

Stochastic particle methods in Bayesian statistical learning

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INRIA & Bordeaux Mathematical Institute & X CMAP

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Some hyper-refs

- ▶ Feynman-Kac formulae, Genealogical & Interacting Particle Systems with appl., Springer (2004)
- ▶ Sequential Monte Carlo Samplers JRSS B. (2006). (joint work with Doucet & Jasra)
- ▶ On the concentration of interacting processes Hal-inria (2011). (joint work with Hu & Wu) [+ Refs]
- ▶ More references on the website <http://www.math.u-bordeaux1.fr/~delmoral/index.html> [+ Links]

Stochastic particle sampling methods

Interacting jumps models

Genetic type interacting particle models

Particle Feynman-Kac models

The 4 particle estimates

Island particle models (\subset Parallel Computing)

Bayesian statistical learning

Nonlinear filtering models

Fixed parameter estimation in HMM models

Particle stochastic gradient models

Approximate Bayesian Computation

Interacting Kalman-Filters

Uncertainty propagations in numerical codes

Concentration inequalities

Current population models

Particle free energy

Genealogical tree models

Backward particle models

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Introduction

Stochastic particle methods
=
Universal adaptive sampling technique

2 types of stochastic interacting particle models:

- ▶ Diffusive particle models with mean field drifts
[McKean-Vlasov style] \longleftrightarrow *Fluid mechanics*

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2 types of stochastic interacting particle models:

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[McKean-Vlasov style] \longleftrightarrow *Fluid mechanics*
- ▶ Interacting jump particle models
[Boltzmann & Feynman-Kac style]
 \longleftrightarrow *Fluid mech. & Physics + Biology + Engineering + Statistics*

Lectures ⊂ Interacting jumps models

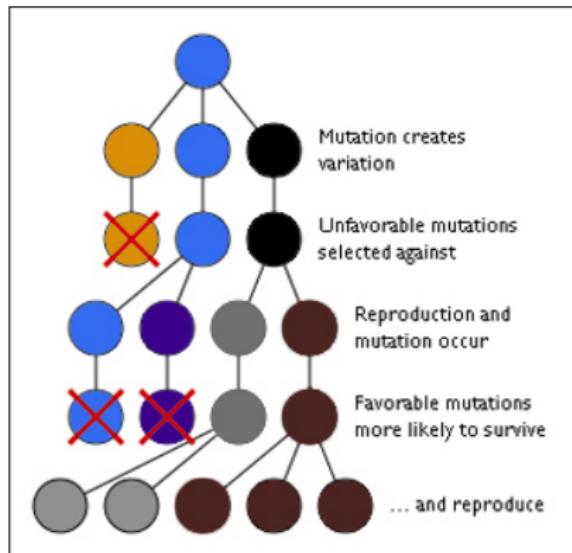


- ▶ Interacting jumps = Recycling transitions =
- ▶ Discrete time models (\Leftrightarrow geometric rejection/jump times)



Genetic type interacting particle models

- ▶ Mutation-Proposals w.r.t. Markov transitions $X_{n-1} \rightsquigarrow X_n \in E_n$.
- ▶ Selection-Rejection-Recycling w.r.t. potential/fitness function G_n .



Equivalent particle algorithms

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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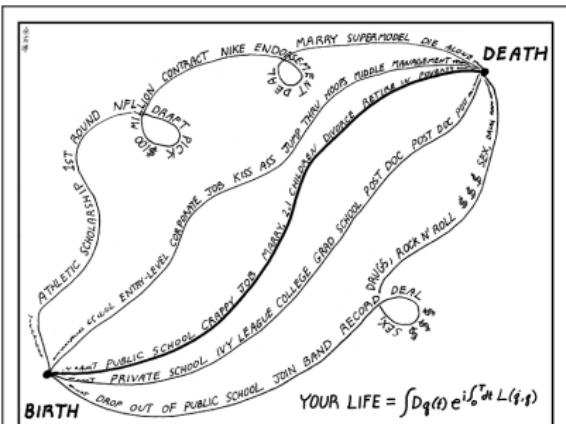
More botanical names:

bootstrapping, spawning, cloning, pruning, replenish, multi-level splitting,
enrichment, go with the winner, ...

$1950 \leq$ Meta-Heuristic style stochastic algorithms ≤ 1996

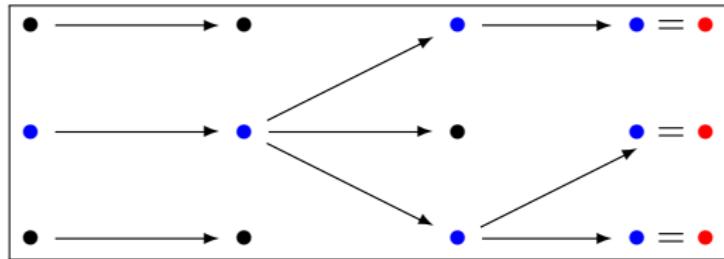
A single stochastic model

Particle interpretation of Feynman-Kac path integrals

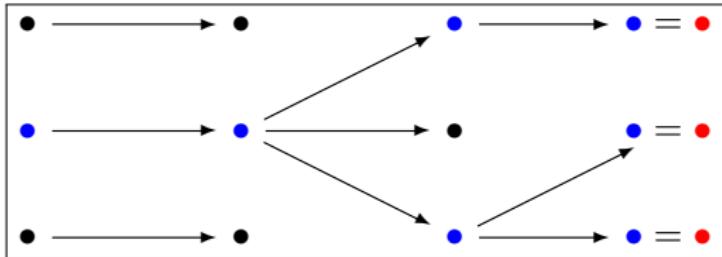


The Path Integral Formulation of Your Life

Genealogical tree evolution (size,time)=(N, n) = (3, 3)



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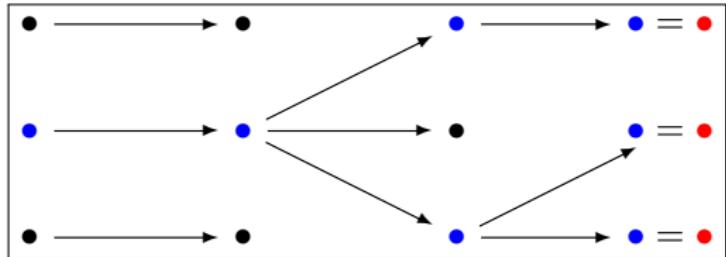


Meta-heuristics \rightsquigarrow "96' Meta-Theorem" :

Ancestral lines \simeq i.i.d. path samples w.r.t. Feynman-Kac measure

$$\mathbb{Q}_n := \frac{1}{\mathcal{Z}_n} \left\{ \prod_{0 \leq p < n} G_p(X_p) \right\} \mathbb{P}_n \quad \text{with} \quad \mathbb{P}_n := \text{Law}(X_0, \dots, X_n)$$

Genealogical tree evolution (size,time)=(N, n) = (3, 3)



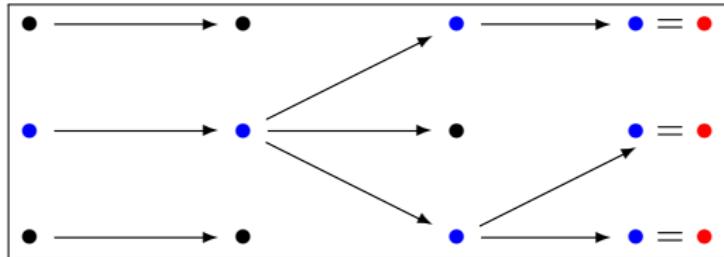
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& Inversely!

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& Inversely! \rightsquigarrow example

$$\mathbb{Q}_n = \text{Law}((X_0, \dots, X_n) \mid X_p \in A_p, \ p < n) \iff G_n = 1_{A_n}$$

Particle estimates

More formally

$(\xi_{0,n}^i, \xi_{1,n}^i, \dots, \xi_{n,n}^i) := i\text{-th ancestral line of the } i\text{-th current individual} = \xi_n^i$



$$\frac{1}{N} \sum_{1 \leq i \leq N} \delta_{(\xi_{0,n}^i, \xi_{1,n}^i, \dots, \xi_{n,n}^i)} \xrightarrow{N \rightarrow \infty} \mathbb{Q}_n$$

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⊕ Current population models

$$\eta_n^N := \frac{1}{N} \sum_{1 \leq i \leq N} \delta_{\xi_n^i} \xrightarrow{N \rightarrow \infty} \eta_n = n\text{-th time marginal of } \mathbb{Q}_n$$

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⊕ Unbiased particle approximation

$$\mathcal{Z}_n^N = \prod_{0 \leq p < n} \eta_p^N(G_p) \xrightarrow{N \rightarrow \infty} \mathcal{Z}_n = \mathbb{E} \left(\prod_{0 \leq p < n} G_p(X_p) \right) = \prod_{0 \leq p < n} \eta_p(G_p)$$

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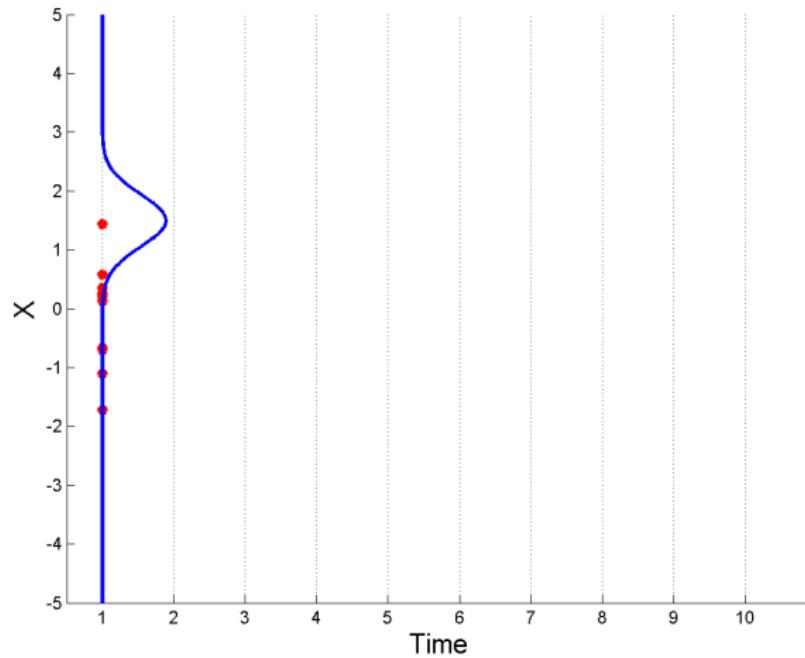
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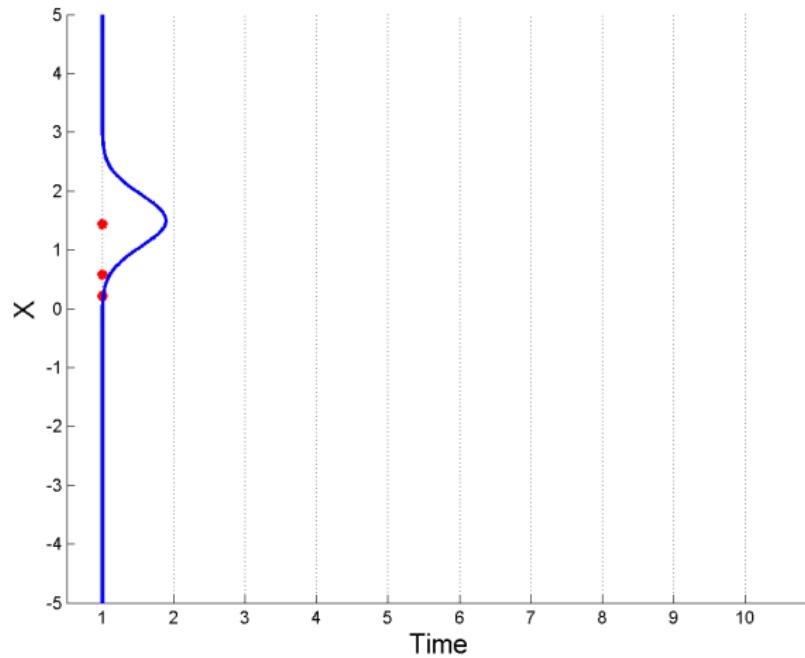
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Ex.: $G_p = 1_{A_p} \rightsquigarrow \mathcal{Z}_n^N = \prod \text{proportion of success} \longrightarrow \mathbb{P}(X_p \in A_p, p < n)$

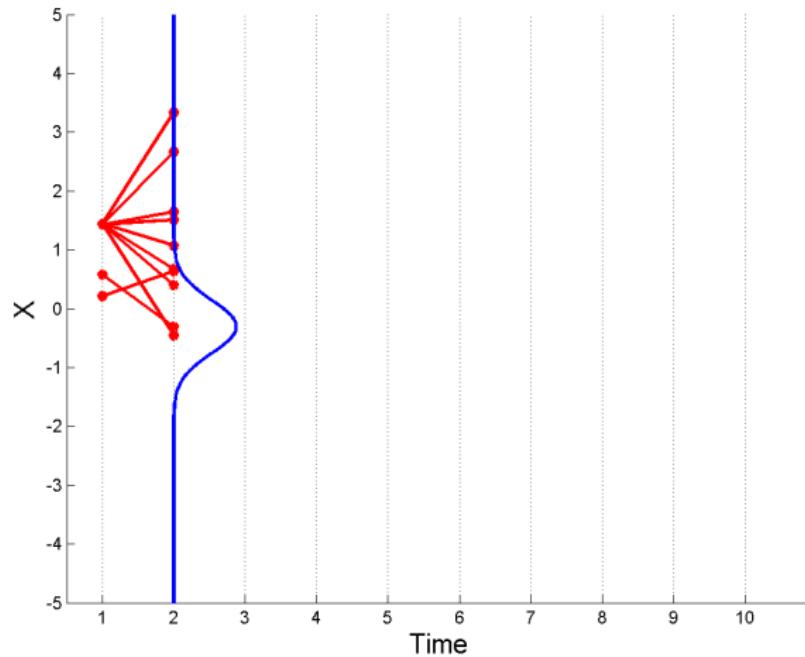
Graphical illustration : $\eta_n^N := \frac{1}{N} \sum_{1 \leq i \leq N} \delta_{\xi_i} \simeq \eta_n$



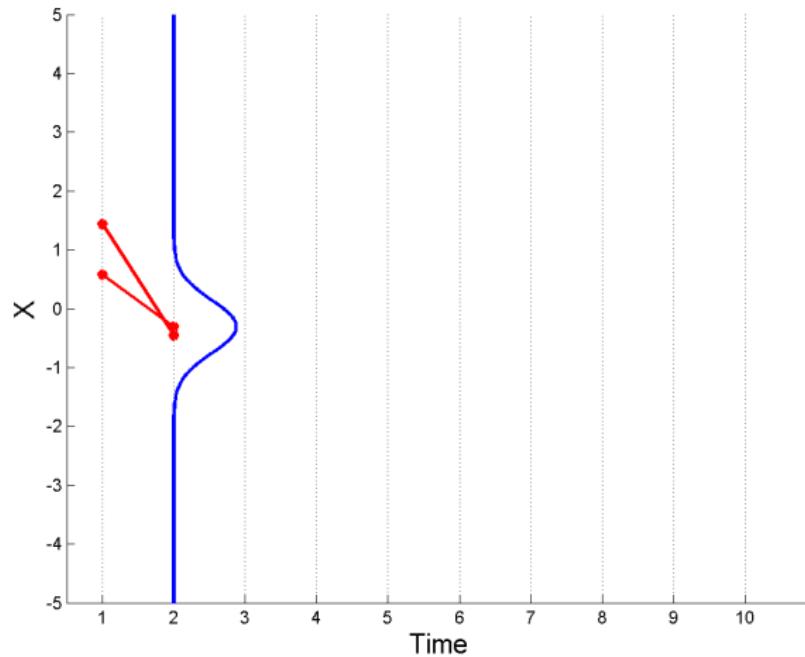
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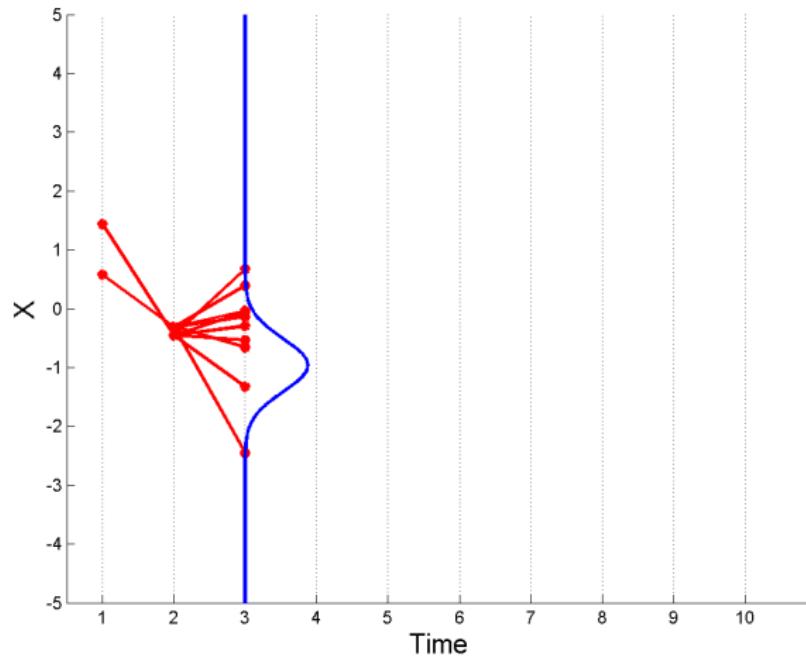
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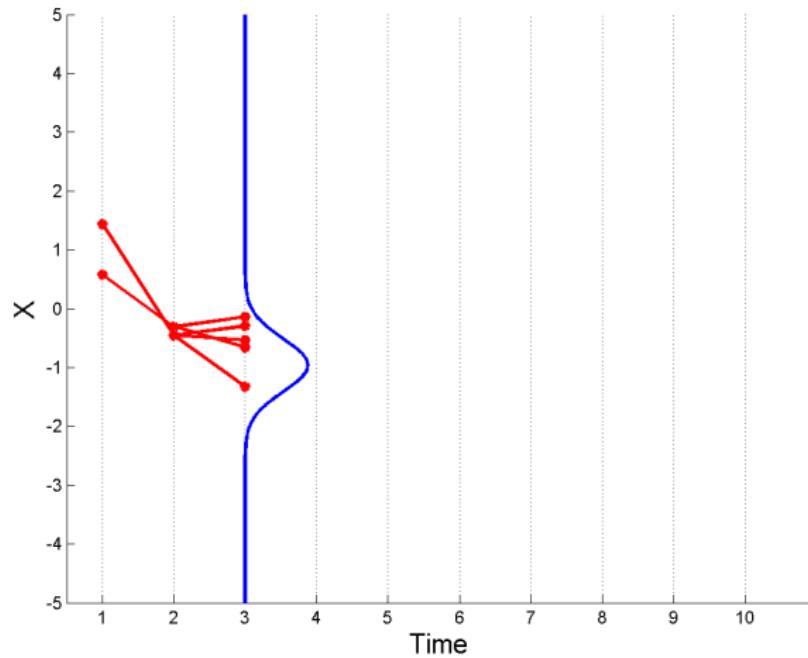
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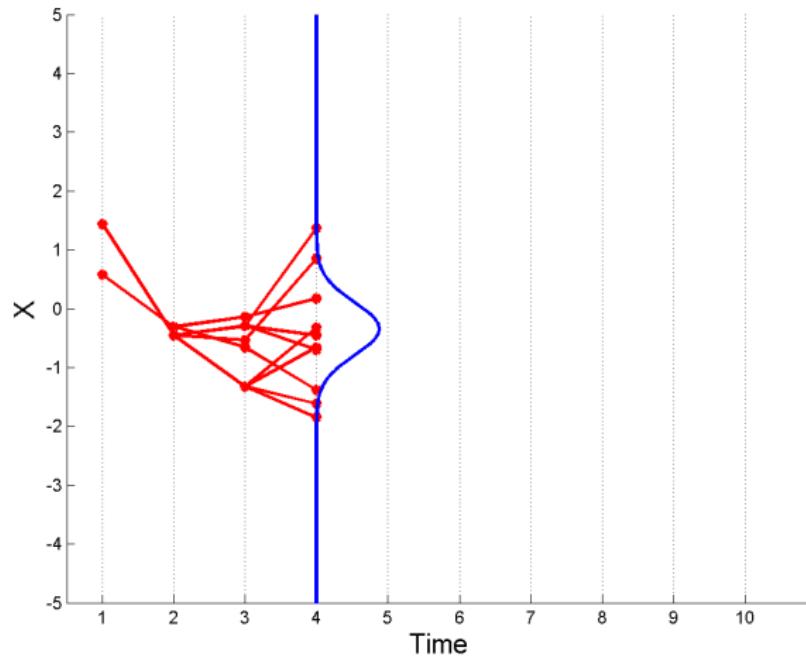
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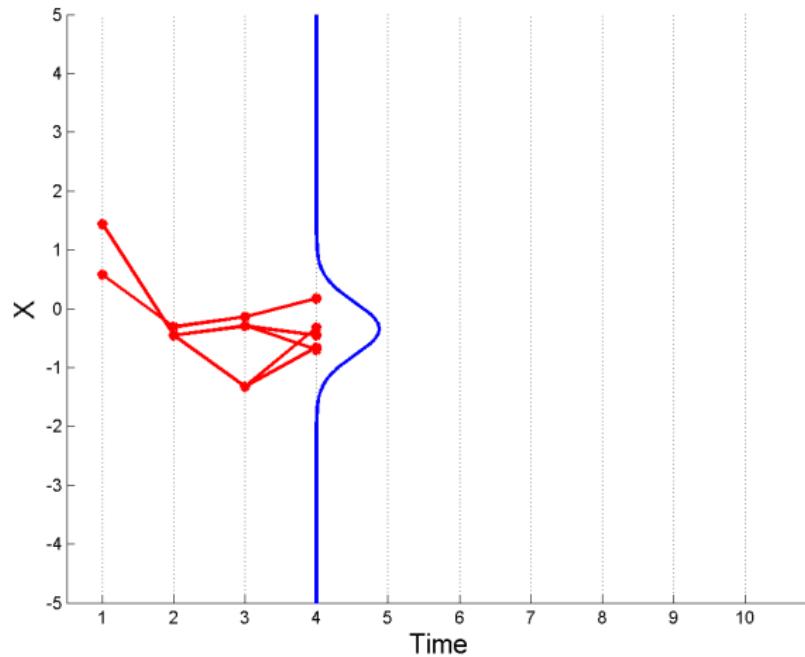
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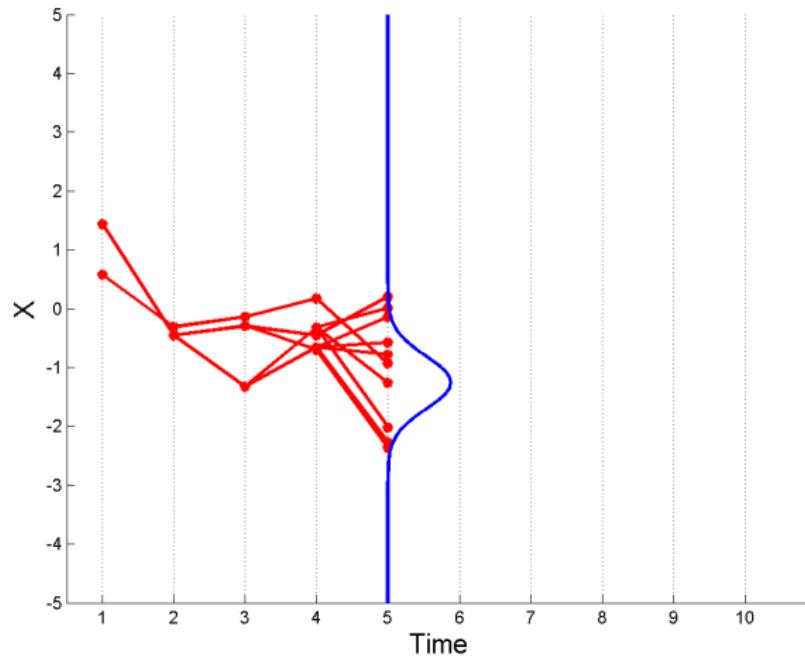
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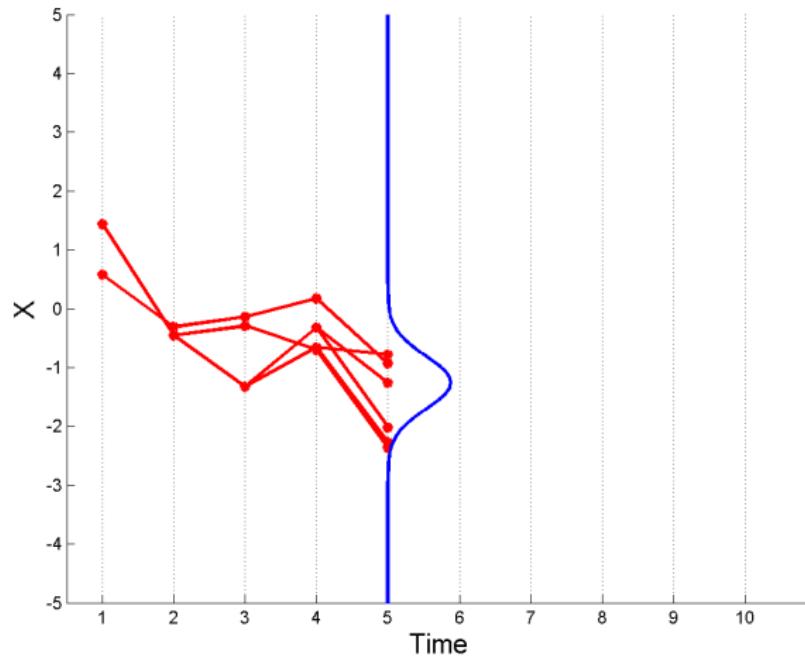
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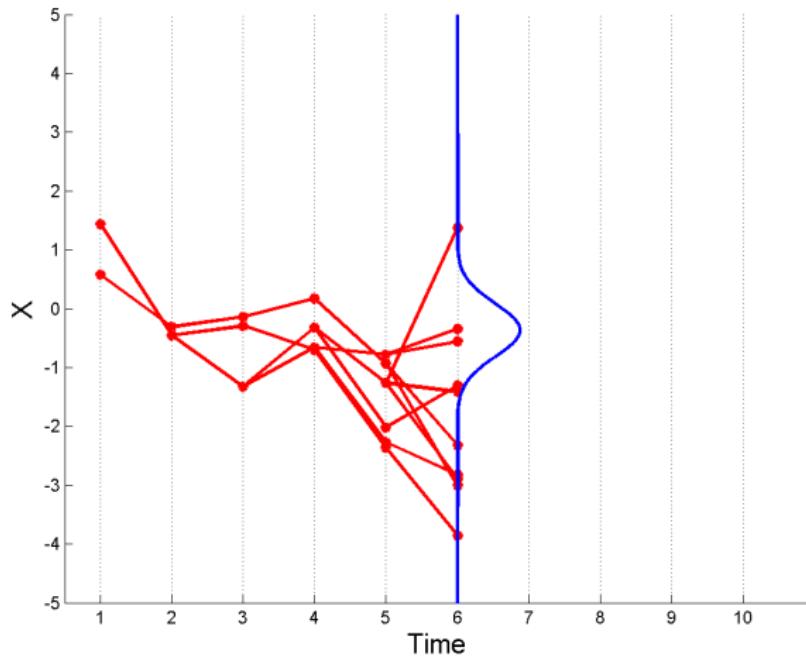
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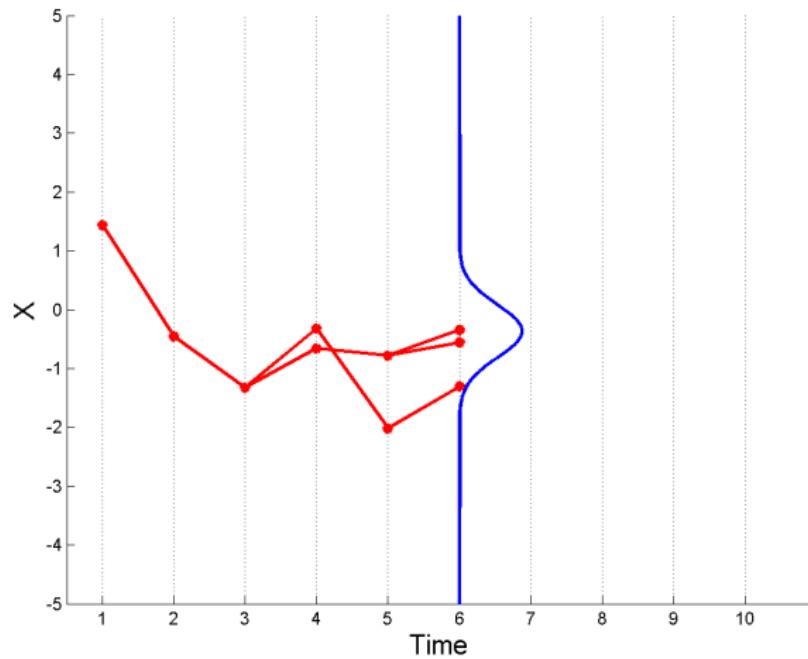
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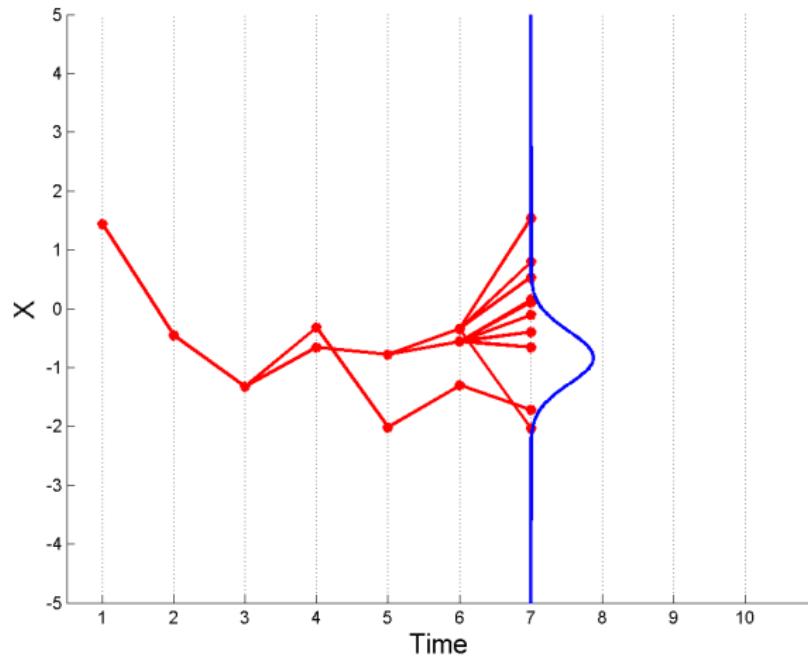
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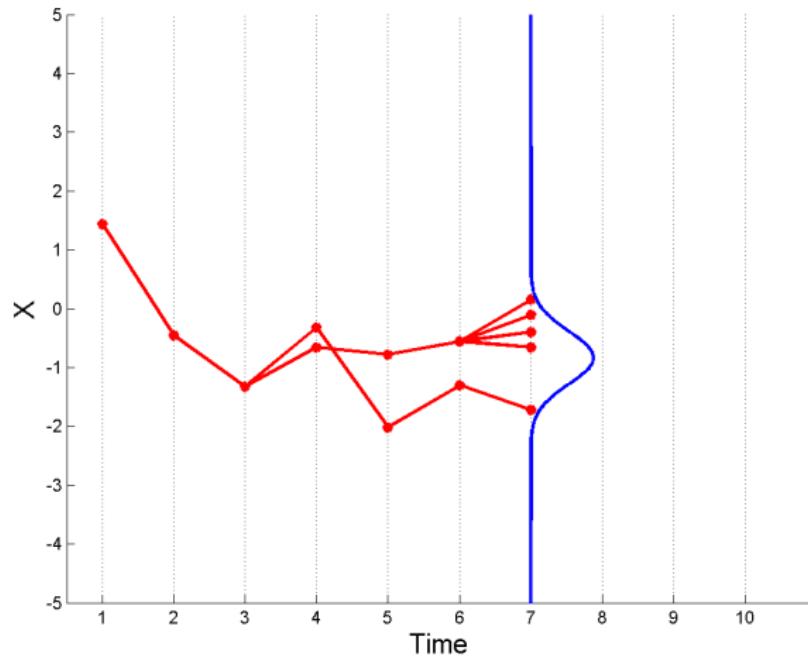
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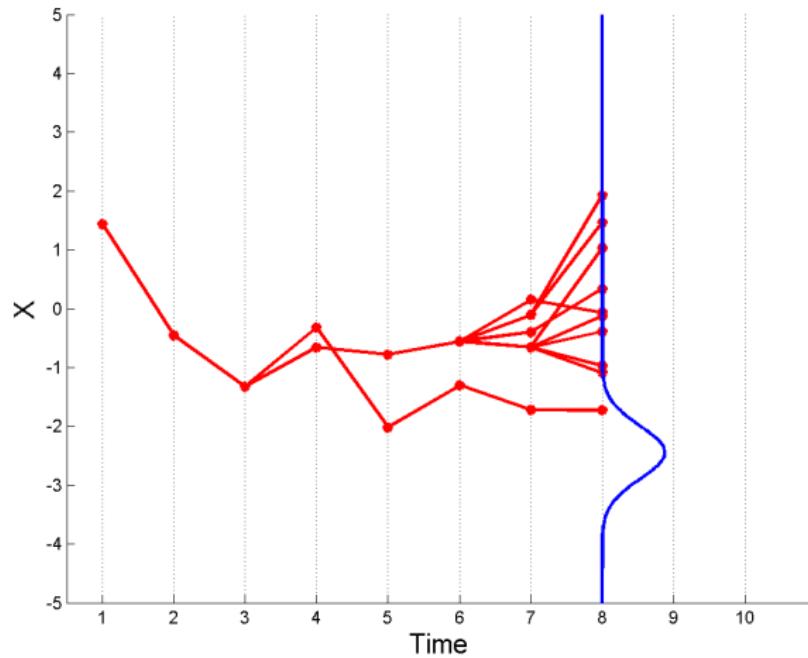
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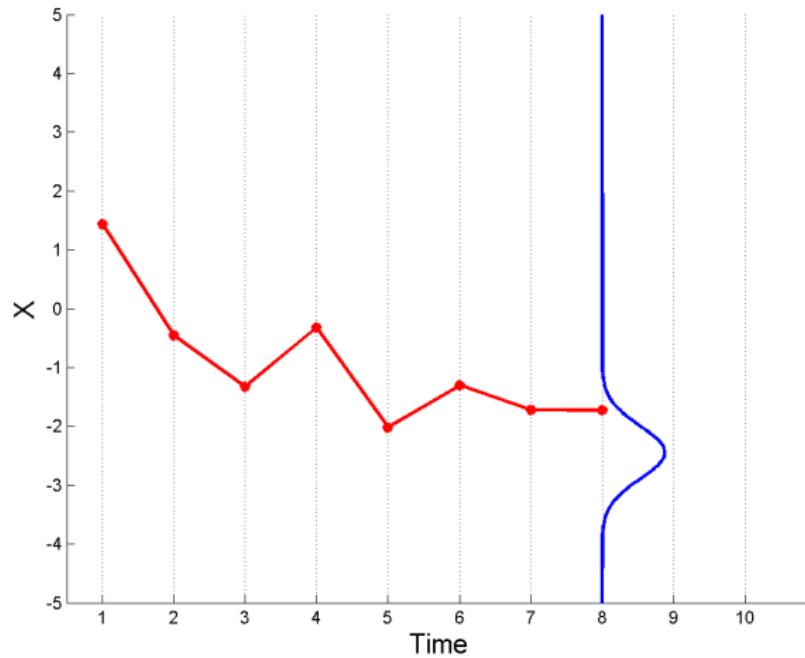
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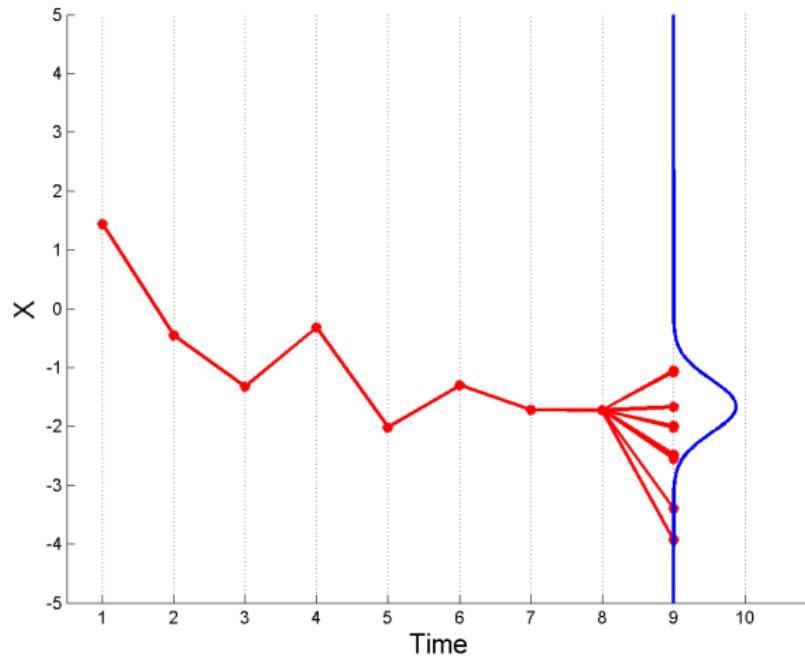
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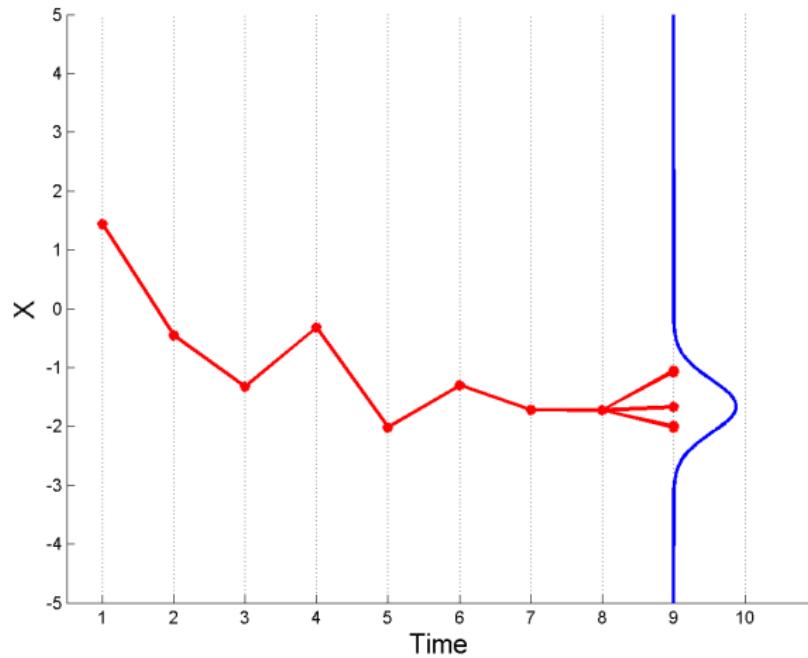
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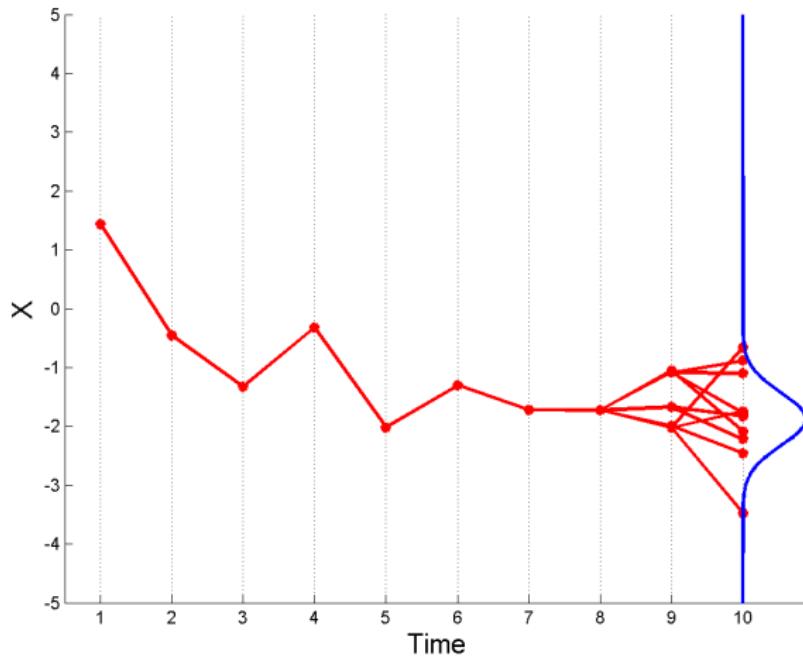
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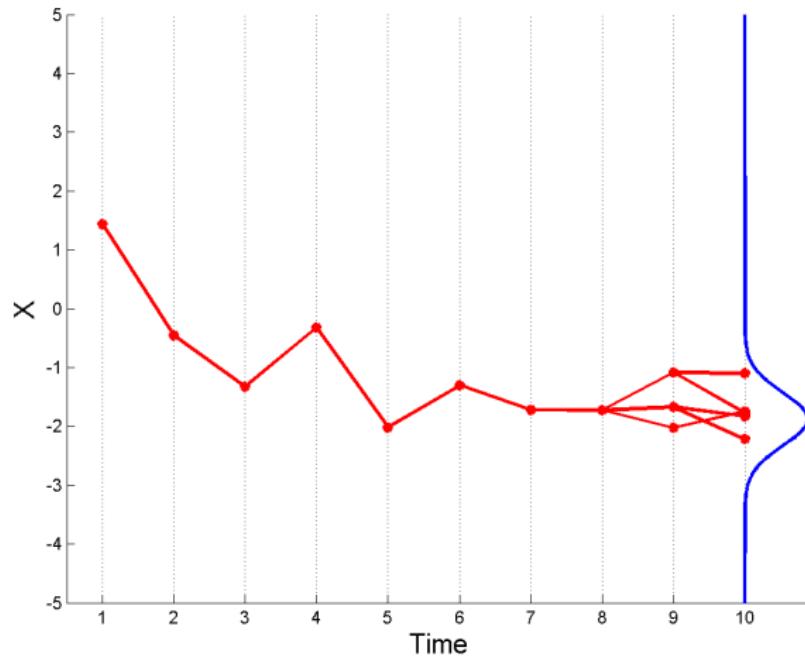
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Complete ancestral tree when $G_{n-1}(x)M_n(x, dy) = H_n(x, y) \lambda(dy)$

Backward Markov chain model

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

with the random particle matrices:

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

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Example: Normalized additive functionals

$$f_n(x_0, \dots, x_n) = \frac{1}{n+1} \sum_{0 \leq p \leq n} f_p(x_p)$$



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

Island models (\subset Parallel Computing)

Reminder : the unbiased property

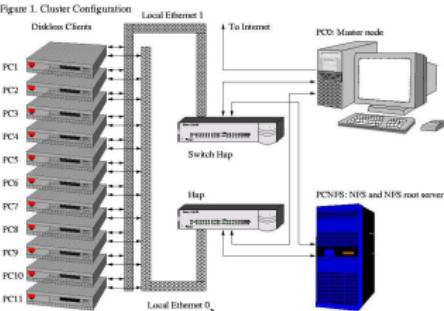
$$\begin{aligned}\mathbb{E} \left(f_n(\mathbf{X}_n) \prod_{0 \leq p < n} G_p(\mathbf{X}_p) \right) &= \mathbb{E} \left(\eta_n^N(f_n) \prod_{0 \leq p < n} \eta_p^N(G_p) \right) \\ &= \mathbb{E} \left(F_n(\mathcal{X}_n) \prod_{0 \leq p < n} G_p(\mathcal{X}_p) \right)\end{aligned}$$

with the Island evolution Markov chain model

$$\mathcal{X}_n := \eta_n^N \quad \text{and} \quad G_n(\mathcal{X}_n) = \eta_n^N(\mathbf{G}_n) = \mathcal{X}_n(\mathbf{G}_n)$$



particle model with $(\mathcal{X}_n, G_n(\mathcal{X}_n)) = \text{Interacting Island particle model}$



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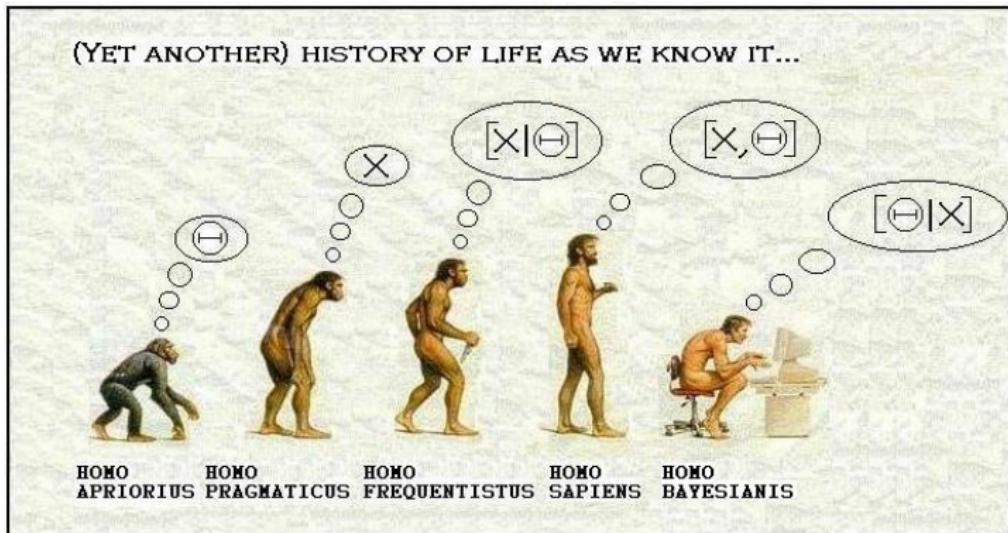
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Bayesian statistical learning



Signal processing & filtering models



Law (**Markov process X** | **Noisy & Partial observations Y**)

- ▶ **Signal X** : target evolution (missile, plane, robot, vehicle, image contours), forecasting models, assets volatility, speech signals, ...
- ▶ **Observation Y** : Radar/Sonar/Gps sensors, financial assets prices, image processing, audio receivers, statistical data measurements, ...

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⊂ **Multiple objects tracking models (highly more complex pb)**

- ▶ On the Stability and the Approximation of Branching Distribution Flows, with Applications to Nonlinear Multiple Target Filtering. Francois Caron, Pierre Del Moral, Michele Pace, and B.-N. Vo (HAL-INRIA RR-7376) [50p]. Stoch. Analysis and Applications Volume 29, Issue 6, 2011.
- ▶ Comparison of implementations of Gaussian mixture PHD filters. M. Pace, P. Del Moral, Fr. Caron 13th International Conference on Information. FUSION, EICC, Edinburgh, UK, 26-29 July (2010)

$$\text{Law} \left(X = \sum_{1 \leq i \leq N_t^X} \delta_{X_t^i} \quad \middle| \quad Y = \sum_{1 \leq i \leq N_t^Y} \delta_{Y_t^i} \right)$$

Filtering (prediction \oplus smoothing)

$$p((x_0, \dots, x_n) \mid (y_0, \dots, y_n)) \quad \& \quad p(y_0, \dots, y_n) \quad ?$$

Bayes' rule

$$p((x_0, \dots, x_n) \mid (y_0, \dots, y_n)) \propto \underbrace{p((y_0, \dots, y_n) \mid (x_0, \dots, x_n))}_{\prod_{0 \leq k \leq n} p(y_k \mid x_k) \leftarrow \text{likelihood functions } G_k} \times p(x_0, \dots, x_n)$$

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↓

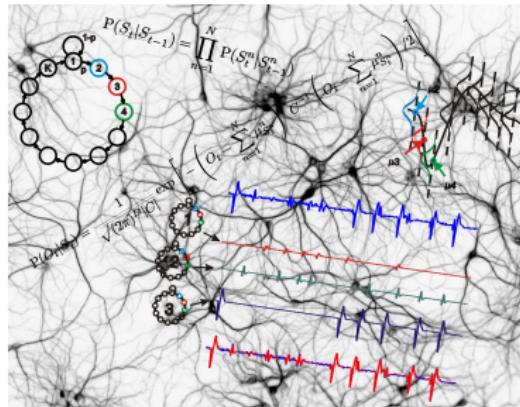
Feynman-Kac models : $G_n(x_n) := p(y_n \mid x_n)$ & $\mathbb{P}_n := \text{Law}(X_0, \dots, X_n)$

$$\text{Law}((X_0, \dots, X_n) \mid Y_p = y_p, p < n) = \frac{1}{Z_n} \left\{ \prod_{0 \leq p < n} G_p(X_p) \right\} \mathbb{P}_n$$

Note : **Not unique stochastic model!**

Hidden Markov chains problems

$\Theta \rightsquigarrow$ Signal $X^\Theta \rightsquigarrow$ observations Y^Θ



Law (fixed parameter Θ | Noisy & Partial observations Y^Θ)

- ▶ **Parameter Θ** : kinetic model unknown parameters, statistical parameters (signal/sensors), hypothesis testing, ..
- ▶ **Signal X^Θ** : Single or multiple targets evolution, forecasting models, financial assets volatility, speech signals, video images, ...
- ▶ **Observation Y^Θ** : Radar/Sonar/Gps sensors, financial assets prices, image processing, statistical data measurements, ...

Posterior density

$$p(\theta | (y_0, \dots, y_n)) \propto \underbrace{p((y_0, \dots, y_n) | \theta)}_{\prod_{0 \leq k \leq n} p(y_k | \theta, (y_0, \dots, y_{k-1}))} \times p(\theta)$$

← likelihood functions

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↓

Multiplicative formulation

$$\text{Law}(\Theta | (y_0, \dots, y_n)) \propto \left\{ \prod_{0 \leq p \leq n} h_p(\theta) \right\} \lambda(d\theta)$$

with

$$h_n(\theta) := p(y_n | \theta, (y_0, \dots, y_{n-1})) \quad \& \quad \lambda := \text{Law}(\Theta)$$

First key observation

$$p((y_0, \dots, y_n) | \theta) = \prod_{0 \leq p \leq n} h_p(\theta) = \mathcal{Z}_n(\theta)$$

with the normalizing constant $\mathcal{Z}_n(\theta)$ of the conditional distribution

$$p((x_0, \dots, x_n) | (y_0, \dots, y_n), \theta)$$

$$= \frac{1}{p((y_0, \dots, y_n) | \theta)} p((y_0, \dots, y_n) | (x_0, \dots, x_n), \theta) p((x_0, \dots, x_n) | \theta)$$

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Second key observation

$h_n(\theta)$ and $\mathcal{Z}_n(\theta)$ easy to compute for linear/gaussian models

Third key observation : Any target measure of the form

$$\eta_n(d\theta) = \frac{1}{Z_n} \left\{ \prod_{0 \leq p \leq n} h_p(\theta) \right\} \times \lambda(d\theta)$$

is the n -th time marginal of the Feynman-Kac measure

$$\mathbb{Q}_n := \frac{1}{Z_n} \left\{ \prod_{0 \leq p < n} G_p(\Theta_p) \right\} \mathbb{P}_n$$

with

$$G_n = h_{n+1} \quad \text{and} \quad \mathbb{P}_n := \text{Law}(\Theta_0, \dots, \Theta_n)$$

where

$\Theta_{p-1} \rightsquigarrow \Theta_p$ as an MCMC move with target measure η_p

Particle auxiliary variables $\theta \rightsquigarrow \xi^\theta \sim P(\theta, d\xi)$

$$\bar{\eta}_n(d\bar{\theta}) \propto \left\{ \prod_{0 \leq p \leq n} \bar{h}_p(\bar{\theta}) \right\}_{=\lambda(d\theta) \times P(\theta, d\xi)}^{\bar{\lambda}(d\bar{\theta})}$$

with $\bar{\theta} = (\theta, \xi)$ and

$$\bar{h}_n(\bar{\theta}) := \frac{1}{N} \sum_{i=1}^N p(y_n \mid \xi_n^{\theta, i}) \underset{N \uparrow \infty}{\simeq} p(y_n \mid \theta, (y_0, \dots, y_{n-1})) = h_p(\theta)$$

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But by the unbiased property the θ -marginal of $\bar{\eta}_n$ coincides with

$$\text{Law}(\Theta \mid (y_0, \dots, y_n)) \propto \left\{ \prod_{0 \leq p \leq n} h_p(\theta) \right\} \lambda(d\theta)$$

Feynman-Kac formulation :

Markov chain $\bar{\Theta}_k = (\Theta_k, \xi^{(k)})$ **MCMC with target** $\bar{\eta}_n$ **and** $G_n = \bar{h}_{n+1}$

Particle gradient models ($\theta \in \mathbb{R}^d$)

$$\mathcal{Z}_n(\theta) = p((y_0, \dots, y_{n-1}) \mid \theta) = \mathbb{E} \left(\prod_{0 \leq q < n} p(y_q \mid \theta, X_q^\theta) \right)$$



$$\Rightarrow \underbrace{\nabla \log \mathcal{Z}_n(\theta)}_{\text{derivative}} = \underbrace{\mathbb{Q}_n^{(\theta)}(\Lambda_n)}_{\text{path-integral}}$$

Just after learning "the steepest descent" method
in optimization class...

with the Feynman-Kac measure $\mathbb{Q}_n^{(\theta)}$ on path space associated with

$$(X_n^\theta, G_n^\theta(x_n)) = (X_n^\theta, p(y_q \mid \theta, x_n))$$

and with the additive functional

$$\Lambda_n(x_0, \dots, x_n) = \sum_{0 \leq q < n} \nabla \log (p(x_{q+1} \mid \theta, x_q) p(y_q \mid \theta, x_q))$$

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~~ Particle gradient algorithm

$$\Theta_n = \Theta_{n-1} + \tau_n \nabla \mathbb{Q}_n^{(\theta)}(\Lambda_n) \simeq \Theta_{n-1} + \tau_n \nabla \mathbb{Q}_n^{(\theta), N}(\Lambda_n)$$

Approximate Bayesian Computation



When $p(y_n|x_n)$ is untractable or impossible to compute in reasonable time

$$\begin{cases} X_n &= F_n(X_{n-1}, W_n) \\ Y_n &= H_n(X_n, V_n) \end{cases} \xrightarrow{\mathcal{X}_n = (X_n, Y_n)} \begin{cases} \mathcal{X}_n &= \mathcal{F}_n(\mathcal{X}_{n-1}, \mathcal{W}_n) \\ Y_n^\epsilon &= Y_n + \epsilon V_n^\epsilon \end{cases}$$



$$\mathbf{Law}(X \mid Y^\epsilon = y) \simeq_{\epsilon \downarrow 0} \mathbf{Law}(X \mid Y = y)$$

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$$\mathbf{Law}(X \mid Y^\epsilon = y) \simeq_{\epsilon \downarrow 0} \mathbf{Law}(X \mid Y = y)$$



Feynman-Kac model with the Markov chain and the potentials :

$$\mathcal{X}_n = (X_n, Y_n) \quad \text{and} \quad G_n(\mathcal{X}_n) = p(Y_n^\epsilon \mid Y_n)$$

Interacting Kalman-Filters

$X_n = (X_n^1, X_n^2)$ with X_n^1 Markov and $(X_n^2, Y_n) | X_n^1$ linear-gaussian model

$$\begin{cases} X_n^2 &= A_n(X_n^1) X_{n-1}^2 + B_n(X_n^1) W_n \\ Y_n &= C_n(X_n^1) X_n^2 + D_n(X_n^1) V_n \end{cases}$$



Law $(X_n^2 \mid X^1, Y_p = y_p, p < n) = \eta_{X^1, n}$ = Kalman gaussian predictor

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Law ($X_n^2 \mid X^1, Y_p = y_p, p < n$) = $\eta_{X^1, n}$ = Kalman gaussian predictor



Law(($X^1, X^2 \mid Y$) = **Feynman-Kac model with**

$$\mathcal{X}_n = (X_n^1, \eta_{X^1, n}) \quad \& \quad G_n(\mathcal{X}_n) = \int p(Y_n \mid (x_n^1, x_n^2)) \eta_{X^1, n}(dx_n^2)$$

► Uncertainty propagations in numerical codes



Law (Inputs \mathcal{I} | Outputs $\mathcal{O} = C(\mathcal{I}) \in \text{Reference or Critical event })$

\Updownarrow

$$\left. \begin{array}{l} \mu = \text{Law}(\mathcal{I}) \\ A = \{\mathcal{I} : C(\mathcal{I}) \in B\} \end{array} \right\} \longrightarrow \mathbb{P}(\mathcal{I} \in A) = \mu(A) \text{ & Law}(\mathcal{I} \mid \mathcal{I} \in A) = \mu_A$$

► Uncertainty propagations in numerical codes



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Multi-level decomposition

$$h_n = 1_{A_n} \text{ with } A_n \downarrow \implies \mu_{A_n}(dx) \propto \left\{ \prod_{0 \leq p \leq n} h_p(x) \right\} \mu(dx)$$

► Uncertainty propagations in numerical codes



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⇒ Feynman-Kac representation

$$(X_{n-1} \rightsquigarrow X_n) = \text{MCMC moves with target } \mu_{A_n} \quad \& \quad G_n = 1_{A_{n+1}}$$

Stochastic particle sampling methods

Bayesian statistical learning

Concentration inequalities

Current population models

Particle free energy

Genealogical tree models

Backward particle models

Current population models

Constants (c_1, c_2) related to (bias, variance), c universal constant
Test funct. $\|f_n\| \leq 1$

- ▶ $\forall (x \geq 0, n \geq 0, N \geq 1)$, the probability of the event

$$[\eta_n^N - \eta_n](f) \leq \frac{c_1}{N} (1 + x + \sqrt{x}) + \frac{c_2}{\sqrt{N}} \sqrt{x}$$

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

- ▶ $y = (y_i)_{1 \leq i \leq d} \rightsquigarrow (-\infty, y] = \prod_{i=1}^d (-\infty, y_i]$ cells in $E_n = \mathbb{R}^d$.

$$F_n(y) = \eta_n(1_{(-\infty, y]}) \quad \text{and} \quad F_n^N(y) = \eta_n^N(1_{(-\infty, y]})$$

$\forall (x \geq 0, n \geq 0, N \geq 1)$, the probability of the following event

$$\sqrt{N} \|F_n^N - F_n\| \leq c \sqrt{d(x+1)}$$

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

Particle free energy models

Constants (c_1, c_2) related to (bias, variance), c universal constant.

- ▶ $\forall (x \geq 0, n \geq 0, N \geq 1, \epsilon \in \{+1, -1\})$, the probability of the event

$$\frac{\epsilon}{n} \log \frac{\mathcal{Z}_n^N}{\mathcal{Z}_n} \leq \frac{c_1}{N} (1 + x + \sqrt{x}) + \frac{c_2}{\sqrt{N}} \sqrt{x}$$

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

Note : $(0 \leq \epsilon \leq 1 \Rightarrow (1 - e^{-\epsilon}) \vee (e^\epsilon - 1) \leq 2\epsilon)$

$$e^{-\epsilon} \leq \frac{z^N}{z} \leq e^\epsilon \Rightarrow \left| \frac{z^N}{z} - 1 \right| \leq 2\epsilon$$

Genealogical tree models := η_n^N (in path space)

Constants (c_1, c_2) related to (bias, variance), c universal constant
 \mathbf{f}_n test function $\|\mathbf{f}_n\| \leq 1$.

- ▶ $\forall (x \geq 0, n \geq 0, N \geq 1)$, the probability of the event

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

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

- ▶ \mathcal{F}_n = indicator fct. \mathbf{f}_n of cells in $\mathbf{E}_n = (\mathbb{R}^{d_0} \times \dots \times \mathbb{R}^{d_n})$
 $\forall (x \geq 0, n \geq 0, N \geq 1)$, the probability of the following event

$$\sup_{\mathbf{f}_n \in \mathcal{F}_n} |\eta_n^N(\mathbf{f}_n) - \mathbb{Q}_n(\mathbf{f}_n)| \leq c (n+1) \sqrt{\frac{\sum_{0 \leq p \leq n} d_p}{N} (x+1)}$$

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

Backward particle models

Constants (c_1, c_2) related to (bias, variance), c universal constant.
 \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 $1 - e^{-x}$.

- ▶ $\mathbf{f}_{a,n}$ normalized additive functional w.r.t. $f_p = 1_{(-\infty, a]}$, $a \in \mathbb{R}^d = E_n$

$\forall (x \geq 0, n \geq 0, N \geq 1)$, the probability of the following event

$$\sup_{a \in \mathbb{R}^d} |\mathbb{Q}_n^N(\mathbf{f}_{a,n}) - \mathbb{Q}_n(\mathbf{f}_{a,n})| \leq c \sqrt{\frac{d}{N}(x+1)}$$

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