

# New Insights on Particle MCMC algorithms

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STM Workshop, IMS Tokyo 2014

## Some hyper-refs

- ▶ [PMCMC - Andrieu, Doucet, Holenstein JRSS-10](#)
- ▶ [On Feynman-Kac and PMCMC models, with R. Kohn and F. Patras \(ArXiv-2014\).](#)
- ▶ On parallel implementation of Sequential Monte Carlo methods: the island particle model, with C. Vergé, C. Dubarry, and E. Moulines. (Statistics and Computing-2013).
- ▶ A Backward Particle Interpretation of Feynman-Kac Formulae, with A. Doucet and S. Singh (Arxiv-2009/M2AN-2010)
- ▶ Feynman-Kac formulae, Springer (2004) [+ Refs]
- ▶ Mean field simulation for Monte Carlo integration. Chapman - Hall (2013) [+ Refs]

Bayes/Conditioning/Feynman-Kac measures

Origins/Equivalent particle algorithms

Ex.: MCMC with product target measures

Particle measures  $\oplus$  2 key formulae

Conditioning and duality formulae

Taylor expansions for PMCMC transitions

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# Conditioning formulae (not<sup>o</sup>: $\mathbf{z}_n = (z_0, \dots, z_n) = z_{0:n}$ )

- ▶ Bayes rule/Filtering

$$p(\mathbf{x}_n | \mathbf{y}_n) \propto p(\mathbf{y}_n | \mathbf{x}_n) \times p(\mathbf{x}_n)$$

with *product* likelihood functions

$$p(\mathbf{y}_n | \mathbf{x}_n) \propto \prod_{0 \leq k \leq n} p(y_k | x_k)$$

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- ▶ Markov path restricted to a tube  $\mathbf{A}_n = (A_0 \times \dots \times A_n)$

$$p(\mathbf{x}_n | \mathbf{x}_n \in \mathbf{A}_n) \propto p(\mathbf{x}_n \in \mathbf{A}_n | \mathbf{x}_n) \times p(\mathbf{x}_n)$$

with *product* indicator functions

$$p(\mathbf{x}_n \in \mathbf{A}_n | \mathbf{x}_n) \propto \prod_{0 \leq k \leq n} 1_A(x_k)$$

► **(Sequential) Importance Sampling**  $\mathbf{x}_n \rightsquigarrow \mathbf{x}_{n+1} = (\mathbf{x}_n, x_{n+1})$

$$\pi_{n+1}(\mathbf{x}_{n+1}) \stackrel{\text{hyp.}}{=} \pi_n(\mathbf{x}_n) q(\mathbf{x}_{n+1}|\mathbf{x}_n) \quad (1)$$

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$$\dots$$

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$$\stackrel{\text{"hyp"}}{\propto} \mathbf{G}_{n+1}(\mathbf{x}_{n+1}) \mathbf{p}(\mathbf{x}_{n+1}|\mathbf{x}_n) \pi_n(\mathbf{x}_n)$$

...

$$\propto \left\{ \prod_{0 \leq k \leq (n+1)} \mathbf{G}_k(\mathbf{x}_k) \right\} \underbrace{\prod_{0 \leq k \leq (n+1)} \mathbf{p}(\mathbf{x}_k|\mathbf{x}_{k-1})}_{=p(x_0, \dots, x_n)}$$



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... or more directly from the initial product formula (1)

$$q(\mathbf{x}_{n+1}|\mathbf{x}_n) = p(\mathbf{x}_{n+1}|\mathbf{x}_n) \underbrace{\frac{q(\mathbf{x}_{n+1}|\mathbf{x}_n)}{p(\mathbf{x}_{n+1}|\mathbf{x}_n)}}_{=\mathbf{G}_{n+1}(\mathbf{x}_{n+1})}$$

All ex. are strictly  $\subset$  Feynman-Kac models ( $\exists \neg!$ )

$$\mathbb{Q}_n(d(x_0, \dots, x_n)) = \frac{1}{Z_n} \left\{ \prod_{0 \leq p < n} G_p(x_p) \right\} \mathbb{P}_n(d(x_0, \dots, x_n))$$

with

$$\mathbb{P}_n := \text{Law}(X_0, \dots, X_n) \quad \text{with } X_n \text{ Markov in } E_n$$

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$\Downarrow$

**Key obs.:**  $\mathbf{X}_n = (X_0, \dots, X_n)$  and  $\mathbf{G}_k(\mathbf{X}_k) = G_k(X_k)$

$$\eta_n(\mathbf{f}) = \mathbb{E} \left( \mathbf{f}(\mathbf{X}_n) \prod_{0 \leq k < n} \mathbf{G}_k(\mathbf{X}_k) \right) = \mathbb{Q}_n(\mathbf{f})$$

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$\Leftrightarrow$ Algo.	$X_{n-1} \rightsquigarrow X_n$	$G_n$
Sequential Monte Carlo	Sampling	Resampling
Particle Filters	Prediction	Updating
Genetic Algorithms	Mutation	Selection
Evolutionary Population	Exploration	Branching-selection
Diffusion Monte Carlo	Free evolutions	Absorption
<b>Quantum Monte Carlo</b>	Walkers motions	Reconfiguration
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bootstrapping, spawning, cloning, pruning, replenish, multi-level splitting, enrichment, go with the winner, quantum teleportation,...

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1947/1948

(Fermi/Kahn-Harris)

$\leq$  Meta-Heuristic style stochastic algo.  $\leq$  1996



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**Convergence/Performance analysis** : CLT, LDP,  $\mathbb{L}_p$ -estimates, Empirical processes, Moderate deviations, propagations of chaos, unif cv w.r.t. time, **new stochastic models**  $\supset$  **PMCMC (2009-2010)**....

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∇ **Interpolating path measures**  $\pi_0 \rightsquigarrow \dots \rightsquigarrow \pi_T$

$$\pi_n(d\theta) \propto \left\{ \prod_{1 \leq k \leq n} h_k(\theta) \right\} \lambda(d\theta)$$

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**As the filtering equation:**

$$\pi_{n-1} \xrightarrow{\text{Correction/Updating}} d\pi_n \propto h_n d\pi_{n-1} \xrightarrow{\pi_n\text{-MCMC/Prediction } M_n} \pi_n$$

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⊂  $n$ -th marginals  $\pi_n = \eta_n$  of a Feynman-Kac model  $\mathbb{Q}_n$

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⊂  **$n$ -th marginals  $\pi_n = \eta_n$  of a Feynman-Kac model  $\mathbb{Q}_n$**

- *Physics*  $\rightsquigarrow$  *Crook/Jarzinsky formula*;
- *Rare event*  $\oplus$  *Black-box*  $\rightsquigarrow$  *subset sampling/multi-level splitting*;
- *Operation Research*  $\rightsquigarrow$  *Interacting simulated annealing* ...

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$$\eta_n \simeq \eta_n^N := \frac{1}{N} \sum_{1 \leq i \leq N} \delta_{(\chi_{0,n}^i, \chi_{1,n}^i, \dots, \chi_{n,n}^i) = i\text{-th ancestral line}}$$

$\rightsquigarrow \mathbb{X}_n^a := \text{uniform ancestral line}$

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## 1) Product formulae/Particle approximation

$$\mathcal{Z}_n = \prod_{0 \leq k < n} \eta_k(G_k) \stackrel{\text{unbias}}{\simeq} \prod_{0 \leq k < n} \eta_k^N(G_k) := \mathcal{Z}_n^N = \prod_{0 \leq k < n} \mathcal{G}_k(\chi_k)$$

with the empirical potential function

$$\mathcal{G}_k(\chi_k) = \eta_k^N(G_k) = \frac{1}{N} \sum_{1 \leq i \leq N} G_k(\chi_k^i)$$

↪ Many-body FK on path space

FK model with  $(\mathbf{X}_n, \mathbf{G}_n) \rightsquigarrow (\mathcal{X}_n, \mathcal{G}_n) = \text{Many-body FK}$



## ↪ Many-body FK on path space

FK model with  $(\mathbf{X}_n, \mathbf{G}_n) \rightsquigarrow (\chi_n, \mathcal{G}_n) = \text{Many-body FK}$

**For any empirical function**  $\mathbf{F}(\chi_n) = \frac{1}{N} \sum_{1 \leq i \leq N} \mathbf{f}(\chi_n^i)$

Theo [MPRF-1996]

$$\mathbb{E} \left( \mathbf{f}(\mathbf{X}_n) \prod_{0 \leq k < n} \mathbf{G}_k(\mathbf{X}_k) \right) = \mathbb{E} \left( \mathbf{F}(\chi_n) \prod_{0 \leq k < n} \mathcal{G}_k(\chi_k) \right)$$

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↪ SC-13 (Island models/Parallel particle models)

↪ FTML-02/Arxiv-2011 (independent Metropolis-Hastings/SMC<sup>2</sup>)

# The 2nd key

## Hypothesis

$$M_{k+1}(x_k, dx_{k+1}) = H_{k+1}(x_k, x_{k+1}) \lambda(dx_{k+1}) \stackrel{\text{ex.}}{\propto} e^{-\frac{1}{2}(x_{k+1} - a(x_k))^2} dx_{k+1}$$

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## 2) Backward formulae/Backward Particle chain

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

with

$$\begin{aligned} & \mathbb{K}_{k+1, \eta_k}(x_{k+1}, dx_k) \\ &= \frac{\eta_k(dx_k) G_k(x_k) H(x_k, x_{k+1})}{\int \eta_k(dx'_k) G_k(x'_k) H(x'_k, x_{k+1})} \end{aligned}$$

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↪ backward random path  $\mathbb{X}_n^b$

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$\oplus$

**Theo 1** [Arxiv-2014]

Law (**Ancestral line** | **Complete tree**)

=

Law of the (**backward particle model**)

## Theo 2 [Duality formula for Many-body FK ([Arxiv-2014](#))]

$$\text{Law}(\mathcal{X}_n^* \mid \mathbf{X}_n = \mathbf{x}) := \text{Law}_{\text{many-body}}(\mathcal{X}_n \mid \mathbb{X}_n^b = \mathbf{x})$$

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 $\stackrel{\text{def.}}{=} \text{Law } N \text{ particles with frozen path } \mathbf{X}_n = \mathbf{x}$

$\Downarrow$

$$\mathbb{E} \left( \mathbf{F}(\mathbb{X}_n^b, \mathcal{X}_n) \prod_{0 \leq k < n} \mathcal{G}_k(\mathcal{X}_k) \right) = \mathbb{E} \left( \mathbf{F}(\mathbf{X}_n, \mathcal{X}_n^*) \prod_{0 \leq k < n} \mathbf{G}_k(\mathbf{X}_k) \right)$$

Proof ingredient  $\chi = (\chi^i)$  i.i.d.  $\sim \eta = \text{Law}(X)$

$$\mathcal{X}^* | X = \text{i.i.d.} \sim \frac{1}{N} \delta_X + \left(1 - \frac{1}{N}\right) \frac{1}{N-1} \sum_{2 \leq i \leq N} \delta_{\chi^i}$$

and

$$\mathbb{X} | \chi \sim \frac{1}{N} \sum_{1 \leq i \leq N} \delta_{\chi^i}$$

$\Downarrow$

$$\mathbb{E}(F(\mathbb{X}, \chi)) = \mathbb{E}(F(X, \mathcal{X}^*))$$

# Direct consequence

Duality  $\Rightarrow$  Andrieu-Doucet-Holenstein Particle Gibbs model



2 reversible transitions  $\mathbb{K}_n(\mathbf{x}, d\mathbf{x}')$  w.r.t.  $Q_n$ :

$$\mathbf{x} \rightsquigarrow \mathcal{X}_n^* \text{ with frozen path } \mathbf{x} \rightsquigarrow \begin{cases} \text{Random backward path } \mathbf{x}' \\ \text{or} \\ \text{Random ancestral line } \mathbf{x}' \end{cases}$$



Direct (but too crude) minorization condition  $\mathbb{K}_n(\mathbf{x}, \cdot) \geq \epsilon_n \eta_n$

## Using the key observation

$\mathbb{X}_n^{\mathbf{b}} \perp \overline{\mathbb{X}}_n^{\mathbf{b}}$  Independent copies

$\Downarrow$

$$\mathbb{E} \left( \mathbf{f}_1(\mathbb{X}_n^{\mathbf{b}}) \mathbf{f}_2(\overline{\mathbb{X}}_n^{\mathbf{b}}) \prod_{0 \leq p < n} \mathcal{G}_p(\mathcal{X}_p) \right) \stackrel{\text{duality}}{=} \mathbb{E} \left( \mathbf{f}_1(\mathbf{X}_n) \mathbb{K}_n(\mathbf{f}_2)(\mathbf{X}_n) \prod_{0 \leq p < n} \mathbf{G}_p(\mathbf{X}_p) \right)$$

⊕ Symmetry argument  $\mathbf{f}_1 \leftrightarrow \mathbf{f}_2$

Bayes/Conditioning/Feynman-Kac measures

Origins/Equivalent particle algorithms

Ex.: MCMC with product target measures

Particle measures  $\oplus$  2 key formulae

Conditioning and duality formulae

Taylor expansions for PMCMC transitions



### Theo 3 [Taylor exp. - ancestral-lines PMCMC (Arxiv-2014)]

$$\mathbb{K}_n(x, \cdot) = \eta_n + \sum_{1 \leq k \leq l} \frac{1}{N^k} d^{(k)} \mathbb{K}_n(x, \cdot) + O\left(\frac{1}{N^{l+1}}\right)$$

at any order  $l$ , with explicit operators  $d^{(k)} \mathbb{K}_n$  in terms of coalescent trees.

⊕ **Taylor exp. for the law of  $q$  particles in the scheme with frozen  $x$**

## Some direct corollaries

- ▶ Bias and variance of PMCMC empirical centered function  $\mathbf{f}_n$ :

$$\text{Var} = \frac{1}{N} \eta_n(\mathbf{f}_n^2) + O\left(\frac{1}{N^2}\right)$$

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- ▶  $m$ -iterates expansions

$$\mathbb{K}_n^m(x, \cdot) = \boldsymbol{\eta}_n + \frac{1}{Nm} \left[ \sum_{0 \leq k \leq l} \frac{1}{N^k} d^{(m+k)} \mathbb{K}_n^m(x, \cdot) + O\left(\frac{1}{N^{l+1}}\right) \right]$$