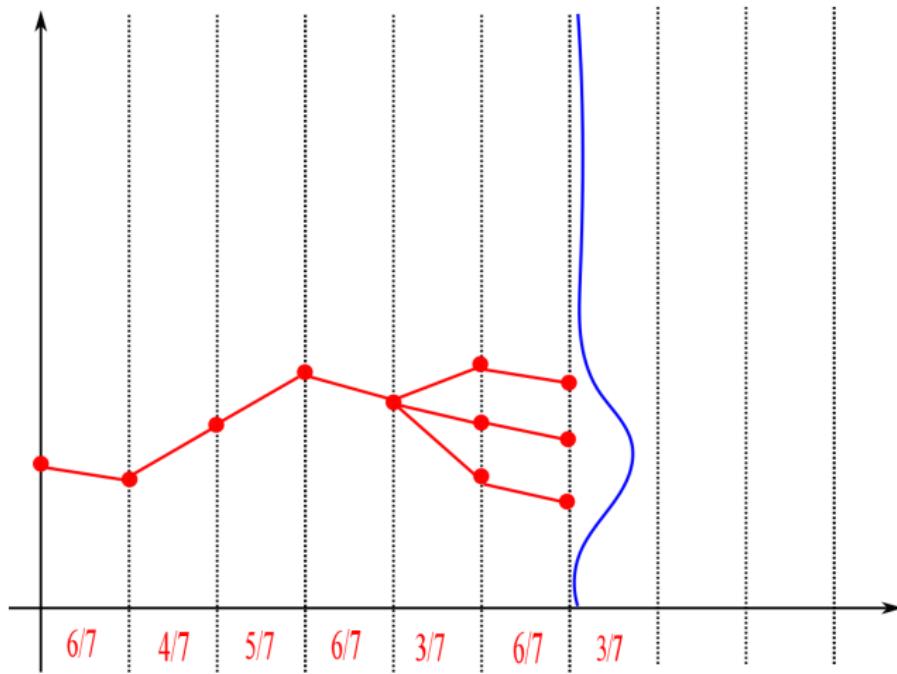
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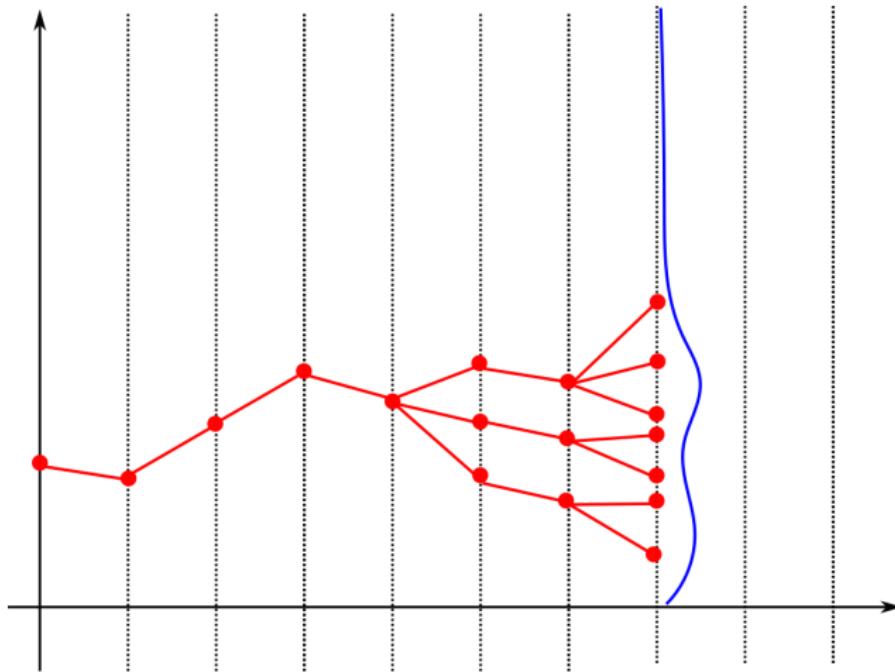
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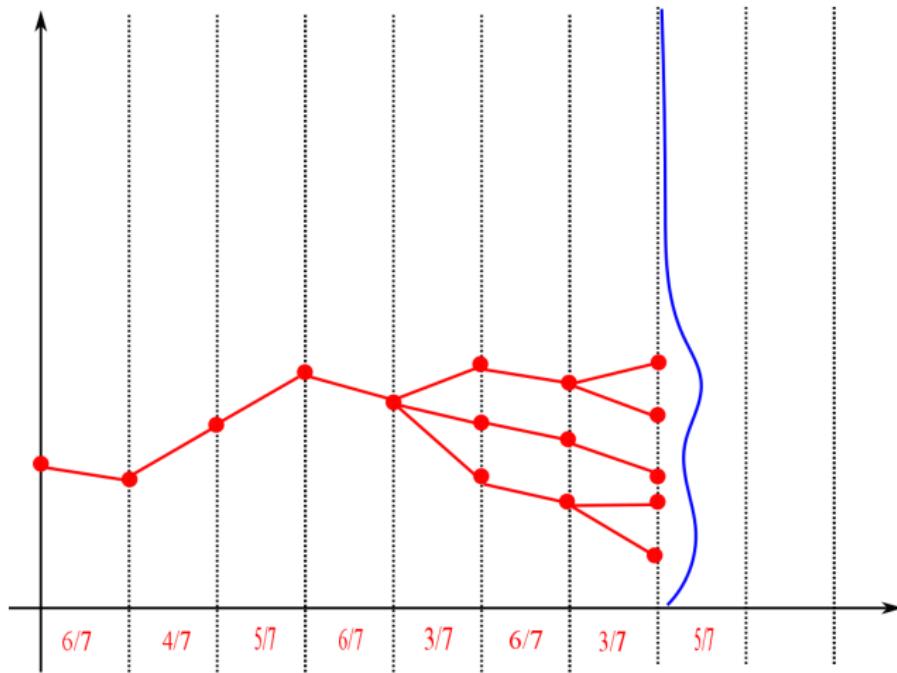
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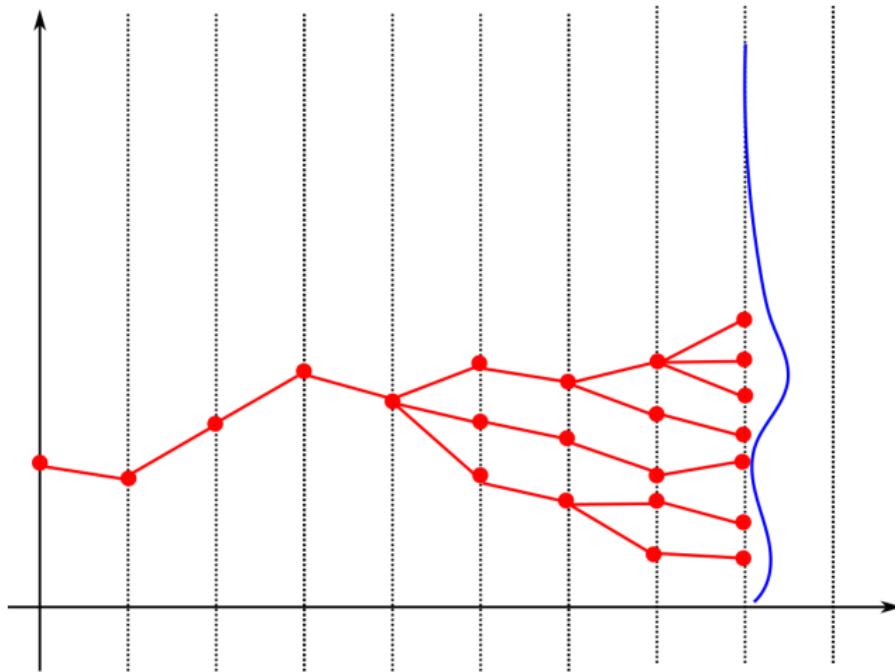
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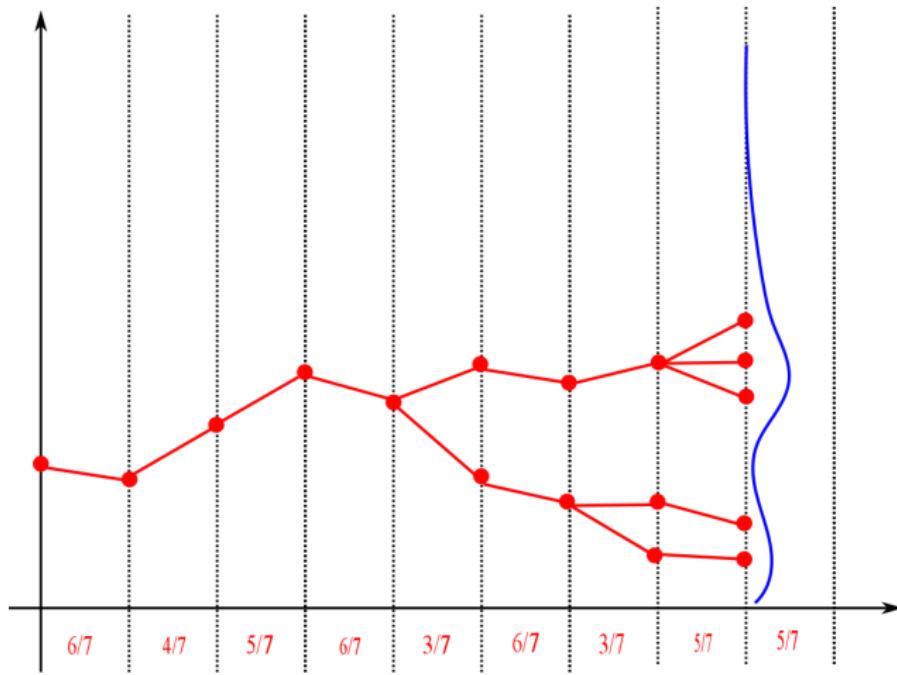
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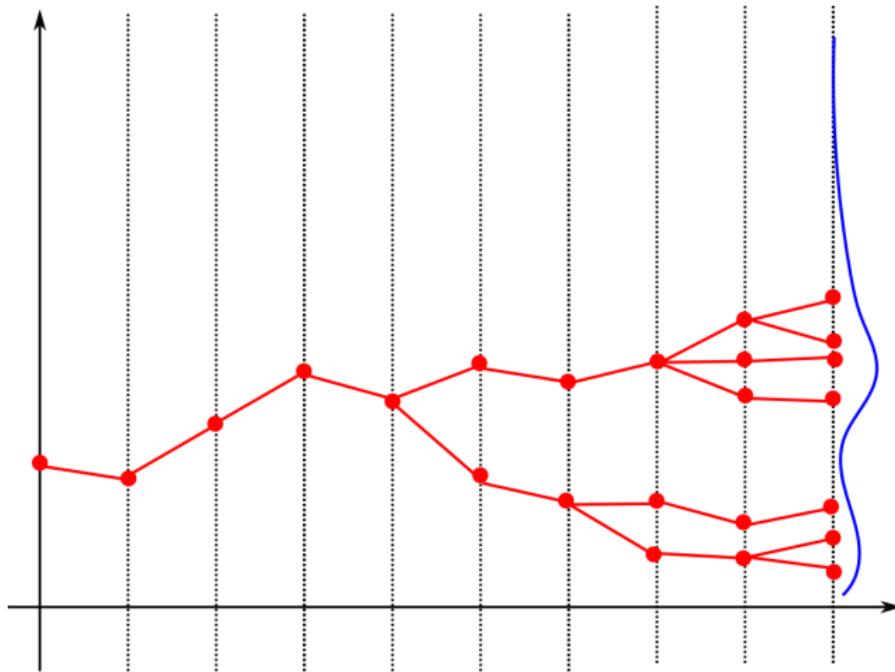
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## Continuous time models $X'_t$ , $t \in \mathbb{R}_+$

►  $X_n = X'_{[t_n, t_{n+1}]}$  and  $G_n(X_n) = \exp \left\{ \int_{t_n}^{t_{n+1}} V_t(X'_t) dt \right\}$



$$d\mathbb{Q}_n = \frac{1}{\mathcal{Z}_n} \exp \left( \int_0^{t_n} V_t(X'_t) dt \right) \mathbb{P}_n$$

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- Euler/Milstein/... discrete time approximations

# Equivalent heuristic like particle algorithms

∈ [1950 – 1996]

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

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## Many other lively buzzwords :

bootstrapping, spawning, cloning, pruning, replenish, splitting,  
enrichment, go with the winner, look-ahead, weighted dynamics, ...

## Remarks

- **Geo. accept. rates  $e^{-V \Delta t}$**   $\rightsquigarrow$  Continuous time interact. jumps

$$\frac{d}{dt} \eta_t(f) = \eta_t(L_{t,\eta_t}(f)) = \eta_t(L_t^X) - [\eta_t(fV) - \eta_t(f)\eta_t(V)]$$

with  $L_{t,\eta_t} = L_t^X + \widehat{L}_{t,\eta_t}$  the jump generator:

$$\widehat{L}_{t,\eta_t}(f)(x) = V(x) \int (f(y) - f(x)) \eta_t(dy)$$

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Law(Branching process with Poisson branching numbers | Size =  $N$ )

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- **Fleming-Viot and Dawson-Watanable :**

► **Different scaling** : higher jump rate  $N \rightsquigarrow N^2$

Ex.: finite state space

genetic selection  $\longrightarrow$  diffusions (at the level of the proportions)

► **Neutral and/or symmetric adaptation**  $V(x,y) = V(y,x)$

# Some open questions

## Finite population model:

- ▶ Invariant measure, limiting occupation measures.
- ▶ Long time behavior : relaxation times, spectral analysis, ...
- ▶  $k$ -Times de common ancestors, population size at each level.
- ▶ Occupation measures of the complete ancestral tree.
- ▶ Effects of multiple energy well envrionement.

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## Some answers [1996 – . . .]:

- ▶ Occupation meas. **complete** ancestral tree  $\rightarrow_{N \uparrow \infty}$  McKean process.
- ▶ Occupation meas. **genealogical** tree  $\rightarrow_{N \uparrow \infty}$  Feynman-Kac model
- ▶ Long time behavior (under mixing and regularity conditions)  
 $\Rightarrow \lim_{t \rightarrow \infty} \lim_{N \rightarrow \infty} = \lim_{N \rightarrow \infty} \lim_{t \rightarrow \infty}$
- ▶ Propagations of chaos expansions, CLT, LDP,  $\mathbb{L}_p$ -estimates,  
Empirical processes, Moderate deviations, stability and contraction  
inequalities, **exponential concentration analysis**

# Some questions

**n-th time marginals:**

$$\eta_n(f) = \mathbb{E} (f(X_n^c) \mid T^{\text{absorption}} \geq n) \quad \text{and} \quad \gamma_n(1) = \mathbb{P} (T^{\text{absorption}} \geq n)$$

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# An MCMC absorption model

Target measures:

$$\eta_n(dx) := \frac{1}{\mathcal{Z}_n} \left\{ \prod_{p=0}^n h_p(x) \right\} \lambda(dx) \quad \text{with} \quad 0 \leq h_p \leq 1$$

A couple of examples:

- ▶  $h_n = 1_{A_n}$  with  $A_n \downarrow \Rightarrow d\eta_n = \frac{1}{\lambda(A_n)} 1_{A_n} d\lambda$
- ▶  $h_n = e^{-(\beta_n - \beta_{n-1})V}$  with  $\beta_n \uparrow \Rightarrow d\eta_n = \frac{1}{\lambda(e^{-(\beta_n - \beta_0)V})} e^{-(\beta_n - \beta_0)V} d\lambda$

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Absorption model  $\rightsquigarrow$  exact sampling & Mean field simulation:

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$$\begin{aligned}\eta_n &= \text{Law}(X_n^c \mid T^{\text{absorption}} \geq n) \quad \text{and} \quad \mathcal{Z}_n = \mathbb{P}(T^{\text{absorption}} \geq n) \\ &= \text{Law}(\text{MCMC at time } n \mid h\text{-rejection time} \geq n)\end{aligned}$$

## Absorption models : A couple of bad tempting ideas

1. **Acceptance-Rejection simulation :**  $X_n^i$  iid copies of  $X_n^c$

$$\mathcal{Z}_n^N := \frac{1}{N} \sum_{1 \leq i \leq N} 1_{T^i \geq n} \quad \simeq_{N \uparrow \infty} \quad \mathcal{Z}_n$$

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~> **Exact sampling but with extremely poor estimates:**

$$N \operatorname{Var}(P_n^N / P_n) = (1 - P_n) \, P_n^{-1} \quad (\text{for Mean field IPS} \quad \leq c \times n)$$

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2. **Weighted models**  $\overset{G_n=1_{A_n}}{\Leftrightarrow}$  **Acceptance-Rejection simulation :**

$$\mathcal{Z}_n^N := \frac{1}{N} \sum_{1 \leq i \leq N} \prod_{0 \leq p < n} G_p(X_p^i) \quad \simeq_{N \uparrow \infty} \quad \mathcal{Z}_n$$

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Introduction

Absorption models

Extended path integration models

Branching processes

Non commutative models

Lyapunov weighted dynamics model

Path integration and sensitivity measures

Interacting Island models

Feynman-Kac models

Stochastic analysis

How & Why it works

Continuous time models

# Branching processes when $G_n \geq 1$

$$\mathcal{X}_n = \sum_{1 \leq i \leq N_n} \delta_{X_n^i} \xrightarrow[\mathbb{E}(g_n(x)) = G_n(x)]{\text{branching w.r.t.}} \widehat{\mathcal{X}}_n = \sum_{1 \leq i \leq \widehat{N}_n} \delta_{\widehat{X}_{n+1}^i} \xrightarrow[M_{n+1}]{\text{exploration}} \mathcal{X}_{n+1}$$

**First moments:**

$$\mathcal{X}_{n+1} = \sum_{1 \leq i \leq N_n} \sum_{1 \leq j \leq g_n^i(X_n^i)} \delta_{X_{n+1}^{i,j}} \Rightarrow \mathbb{E}(\mathcal{X}_{n+1}(f) \mid \mathcal{X}_n) = \mathcal{X}_n(G_n M_{n+1}(f))$$

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**Path space first moments given by the Feynman-Kac measures**

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

with

$$\mathbb{P}_n = \text{Law}(X_0, \dots, X_n) \quad \text{and} \quad \mathcal{Z}_n = \mathbb{E}(N_n)$$

# Some questions

**n-th time marginals:**

$$\eta_n(f) = \mathbb{E}(\mathcal{X}_n(f)) / \mathbb{E}(\mathcal{X}_n(1)) \quad \text{and} \quad \gamma_n(1) = \mathbb{E}(\mathcal{X}_n(1))$$

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Adding mass (notation :  $Q_{n+1}(f) = G_n M_{n+1}(f)$ )

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$$\begin{aligned}\mathbb{E}(\mathcal{X}_{n+1}(f)) &= \gamma_{n+1}(f) = \gamma_n(G_n M_{n+1}(f)) + \mu_n(f) \quad \text{with } \mu_n \text{ positive} \\ \eta_n(f) &:= \gamma_n(f)/\gamma_n(1) \quad \text{Normalized measures}\end{aligned}$$

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### Three typical scenarios when

$$(G_n, M_n, Q_n, \mu_n, \gamma_0) = (G, M, Q, \mu, \mu) \quad \text{and} \quad g_- := \inf G \leq \sup G := g_+$$

Adding mass (notation :  $Q_{n+1}(f) = G_n M_{n+1}(f)$ )

### First moment evolution equation

$$\begin{aligned}\mathbb{E}(\mathcal{X}_{n+1}(f)) &= \gamma_{n+1}(f) = \gamma_n(G_n M_{n+1}(f)) + \mu_n(f) \quad \text{with } \mu_n \text{ positive} \\ \eta_n(f) &:= \gamma_n(f)/\gamma_n(1) \quad \text{Normalized measures}\end{aligned}$$



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1.  $G = 1$  &  $\eta_\infty := \eta_\infty M$  (independent of  $\mu$ )

$$\gamma_n(1) = \gamma_0(1) + \mu(1) n \quad \text{and} \quad \|\eta_n - \eta_\infty\|_{\text{tv}} = O(1/n)$$

2.  $g_+ < 1$  &  $\eta_\infty := \gamma_\infty / \gamma_\infty(1)$  with  $\gamma_\infty$  given by

$$\gamma_\infty := \sum_{n \geq 0} \mu Q^n \iff \text{Poisson equation } \gamma_\infty (Id - Q) = \mu$$

and

$$|\gamma_n(f) - \gamma_\infty(f)| \vee |\eta_n(f) - \eta_\infty(f)| \leq c g_+^n \|f\|$$

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**Continuous time models**  $G = e^{-V\Delta t}$  &  $M = Id + L \Delta t$

$$\gamma_t = \int_0^t \mathbb{E}_\mu \left( f(X_s) \exp \left( - \int_0^s V(X_r) dr \right) \right) ds$$

$t \rightarrow \infty \rightsquigarrow$  Poisson equation  $\gamma_\infty L^V = \mu$  with  $L^V = L + V$

3.  $g_- > 1$  &  $\eta_\infty(f) := \eta_\infty Q(f)/\eta_\infty Q(1)$  (independent of  $\mu$ )

$\eta_\infty$  = Fixed point of FK-sg [quasi-inv. meas., ground states, etc.]

$$\lim_{n \rightarrow \infty} \frac{1}{n} \log \gamma_n(1) = \log \eta_\infty(G) \quad \text{and} \quad \|\eta_n - \eta_\infty\|_{\text{tv}} \leq c e^{-\lambda n}$$

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Hyper-references (including Mean field simulation schemes) :

- ▶ Particle approximations of a class of branching distribution flows arising in multi-target tracking (with Caron, Doucet, Pace) SIAM (2011).
- ▶ Mean field simulation for Monte Carlo integration. Chapman & Hall CRC Press (2013)

## Non commutative models

- ▶  $G_n(x_n) \in \mathbb{R}^{d \times d}$  s.t.  $\forall u \in \mathbb{S}^{d-1} := \{|u| = 1\}$  we have  $\|G_n(x) \cdot u\| > 0$
- ▶  $f_n(x_0, \dots, x_n) \in \mathbb{R}^d$  and  $\prod_{0 \leq p \leq n} A_p = A_0 A_1 \dots A_n$

$$\Gamma_n(f_n) \cdot u_0 := \mathbb{E} \left( f_n(X_0, \dots, X_n) \prod_{0 \leq p < n} G_p(X_p) \cdot u_0 \right)$$

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with

$$\mathbf{X}_n = (X_n, U_n) \in (E_n \times \mathbb{S}^{d-1}) \quad \text{and} \quad \mathbf{G}_n(\mathbf{X}_n) = \|G_n(X_n) \cdot U_n\|$$

and the walk on the sphere model

$$U_{n+1} = \frac{G_n(X_n) \cdot U_n}{\|G_n(X_n) \cdot U_n\|}$$

$\nabla$  of  $P_n(\varphi)(x) = \mathbb{E}_x(\varphi(Y_n))$  with  $Y_{n+1} = F_n(Y_n, W_n)$

### First variational equation

$$\begin{aligned}\text{Jac}(Y_{n+1}) &= G_n(Y_n, W_n) \text{ Jac}(Y_n) \quad \text{with} \quad G_n^{i,j} = \partial_{x^j} F_n^i \\ &= \prod_{0 \leq p \leq n} G_p(X_p) \quad \text{with} \quad X_n = (Y_n, W_n)\end{aligned}$$

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$\Leftrightarrow$  FK model w.r.t.  $Y_n$  weighted with the directional Lyap. exp.

$$\prod_{0 \leq p \leq n} G_p(X_p) = \|\text{Jac}(Y_n) \cdot u_0\| = \prod_{0 \leq p \leq n} \frac{\|\text{Jac}(Y_p) \cdot u_0\|}{\|\text{Jac}(Y_{p-1}) \cdot u_0\|}$$

## Related Feynman-Kac model

$$\mathbf{X}_n = (X_n, X_{n+1}) \quad \text{and} \quad \mathbf{G}_n(\mathbf{X}_n) = \|\text{Jac}(X_{n+1})\|^{\alpha} / \|\text{Jac}(X_n)\|^{\alpha}$$

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Feynman-Kac model = The Lyapunov weighted dynamics model

$$d\mathbf{Q}_n = \frac{1}{Z_n} \|\text{Jac}(X_n)\|^{\alpha} d\mathbf{P}_n$$

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Hyper-references :

- ▶ T Laffargue, K.D. Nguyen Thu Lam, J. Kurchan, J. Tailleur LDP of Lyapunov exp. (2013)
- ▶ S. Tanese Nicola, J. Kurchan. Metastable states, transitions, basins and borders at finite temperature J. Stat. Phys. (2004).
- ▶ J. Tailleur, S. Tanese Nicola, J. Kurchan. Kramers equations an supersymmetry J. Stat. Phys. (2006).
- ▶ J. Tailleur, J. Kurchan. Probing rare physical trajectories with Lyapunov weighted dynamics, Nature Physics (2007)
- ▶ C Genealogical particle analysis of aare events (joint work with J. Garnier) AAP (2005).

# Sensitivity measures

**hypothesis :**  $\theta \in \mathbb{R}^d \mapsto G_{\theta,n-1}(x)M_{\theta,n}(x, dy) = H_{\theta,n}(x, y) \lambda_n(dy)$

$$\Gamma_{\theta,n}(\mathbf{f}_n) = \mathbb{E} \left( \mathbf{f}_n(X_0^{(\theta,c)}, \dots, X_n^{(\theta,c)}) \mid T^{(\theta,\text{absorption})} \geq n \right)$$

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and the *additive functional*

$$\mathbb{L}_{\theta,n}(x_0, \dots, x_n) := \sum_{p=1}^n \log(H_{\theta,p}(x_{p-1}, x_p))$$

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**Derivation = Integration of additive functionals**

$$\begin{aligned}\nabla \Gamma_{\theta,n}(\mathbf{f}_n) &= \Gamma_{\theta,n}(\mathbf{f}_n \nabla \mathbb{L}_{\theta,n}) \\ \nabla^2 \Gamma_{\theta,n}(\mathbf{f}_n) &= \Gamma_{\theta,n} [\mathbf{f}_n (\nabla \mathbb{L}_{\theta,n})' \nabla \mathbb{L}_{\theta,n} + \mathbf{f}_n \nabla^2 \mathbb{L}_{\theta,n}], \dots\end{aligned}$$

# Some examples

Potential perturbation:

$$\log G_n = [V_n + \theta V'_n]$$



$$\frac{\partial}{\partial \theta} \sum_{1 \leq p \leq n} \log (H_{\theta,p}(x_{p-1}, x_p)) = - \sum_{0 \leq p < n} V'_p(x_p)$$

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Derivative of the non absorption probability:

$$\frac{1}{n} \frac{\partial}{\partial \theta} \log \Gamma_{\theta,n}(1) = \frac{1}{n} \frac{\partial}{\partial \theta} \log \mathbb{P} \left( T^{(\theta, \text{absorption})} \geq n \right) = -\mathbb{Q}_{\theta,n}(f_n)$$

with the normalized additive functional

$$f_n(x_0, \dots, x_n) = \frac{1}{n} \sum_{0 \leq p < n} V'_p(x_p)$$

# Some examples

**Diffusion perturbation:**

$$X_n^{(\theta)} - X_{n-1}^{(\theta)}$$

$$= b \left( X_{n-1}^{(\theta)} \right) \Delta + \left[ \sigma \left( X_{n-1}^{(\theta)} \right) + \theta \sigma' \left( X_{n-1}^{(\theta)} \right) \right] (W_{t_n} - W_{t_{n-1}}) \in \mathbb{R}$$

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⇓

$$\frac{\partial}{\partial \theta} \sum_{p=1}^n \log (H_{\theta,p}(x_{p-1}, x_p))$$

$$= \sum_{p=1}^n \frac{\sigma'(x_{p-1})}{\sigma(x_{p-1}) + \theta \sigma'(x_{p-1})} \left[ \left( \frac{(x_p - x_{p-1}) - b(x_{p-1})\Delta}{(\sigma(x_{p-1}) + \theta \sigma'(x_{p-1}))\sqrt{\Delta}} \right)^2 - 1 \right]$$

# Some examples

**Drift perturbation:**

$$X_n^{(\theta)} - X_{n-1}^{(\theta)}$$

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$$\frac{\partial}{\partial \theta} \sum_{p=1}^n \log(H_{\theta,p}(x_{p-1}, x_p))$$

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**FK (absorption) model :**  $\theta \mapsto (M_{\theta,n}, G_{\theta,n})$  and  $\Theta \sim \nu(d\theta)$

$$\mathbb{Q}_{\theta,n} = \text{Law}((X_0^c, \dots, X_n^c) \mid T^{\text{absorption}} \geq n, \Theta = \theta) \rightsquigarrow n\text{-th marginal } \eta_{\theta,n}$$



## Multiplicative formula

$$\mathcal{Z}_{\theta,n} = \mathbb{P}(T^{\text{absorption}} \geq n, \Theta = \theta) = \prod_{0 \leq p < n} \underbrace{\eta_{\theta,p}(G_{\theta,p})}_{=h_p(\theta)}$$

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### Conditional distribution of the environment w.r.t. non absorption:

$$\mathbb{P}(\Theta \in d\theta \mid T^{\text{absorption}} \geq n) = \frac{1}{\mathcal{Z}_n} \left[ \prod_{0 \leq p < n} h_p(\theta) \right] \times \nu(d\theta)$$

when  $h_n$  are known :

$\rightsquigarrow$  use the MCMC absorption model  $\oplus$  Mean field particle approximation

# Interacting Island models

$\xi_{\theta,n}$  = particle Feynman-Kac model  $\sim (M_{\theta,n}, G_{\theta,n})$  and  $\Theta \sim \nu(d\theta)$

$$\left. \begin{aligned} x &= (\theta, (\xi_{\theta,n})_{n \in [0, T]}) \\ h_n(x) &= \eta_{\theta,n}^N(G_{\theta,n}) \end{aligned} \right\} \rightarrow \mu_n(dx) = \frac{1}{\mathcal{Z}_n} \left\{ \prod_{0 \leq p < n} h_p(x) \right\} \lambda(dx)$$

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By the unbiased property

$$\mu_n \circ \Theta^{-1} = \frac{1}{\mathcal{Z}_n} \left\{ \prod_{0 \leq p < n} \eta_{\theta,n}(G_{\theta,n}) \right\} \nu(d\theta)$$

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- MCMC shaking moves in (parameter-island)-spaces

$$\mathbb{P}(X_n \in dx \mid X_{n-1}) = M_n(X_{n-1}, dx) \quad \text{s.t.} \quad \mu_n M_n = \mu_n$$

- Updating w.r.t. the average fitness of the islands  $\eta_{\theta,n}^N(G_{\theta,n})$

Introduction

Absorption models

Extended path integration models

Feynman-Kac models

Nonlinear evolution equations

Historical processes

Mean field particle models

Some particle estimates

Stochastic analysis

How & Why it works

Continuous time models

**FK model:**  $\forall G_n \geq 0$  and  $M_n = \text{Markov transition of } X_n$

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$\eta_n$ = $n$ -marginal measures of  $\mathbb{Q}_n$  and the unnormalized  $\gamma_n = Z_n \times \eta_n$

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**Key formula**  $\rightsquigarrow Z_n = \prod_{0 \leq p < n} \eta_p(G_p)$

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## Two more key observations

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### Example

$$G_n = 1_{A_n} = \text{Hard} \rightsquigarrow \text{Soft obstacles} = \hat{G}_{n-1}(x) = \mathbb{P}(X_n \in A_n \mid X_{n-1} = x)$$

# Mean field and Interacting particle models

- **Nonlinear McKean Markov models**  $\eta_{n+1} = \eta_n K_{n+1, \eta_n}$

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⇓

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Mean field particle model when  $K_{n+1,\eta} = S_{n,\eta} M_{n+1}$

**Mean field simulation:**

$$K_{n+1,\eta_n^N} = \underbrace{S_{n,\eta_n^N}}_{selection} \quad \underbrace{M_{n+1}}_{mutation} \Leftrightarrow \text{Genetic type interacting particle system}$$

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Genealogical tree occupation measures

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- ▶ Individuals  $\xi_n^i$  "almost" iid with law  $\eta_n \simeq_{N \uparrow \infty} \eta^{\textcolor{red}{N}} = \frac{1}{N} \sum_{1 \leq i \leq N} \delta_{\xi_n^i}$

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- ▶ Normalizing constants

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$$\gamma_n = \mathcal{Z}_n \times \eta_n \simeq_{N \uparrow \infty} \gamma_n^{\textcolor{red}{N}} = \mathcal{Z}_n^{\textcolor{red}{N}} \times \eta_n^{\textcolor{red}{N}} \quad (\text{Unbiased})$$

# Important observation

## Exponential rate of the normalizing constants

$$\frac{1}{n} \log \mathcal{Z}_n = \frac{1}{n} \sum_{0 \leq p < n} \log \eta_p(G_p) \simeq \frac{1}{n} \log \mathcal{Z}_n^N = \frac{1}{n} \sum_{0 \leq p < n} \log \eta_p^N(G_p)$$

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Time homogeneous models  $(G_n, M_n) = (G, M)$ :

Link to the long time behavior of  $\eta_n$  and/or  $\eta_n^N$

$$\frac{1}{n} \log \mathcal{Z}_n \xrightarrow{n \uparrow \infty} \log \eta_\infty(G) \simeq_{N \uparrow \infty} \log \eta_\infty^N(G) \xleftarrow{n \uparrow \infty} \frac{1}{n} \log \mathcal{Z}_n^N$$

Introduction

Absorption models

Extended path integration models

Feynman-Kac models

## Stochastic analysis

Stability and contraction properties

Uniform concentration inequalities

Coalescent tree based expansions

Ground states and  $h$ -processes

Som derivation properties

Backward particle models

How & Why it works

Continuous time models

# Long time behavior of the FK-sg $\Phi_{p,n}(\eta_p) = \eta_n$

## Theorem:

- $M_n$ -mixing conditions and  $G_n$  unif. lower-upper bounded
- or  $\widehat{M}_n$ -mixing conditions and  $\widehat{G}_n$  unif. lower-upper bounded

$$\widehat{G}_n(x) \widehat{M}_{n+1}(x, dy) = M_{n+1}(G_{n+1})(x) \times \frac{M_{n+1}(x, dy) G_{n+1}(y)}{M_{n+1}(G_{n+1})(x)}$$

↓

$$\exists(a, b) \in \mathbb{R}_+ \quad \sup_{\mu_1, \mu_2} \|\Phi_{p,n}(\mu_1) - \Phi_{p,n}(\mu_2)\|_{\text{tv}} \leq a e^{-b(n-p)}$$

$$\beta(P_{p,n}) := \sup_{\mu_1, \mu_2} \|\Phi_{p,n}(\mu_1) - \Phi_{p,n}(\mu_2)\|_{\text{tv}}$$

*with the Dobrushin ergodic coefficient of the Markov transition*

$$P_{p,n}(x, dy) = \mathbb{P}_{p,x} (X_n^c \in dy)$$

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$$P_{p,n}(x, dy) = \mathbb{P}_{p,x} (X_n^c \in dy) = \left( R_{p+1}^{(n)} R_{p+2}^{(n)} \dots R_n^{(n)} \right) (x, dy)$$

and the non absorption transitions (for absorption type models)

$$R_{p+1}^{(n)}(x, dy) = \mathbb{P}_{p,x} (X_{p+1}^c \in dy \mid X_p^c = x, T \geq n)$$

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**Example :**

$$\begin{aligned} \epsilon \nu(dy) &\leq M(x, dy) \leq \epsilon^{-1} \nu(dy) \Rightarrow R_{p+1}^{(n)}(x, dy) \geq \epsilon^2 \nu_{p,n}(dy) \\ &\Rightarrow \beta \left( R_{p+1}^{(n)} \right) \leq (1 - \epsilon^2) \\ &\Rightarrow \beta(P_{p,n}) \leq (1 - \epsilon^2)^{(n-p)} \end{aligned}$$

$$\beta(P_{p,n}) := \sup_{\mu_1, \mu_2} \|\Phi_{p,n}(\mu_1) - \Phi_{p,n}(\mu_2)\|_{\text{tv}}$$

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~~~ nice extensions/characterizations of exponential stability  
by N. Champagnat & D. Villemonais

# Time homogeneous models $\Phi_{p,n} = \Phi^{(n-p)}$

**Corollary:**

$$\exists! \eta_\infty = \Phi(\eta_\infty) \quad \text{and} \quad \left\| \Phi^{(n)}(\mu_1) - \Phi^{(n)}(\eta_\infty) \right\|_{\text{tv}} \leq a e^{-b n}$$

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$$\frac{1}{n} \log \mathbb{P}(T^{\text{absorption}} > n) = \log \eta_\infty(G) + O\left(\frac{1}{n}\right)$$

Some hyper-references [▷ Continuous time models; ex.: non degenerate diffusion ⊂ compact]

- ▶ Branching and interacting particle systems. (with L. Miclo) Sémin. Proba. de Strasbourg (2000).
- ▶ On the stability of interacting processes (with A. Guionnet) IHP (2001).
- ▶ On the Stability of Feynman-Kac sg. (with L. Miclo) Annales de la Fac. Sci. Toulouse (2002)
- ▶ Particle Lyapunov exponents connected to Schrödinger op. (with L. Miclo) ESAIM PS (2003).
- ▶ Particle Motions in Absorbing Medium with Hard and Soft Obst. (with A. Doucet) SAA (2004).
- ▶ Feynman-Kac formulae, Genealogical & Interacting Particle Systems, Springer (2004).

## Some consequences

Cts  $(c, c_1, c_2) \sim (\text{bias}, \text{variance}, a, b)$ ,  $\|f_n\| \leq 1$ ,  $\forall (x \geq 0, n \geq 0, N \geq 1)$ .

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$$|\frac{1}{n} \log \mathcal{Z}_n^N - \log \eta_\infty(G)| \leq \frac{c}{n} + \frac{c_1}{N} (1 + x + \sqrt{x}) + \frac{c_2}{\sqrt{N}} \sqrt{x}$$

# Coalescent tree based expansions

## Weak propagation of chaos Taylor's type expansions

$$\begin{aligned}\mathbb{P}^{(N,q)} &= \text{Law of the first } q \leq N \text{ ancestral lines} \\ &= \mathbb{Q}^{\otimes q} + \sum_{1 \leq l \leq m} \frac{1}{N^l} d_l \mathbb{P}_n^{(q)} + O\left(\frac{1}{N^{m+1}}\right)\end{aligned}$$

with signed measures  $d_l \mathbb{P}_n^{(q)}$  expressed in terms of *l-coalescent trees*.

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**Romberg-Richardson interpolation:** For any order  $l \geq 1$

$$\sum_{1 \leq m \leq l} \frac{(-1)^{l-m}}{m!} \frac{m^l}{(l-m)!} \mathbb{P}^{(mN,q)} = \mathbb{Q}^{\otimes q} + O\left(\frac{1}{N^l}\right)$$

### Some hyper-references

- ▶ Coalescent tree based functional representations for some Feynman-Kac particle models (with F. Patras, S. Rubenthaler) AAP (2009)
- ▶ U-statistics for interacting particle systems (with F. Patras, S. Rubenthaler) JTP (2011).

## Time homogeneous models $(G_n, M_n) = (G, M)$

$$Q(x, dy) = G(y) M(x, dy) \quad \text{with} \quad G(x) \leq 1 \quad (\rightsquigarrow \text{Sub-Markov})$$

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- ▶ Reversibility condition :  $\mu(dx)M(x, dy) = \mu(dy)M(y, dx)$

$$\frac{1}{n} \log \mathbb{P}(T^{\text{absorption}} \geq n) = \frac{1}{n} \sum_{0 \leq p < n} \log \eta_p(G) \simeq \log \lambda = \log \eta_\infty(G)$$

with  $\lambda = \text{top eigenvalue of}$

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- ▶  $Q(h) = \lambda h \rightsquigarrow \text{Doob } h\text{-process } X^h$

$$M^h(x, dy) = \frac{1}{\lambda} h^{-1}(x) Q(x, dy) h(y) = \frac{Q(x, dy) h(y)}{Q(h)(x)} = \frac{M(x, dy) h(y)}{M(h)(x)}$$

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$$\mathbb{Q}_n(d(x_0, \dots, x_n)) \propto \mathbb{P}((X_0^h, \dots, X_n^h) \in d(x_0, \dots, x_n)) h^{-1}(x_n)$$

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- *Invariant measure  $\mu_h = \mu_h M^h$  & normalized additive functionals*

$$\bar{F}_n(x_0, \dots, x_n) = \frac{1}{n+1} \sum_{0 \leq p \leq n} f(x_p) \implies \mathbb{Q}_n(\bar{F}_n) \simeq_n \mu_h(f)$$

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- If  $G = G^\theta$  depends on some  $\theta \in \mathbb{R}$   $\rightsquigarrow f := \frac{\partial}{\partial \theta} \log G^\theta$

$$\underbrace{\frac{\partial}{\partial \theta} \log \lambda^\theta}_{\text{derivation}} \simeq_n \frac{1}{n+1} \underbrace{\frac{\partial}{\partial \theta} \log \mathcal{Z}_{n+1}^\theta}_{\text{path-integration}} = \underbrace{\mathbb{Q}_n(\bar{F}_n)}_{\text{path-integration}}$$

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NB : Similar expression when  $M^\theta$  depends on some  $\theta \in \mathbb{R}$ .

# The last key

- ▶ Backward Markov models

$$\mathbb{Q}_n(dx_0, \dots, dx_n) \propto \eta_0(dx_0) Q_1(x_0, dx_1) \dots Q_n(x_{n-1}, dx_n)$$

with

$$\begin{aligned} Q_n(x_{n-1}, dx_n) &:= G_{n-1}(x_{n-1}) M_n(x_{n-1}, dx_n) \\ &\stackrel{\textcolor{red}{hyp}}{=} H_n(x_{n-1}, x_n) \nu_n(dx_n) \end{aligned}$$

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If we set

$$\mathbb{M}_{n+1, \eta_n}(x_{n+1}, dx_n) = \frac{\eta_n(dx_n) H_{n+1}(x_n, x_{n+1})}{\eta_n(H_{n+1}(\cdot, x_{n+1}))}$$

then we find the backward equation

$$\eta_{n+1}(dx_{n+1}) \mathbb{M}_{n+1, \eta_n}(x_{n+1}, dx_n) = \frac{1}{\eta_n(G_n)} \eta_n(dx_n) Q_{n+1}(x_n, dx_{n+1})$$

## The last key (continued)

$$\mathbb{Q}_n(d(x_0, \dots, x_n)) \propto \eta_0(dx_0) Q_1(x_0, dx_1) \dots Q_n(x_{n-1}, dx_n)$$

$\oplus$

$$\eta_{n+1}(dx_{n+1}) \mathbb{M}_{n+1, \eta_n}(x_{n+1}, dx_n) \propto \eta_n(dx_n) Q_{n+1}(x_n, dx_{n+1})$$

# The last key (continued)

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⊕

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⇓

Backward Markov chain model :

$$\mathbb{Q}_n(d(x_0, \dots, x_n)) = \eta_n(dx_n) \mathbb{M}_{n, \eta_{n-1}}(x_n, dx_{n-1}) \dots \mathbb{M}_{1, \eta_0}(x_1, dx_0)$$

with the dual/backward Markov transitions

$$\mathbb{M}_{n+1, \eta_n}(x_{n+1}, dx_n) \propto \eta_n(dx_n) H_{n+1}(x_n, x_{n+1})$$

# How to use the full ancestral tree model ?

$$\mathbb{Q}_n(dx_0, \dots, dx_n) = \eta_n(dx_n) \underbrace{\mathbb{M}_{n,\eta_{n-1}}(x_n, dx_{n-1})}_{\propto \eta_{n-1}(dx_{n-1}) H_n(x_{n-1}, x_n)} \dots \mathbb{M}_{1,\eta_0}(x_1, dx_0)$$

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Particle approximation

$$\mathbb{Q}_n^N(d(x_0, \dots, x_n)) = \eta_n^N(dx_n) \mathbb{M}_{n, \eta_{n-1}^N}(x_n, dx_{n-1}) \dots \mathbb{M}_{1, \eta_0^N}(x_1, dx_0)$$

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## Particle approximation

$$\mathbb{Q}_n^N(d(x_0, \dots, x_n)) = \eta_n^N(dx_n) \mathbb{M}_{n, \eta_{n-1}^N}(x_n, dx_{n-1}) \dots \mathbb{M}_{1, \eta_0^N}(x_1, dx_0)$$

Ex.: *Additive functionals*       $\mathbf{f}_n(x_0, \dots, x_n) = \frac{1}{n+1} \sum_{0 \leq p \leq n} f_p(x_p)$

$$\underbrace{\mathbb{Q}_n^N(\mathbf{f}_n)}_{\text{path-integration}} := \frac{1}{n+1} \sum_{0 \leq p \leq n} \eta_n^N \underbrace{\mathbb{M}_{n, \eta_{n-1}^N} \dots \mathbb{M}_{p+1, \eta_p^N}(f_p)}_{\text{recursive matrix operations}}$$

## Backward particle models

Cts ( $c_1, c_2$ ) related to (bias, variance, a, b)  $\mathbf{f}_n$  normalized additive functional with  $\|f_p\| \leq 1$ ,  $\forall (x \geq 0, n \geq 0, N \geq 1)$



The probability of the event

$$[\mathbb{Q}_n^N - \mathbb{Q}_n](\bar{\mathbf{f}}_n) \leq c_1 \frac{1}{N} (1 + (x + \sqrt{x})) + c_2 \sqrt{\frac{x}{N(n+1)}}$$

is greater than  $1 - e^{-x}$ .

Introduction

Absorption models

Extended path integration models

Feynman-Kac models

Stochastic analysis

## How & Why it works

A local fluctuation theorem

Second order decompositions

Uniform concentration w.r.t. time

Particle free energy expansions

Continuous time models

# How & Why it works (general mean field models)

- ▶ (Computer Sci.) Stochastic adaptive grid approximation.

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~~> New concentration inequalities for (general) interacting processes

# A stochastic perturbation analysis

Key telescoping decomposition

$$\eta_n^N - \eta_n = \sum_{p=0}^n [\Phi_{p,n}(\eta_p^N) - \Phi_{p,n}(\Phi_p(\eta_{p-1}^N))]$$

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⊕ First order expansion

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with  $\underbrace{\text{a predictable } D_{p,n} - \text{first order operator}}_{\text{fluctuation term}} \oplus \underbrace{\text{2nd-order measure } R_{p,n}^N}_{\text{bias-term}}$

# Uniform concentration w.r.t. time

Stochastic perturbation model

$$W_n^{\eta, N} := \sqrt{N} [\eta_n^N - \eta_n] = \sum_{0 \leq p \leq n} V_p^N D_{p,n} + \frac{1}{\sqrt{N}} R_n^N$$

Under some mixing condition on the limiting FK semigroups  $\Phi_{p,n}$

$$\text{osc}(D_{p,n}(f)) \leq Cte e^{-(n-p)\alpha}$$

and

$$\mathbb{E}(|R_n^N(f)|^m) \leq Cte 2^{-m} (2m)! / m!$$

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Uniform concentration estimates w.r.t. the time parameter

# Particle free energy expansions

## Multiplicative formulae

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

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## Taylor first order expansion

$$\forall x, y > 0 \quad \log y - \log x = \int_0^1 \frac{(y-x)}{x+t(y-x)} dt$$

⇓

$$\log (\gamma_n^N(1)/\gamma_n(1))$$

$$= \sum_{0 \leq p < n} (\log \eta_p^N(G_p) - \log \eta_p(G_p))$$

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$$= \sum_{0 \leq p < n} \left( \log \left( \eta_p(G_p) + \frac{1}{\sqrt{N}} W_p^{\eta, N}(G_p) \right) - \log \eta_p(G_p) \right)$$

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$$= \frac{1}{\sqrt{N}} \sum_{0 \leq p < n} \int_0^1 \frac{W_p^{\eta, N}(G_p)}{\eta_p(G_p) + \frac{t}{\sqrt{N}} W_p^{\eta, N}(G_p)} dt$$

~ first order expansion [exercice]

Introduction

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How & Why it works

## Continuous time models

Discrete time formulations

Fully continuous time models

Some examples of McKean models

## ▷ Continuous time models

- ▶ ▷ Continuous time models with  $X_n := X'_{[t_n, t_{n+1}[}$

$$G_n(X_n) = \exp \int_{t_n}^{t_{n+1}} V_s(X'_s) ds$$

or

$$G_n(X_n) = \exp \int_{t_n}^{t_{n+1}} [V_s^1(X'_s) dW_s + V_s^2(X'_s) ds]$$

- ▶ ▷ Euler style approximations

# Fully continuous time Feynman-Kac models

$$d\mathbb{Q}_t := \frac{1}{Z_t} \exp \left\{ \int_0^t V_s(X_s) ds \right\} d\mathbb{P}_t \quad \text{with} \quad \mathbb{P}_n = \text{Law}(X_{[0,t]})$$

and

$$Z_t = \mathbb{E} \left( \exp \int_0^t V_s(X_s) ds \right)$$

$\eta_t$  =  $t$ -marginal measures of  $\mathbb{Q}_t$  and the unnormalized  $\gamma_t = Z_t \times \eta_t$



**Key formula:**  $\frac{1}{t} \log Z_t = \frac{1}{t} \int_0^t \eta_s(V_s) ds$

$\Downarrow$  ( $L_t$  = generator of  $X_t$ )

$$\frac{d}{dt} \gamma_t(f) = \gamma_t(L_t^V(f)) \quad \text{with} \quad L_t^V = L_t + V_t$$

$$\frac{d}{dt} \eta_t(f) = \eta_t(L_{t,\eta_t}(f)) \quad \text{with} \quad L_{t,\eta_t} = L_t + V_t - \eta_t(V_t)$$

Example :  $V_t = -U \leq 0$  and  $L_t = L$

**Absorption model**  $E^c = E \cup \{c\}$ :

$$L^V(f)(x) = L(f)(x) + \underbrace{U(x)}_{\text{absorption rate}} \int (f(y) - f(x)) \delta_c(dy)$$

**Interacting jump generator**

$$L_{\eta_t}(f)(x) = \underbrace{L(f)(x)}_{\text{free exploration}} + \underbrace{U(x)}_{\text{acceptance/jump rate}} \int (f(y) - f(x)) \underbrace{\eta_t(dy)}_{\text{interacting jump law}}$$



**Particle model when**  $\eta_t \simeq \eta_t^N = \frac{1}{N} \sum_{1 \leq i \leq N} \delta_{\xi_t^i}$

Survival-acceptance rates  $\oplus$  Interacting-recycling jumps

## Other examples (non uniqueness of McKean models)

$V_t = U > 0$  and  $L_t = L$  Interacting jump generator

$$L_{\eta_t}(f)(x) = \underbrace{L(f)(x)}_{\text{free exploration}} + \underbrace{\eta_t(U)}_{\text{acceptance/jump rate}} \int (f(y) - f(x)) \underbrace{\Psi_{U_t}(\eta_t)(dy)}_{\text{interacting jump law}}$$

$\forall V_t$  and  $L_t = L$  Interacting jump generator

$$L_{\eta_t}(f)(x) = \underbrace{L(f)(x)}_{\text{free exploration}} + \underbrace{\eta_t((V - V(x))_+)}_{\text{acceptance/jump rate}} \int (f(y) - f(x)) \underbrace{\Psi_{(V-V(x))_+}(\eta_t)(dy)}_{\text{interacting jump law}}$$

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$$L_{\eta_t}(f)(x) = \underbrace{L(f)(x)}_{\text{free exploration}} + \underbrace{\eta_t((V - V(x))_+)}_{\text{acceptance/jump rate}} \int (f(y) - f(x)) \underbrace{\Psi_{(V-V(x))_+}(\eta_t)(dy)}_{\text{interacting jump law}}$$

In all cases, in practice we work with the discrete time models

- Geometric clocks (discrete time)  $\rightsquigarrow$  Poisson interacting jump rates (continuous time)

Feynman-Kac particle integration with geometric interacting jumps (with P. Jacob, A. Lee, L. Murray, G.W. Peters). ArXiv preprint arXiv:1211.7191 (2012).