New Insights on Particle MCMC algorithms

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ASC-IMS 2014 Conference

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 & Feynman-Kac models

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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Taylor expansions for PMCMC transitions

$$p(x_{0:n} \mid y_{0:n}) \propto \underbrace{p(y_{0:n} \mid x_{0:n})}_{\prod_{0\le k\le n} p(y_k|x_k) \leftarrow \text{likelihood functions } G_k(x_k)} \times \underbrace{p(x_{0:n})}_{\rightsquigarrow \text{density of } \mathbb{P}_n}$$

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strictly $\subset$ Feynman-Kac models ($\exists\neg!$)

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

Notation : η_n n-th marginal distribution

Key obs.: $\mathbf{X_n} = (X_0,\ldots,X_n)$ and $\mathbf{G_k}(\mathbf{X_k}) = G_k(X_k)$

$$\eta_n(\mathbf{f}) = \mathbb{E}\left(\mathbf{f}(\mathbf{X_n}) \prod_{0\leq k<n} \mathbf{G_k}(\mathbf{X_k})\right) = \mathbb{Q}_n(\mathbf{f})$$

$\Leftrightarrow$ **Algo.**	$\mathbf{X_{n-1} \rightsquigarrow X_n}$	$\mathbf{G_n}$
Sequential Monte Carlo	Sampling	Resampling
Particle Filters	Prediction	Updating
Genetic Algorithms	Mutation	Selection
Evolutionary Population	Exploration	Branching-selection
Diffusion Monte Carlo	Free evolutions	Absorption
Quantum Monte Carlo	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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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....

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

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

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

$$\eta_{\mathbf{n}} \simeq \eta_{\mathbf{n}}^{\mathbf{N}} := \frac{1}{N} \sum_{1 \leq i \leq N} \delta_{\left(\mathcal{X}^i_{0,n}, \mathcal{X}^i_{1,n}, \ldots, \mathcal{X}^i_{n,n}\right) = \text{i-th ancestral line}}$$

$\rightsquigarrow$ $\mathbb{X}_{\mathbf{n}} :=$ uniform ancestral line

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1) Product formulae/Particle approximation

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

with the empirical potential function

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

$\rightsquigarrow$ Many-body FK on path space

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

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For any empirical function $\mathbf{F}(\mathcal{X}_\mathbf{n}) = \frac{1}{N}\sum_{1\leq i\leq N} \mathbf{f}(\mathcal{X}^\mathbf{i}_\mathbf{n})$

Theo [**MPRF-1996**]

$$\mathbb{E}\left(\mathbf{f}(\mathbf{X_n}) \prod_{0\leq k<n} \mathbf{G_k}(\mathbf{X_k})\right) = \mathbb{E}\left(\mathbf{F}(\mathcal{X}_\mathbf{n}) \prod_{0\leq k<n} \mathcal{G}_\mathbf{k}(\mathcal{X}_\mathbf{k})\right)$$

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$\rightsquigarrow$ **SC-13 (Island models/Parallel particle models)**

$\rightsquigarrow$ **FTML-02/Arxiv-2011 (independent Metropolis-Hastings/SMC^2)**

The 2nd key

Hypothesis

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

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2) Backward formulae/Backward Particle chain

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

with

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

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$\rightsquigarrow$ backward random path $\mathbb{X}_\mathbf{n}$

Unbias Many-body FK (cf. M2AN-2010/ Arxiv-2014)

$$\mathbb{X}_n = \text{Uniform ancestral line}$$
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$$\oplus$$

Law (**Ancestral line** | **complete tree**) = Law of the **backward particle model**

Theo 1 [Duality formula for Many-body FK (Arxiv-2014)]

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

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Two Feynman-Kac - reversible transitions $\mathbb{K}_n(\mathbf{x}, \mathbf{dx}')$

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

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

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$$\mathbb{K}_n(x,\,.\,) = \boldsymbol{\eta}_\mathbf{n} + \sum_{1\leq k\leq l} \frac{1}{N^k}\; d^{(k)}\mathbb{K}_n(x,\,.\,) + \mathrm{O}\left(\frac{1}{N^{l+1}}\right)$$

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

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Some direct corollaries

- Bias and variance of PMCMC empirical centered function $\mathbf{f_n}$:

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- $m-$Iterates expansions

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