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A duality formula for Feynman–Kac path particle models


Une formule de dualité pour des modèles particuliers de type Feynman–Kac trajectoriels
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ARTICLE INFO

Article history:

Received 27 October 2014

Accepted after revision 25 February 2015

Available online 29 March 2015

Presented by the Editorial Board

ABSTRACT

This Note and its extended version [10] present a new duality formula between genetic type genealogical tree based particle models and Feynman–Kac measures on path spaces. Among others, this formula allows us to design reversible Gibbs–Glauber Markov chains for Feynman–Kac integration on path spaces. Our approach yields new Taylor series expansions of the particle Gibbs–Glauber semigroup around its equilibrium measure w.r.t. the size of the particle system, generalizing the recent work of Andrieu, Doucet, and Holenstein [1]. We analyze the rate of convergence to equilibrium in terms of the ratio of the length of the trajectories to the number of particles. The analysis relies on a tree-based functional and combinatorial representation of a class of Feynman–Kac particle models with a frozen ancestral line. We illustrate the impact of these results in the context of Quantum and Diffusion Monte Carlo methods.

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RÉSUMÉ

Cette Note et sa version étendue [10] présentent une nouvelle formule de dualité entre des modèles d'arbres généalogiques associés à des algorithmes génétiques particuliers et des mesures de Feynman–Kac sur des espaces trajectoriels. Cette formule permet de définir des processus de Markov réversibles de type Gibbs–Glauber pour intégrer des mesures de Feynman–Kac sur des espaces de trajectoires. Notre étude présente aussi de nouveaux développements de Taylor par rapport à la taille des systèmes de particules du semi-groupe de ces processus autour de leur mesure d'équilibre. Ces résultats étendent les travaux récents d'Andrieu, Doucet and Holenstein [1]. En particulier, nous obtenons une vitesse de convergence à l'équilibre liée au rapport entre longueurs des trajectoires et taille des systèmes de particules. La preuve de ces résultats est fondée sur une représentation fonctionnelle et combinatoire des lois de modèles particuliers de type Feynman–Kac ayant une trajectoire ancestrale fixée. Nous en donnons une illustration dans le cadre des méthodes de Monte Carlo quantiques.

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Version française abrégée

Les mesures de Feynman–Kac (1) donnent une interprétation probabiliste de nombreux problèmes issus de traitement du signal, de la statistique, des mathématiques financières et de l'analyse de risque. Ces domaines d'applications sont développés dans les références [4,5,7,8,12]. En chimie moléculaire ainsi qu'en physique statistique, les formules d'intégration sur des espaces de trajectoires (3) sont liées à la résolution d'équations de Schrödinger à temps imaginaire. Leurs interprétations particulières décrites en (2) correspondent aux méthodes « diffusion Monte Carlo », parfois appelées aussi *Resampled Monte Carlo Methods* dans la littérature anglo-saxonne.

Ces méthodes de Monte Carlo sont des interprétations particulières de type champ moyen des flots de mesures de Feynman–Kac décrits en (1) en termes d'une chaîne de Markov X_n et d'une suite de fonctions « potentiel » positives G_n . Elles sont fondées sur des modèles d'évolution d'arbres généalogiques χ_n de processus de branchement χ'_n de type génétique. Les mutations des individus sont liées au processus X_n , la sélection et les taux de branchement des individus étant caractérisés par les fonctions G_n . Une description plus formelle de ces transitions est donnée par la formule (2).

Les propriétés non biaisées des mesures d'occupation dénormalisées des arbres généalogiques sont caractérisées par les formules de Feynman–Kac multi-corps (many-body) π_n décrites en (6). La procédure de dénormalisation est définie en multipliant les mesures d'occupation des lignes ancestrales par les dérivées de Radon–Nikodym $Z_n(\chi)$ décrites dans le Théorème 2.1. Ce théorème démontre par ailleurs que les lignes ancestrales de ces arbres généalogiques, conditionnellement aux populations d'ancêtres du modèle, sont équivalentes à des chaînes de Markov remontant le temps en choisissant les ancêtres aux niveaux inférieurs selon les transitions à rebours décrites en (5).

La formule de dualité (4) est l'un des principaux résultat de cette Note. Elle exprime la mesure π_n en fonction d'un système particulaire identique au précédent, avec toutefois une ligne ancestrale fixée, distribuée selon la mesure de Feynman–Kac originelle (1). La transition \mathbb{K}_n du processus de Gibbs–Glauber (7) – appelé aussi échantillonneur de Gibbs, ou tout simplement dynamique de Glauber – réversible par rapport à la mesure π_n , est définie en deux temps. La première étape revient à simuler un arbre généalogique ayant une trajectoire ancestrale fixée. On choisit ensuite au hasard une de ses lignes ancestrales. De manière alternative, on simule une ligne ancestrale à rebours selon le processus de sélection d'ancêtres aux niveaux inférieurs décrit précédemment (en choisissant au hasard l'un des individus au temps terminal). La réversibilité de \mathbb{K}_n et celle de la transition \mathbb{K}_n^b , basée sur des lignes ancestrales sélectionnées à rebours, est décrite dans le Corollaire 3.1. La formule (8), souligne l'ergodicité uniforme des chaînes de Markov sous-jacentes pour des modèles de Feynman–Kac généraux. Lorsque le semigrroupe de Feynman–Kac satisfait la condition de stabilité décrite au-dessus du Théorème 4.1, une majoration plus fine du coefficient de contraction de Dobrushin $\beta(\mathbb{K}_n)$ de \mathbb{K}_n est décrite en (11) pour des tailles de populations suffisamment élevées, et proportionnelles à la longueur des trajectoires. Ce résultat découle d'un développement de Taylor de la transition \mathbb{K}_n autour de la mesure d'équilibre π_n , en fonction de l'inverse de la taille des systèmes de particules dans le modèle de Feynman–Kac multi-corps. Ces développements décrits dans le Théorème 4.1 permettent de préciser de façon exacte les normes d'erreur (10) dans les espaces $\mathbb{L}_p(\eta_n)$ entre les itérées des noyaux \mathbb{K}_n et leur mesure d'équilibre. La version étendue [10] de cette Note offre une description explicite des opérateurs dérivés en termes d'arbres de coalescences colorés.

1. Feynman–Kac particle models

We consider a Markov chain X_n and some $[\epsilon, 1]$ -valued potential functions G_n on measurable state spaces S_n , with $\epsilon \in]0, 1]$. We also let M_n be the Markov transitions of X_n from S_{n-1} into S_n .

We let η_n be the probability measures defined for any bounded measurable function f_n on S_n by the Feynman–Kac formula

$$\eta_n(f_n) \propto \mathbb{E}(f_n(X_n)Z_n(X)) \quad \text{with the Radon–Nikodym derivative} \quad Z_n(X) := \prod_{0 \leq p < n} G_p(X_p) \tag{1}$$

The N -mean field genetic type particle model associated with these measures is a Markov chain $\chi_n = (\chi_n^i)_{1 \leq i \leq N}$ on the product space $S_n := S_n^N$ starting with N independent copies of X_0 , for some $N > 1$. Given χ_n , the population of individual χ_{n+1} consists of N independent S_{n+1} -valued random variables with common distribution

$$\sum_{1 \leq i \leq N} \frac{G_n(\chi_n^i)}{\sum_{1 \leq j \leq N} G_n(\chi_n^j)} M_{n+1}(\chi_n^i, dx) \tag{2}$$

We further assume that $X_n := (X'_0, \dots, X'_n)$ is the historical process associated with some auxiliary Markov chain X'_n , and that $G_n(X_n) = G'_n(X'_n)$ only depends on the terminal state. In this situation, the path-particle $\chi_n^i = (\chi_{p,n}^i)_{0 \leq p \leq n}$ identifies with the ancestral line of the i -th individual $\chi_n^i = \chi_{i,n}^i$ of the Markov chain $\chi'_n \in S'_n := S_n^N$, defined as above by replacing (G_n, M_n) by (G'_n, M'_n) . Notice that the Feynman–Kac measures η'_n on S'_n associated with (G'_n, M'_n) reduce to the n -th time marginal of η_n .

Feynman–Kac models appear in numerous fields, including signal processing, statistics, mathematical finance, biology, rare event analysis, chemistry, and statistical physics; see [4,5,7,8,12]. Their interpretation depends on the application domain. For instance, in molecular and quantum physics, Feynman–Kac path integrals provide a probabilistic interpretation of imaginary time Schrödinger equations. To be more precise, let $M'_n \simeq_{\Delta t \downarrow 0} Id + L \Delta t$ be the Markov kernel associated with some discretization of a continuous-time stochastic process X'_t with infinitesimal generator L' on some time mesh $t_{n+1} - t_n := \Delta t \ll 1$, with $t_n = n\lfloor t/n \rfloor$. We also assume the existence of a potential V and introduce the functions $G'_n = e^{-V \Delta t}$. Replacing the chain X'_n above by the discrete time approximation model X'_{t_n} , we have:

$$\eta_n(f) \propto \mathbb{E} \left(f(X'_{t_0}, \dots, X'_{t_n}) e^{-\sum_{0 \leq t_k < t_n} V(X'_{t_k})(t_{k+1} - t_k)} \right) \simeq_{\Delta t \downarrow 0} \mathbb{E} \left(f(X'_s, s \leq t) e^{-\int_0^t V(X'_s) ds} \right) \tag{3}$$

The marginal γ_t w.r.t. the terminal time t of the r.h.s. measures is often defined, in a weak sense, by the imaginary time Schrödinger equation $\frac{d}{dt} \gamma_t(f) = \gamma_t(L^V(f))$, with $L^V(f) = L(f) - Vf$. In computational physics and chemistry, the genetic particle models discussed above belong to the class of Quantum Monte Carlo methods. They are often termed Resampled Monte Carlo methods, or Diffusion Monte Carlo methodologies. For a more thorough discussion of these continuous-time models and their applications in chemistry and physics, see [2,3,11,13–16], the recent monograph [8], and the references therein.

2. A duality theorem

Given some random path $X := (X_k)_{k \geq 0}$ of the Markov chain introduced in (1), we let \mathcal{X}_n be the N -particle Markov chain defined as χ_n but with one frozen state $\mathcal{X}_n^{I_n} = X_n$ at each time step, where I_n stands for a sequence of independent uniform random variables on the set $[N] := \{1, \dots, N\}$. More formally, given \mathcal{X}_n (and X), we select randomly an index $I_{n+1} = i \in [N]$ and we set $\mathcal{X}_{n+1}^i = X_{n+1}$. The other random variables \mathcal{X}_{n+1}^j , with $j \in [N] - \{i\}$, are $(N - 1)$ conditionally independent random variables with distribution defined as in (2) by replacing χ_n by \mathcal{X}_n . In the further development of the article, we use the bold letters $\mathbf{Y}_n := (Y_p)_{0 \leq p \leq n}$ to denote the historical processes of a Markov chain Y_n evolving in state spaces E_n . In this notation, $\boldsymbol{\chi}_n$ and $\boldsymbol{\chi}'_n$ take values in $\mathbf{S}_n := \prod_{0 \leq p \leq n} S_k$ and in $\mathbf{S}'_n := \prod_{0 \leq p \leq n} S'_k$. The r.v. $\boldsymbol{\chi}'_n$ can be interpreted as the complete populations of the genetic model χ'_n .

Theorem 2.1. For any $n \geq 0$, $N > 1$, and any bounded measurable function f_n on $(S_n \times \mathbf{S}_n)$ (symmetric on the product spaces S_k^N , with $0 \leq k \leq n$), we have the duality formula

$$\mathbb{E} (f_n(\mathbb{X}_n, \boldsymbol{\chi}_n) \mathcal{Z}_n(\chi)) = \mathbb{E} (f_n(X_n, \boldsymbol{\mathcal{X}}_n) Z_n(X)) \tag{4}$$

with a randomly chosen ancestral line \mathbb{X}_n with distribution $m(\chi_n) := \frac{1}{N} \sum_{1 \leq i \leq N} \delta_{\chi_n^i}$, the Radon–Nikodym derivatives $\mathcal{Z}_n(\chi) := \prod_{0 \leq k < n} \mathcal{G}_k(\chi_k)$, and the potential functions $\mathcal{G}_k(\chi_k) := \frac{1}{N} \sum_{1 \leq i \leq N} G_k(\chi_k^i)$.

Assume that $G'_{n-1}(x)M'_n(x, dy)$ have a density $H'_n(x, y)$ w.r.t. some measure $\nu'_n(dy)$ on S'_n . In this situation, given $\boldsymbol{\chi}'_n$, the sequence of r.v. $(\chi_k)_{0 \leq k \leq n}$ is a Markov chain starting at $\chi_0 = \chi'_0$, with elementary transitions defined for any $0 \leq k < n$ and bounded measurable function f on S_n by the formula

$$\mathbb{E} (f(\chi_{k+1}) | \chi_k, \chi'_{k+1}) \propto \int \left\{ \prod_{1 \leq i \leq N} m(\chi_k)(d\chi_k^i) H'_{k+1}(\chi_k^i, \chi'_{k+1}) \right\} f((\chi_k^i, \chi'_{k+1})_{1 \leq i \leq N}) \tag{5}$$

where $\mathbf{x}_k^i := (\mathbf{x}_{l,k}^i)_{0 \leq l \leq k}$ stands for an ancestral line of length k . In particular, given $\boldsymbol{\chi}'_n$ the ancestral line \mathbb{X}_n has the same (conditional) distribution as the backward Markov chain $\mathbb{X}_n^b = (\mathbb{X}_{k,n}^b)_{0 \leq k \leq n}$ with distribution $m(\chi'_n)$ at time n , and backward Markov transitions from S'_{k+1} into S'_k defined by

$$\mathbb{P} \left(\mathbb{X}_{k,n}^b \in d\mathbf{x}_k \mid \mathbb{X}_{k+1,n}^b, \chi'_k \right) \propto m(\chi'_k)(d\mathbf{x}_k) H'_{k+1}(\mathbf{x}_k, \mathbb{X}_{k+1,n}^b) \quad \text{with } 0 \leq k < n.$$

3. Particle Gibbs–Glauber dynamics

We let π_n be the many-body Feynman–Kac probability measures on $(S_n \times \mathbf{S}_n)$ defined for any bounded measurable function f_n on $(S_n \times \mathbf{S}_n)$ (symmetric on the product spaces S_k , with $0 \leq k \leq n$) by

$$\pi_n(f_n) \propto \mathbb{E} (f_n(\mathbb{X}_n, \boldsymbol{\chi}_n) \mathcal{Z}_n(\chi)) \tag{6}$$

The transition probabilities of the Gibbs–Glauber dynamics (also known as Gibbs sampling or simply Glauber dynamics) of the target multivariate distribution π_n on the product space $(S_n \times \mathbf{S}_n)$ are described by the synthetic diagram:

$$\left\{ \begin{array}{l} \mathbb{X}_n = x \\ \mathcal{X}_n = x \end{array} \right\} \longrightarrow \left\{ \begin{array}{l} \bar{\mathbb{X}}_n = \bar{x} \sim (\mathbb{X}_n | \mathcal{X}_n = x) \\ \mathcal{X}_n = x \end{array} \right\} \longrightarrow \left\{ \begin{array}{l} \bar{\mathbb{X}}_n = \bar{x} \\ \bar{\mathcal{X}}_n = \bar{x} \sim (\mathcal{X}_n | \mathbb{X}_n = \bar{x}) \end{array} \right\} \tag{7}$$

In the above display, $(\mathbb{X}_n | \mathcal{X}_n)$ and $(\mathcal{X}_n | \mathbb{X}_n)$ is a shorthand notation for the π_n -conditional distributions of \mathbb{X}_n given \mathcal{X}_n , and \mathcal{X}_n given \mathbb{X}_n . Notice that the first transition of the Gibbs–Glauber dynamics reduces to the uniform sampling of an ancestral line. In addition, by (4), the second transition amounts to sampling a genetic particle model with a frozen ancestral line:

$$\bar{\mathcal{X}}_n = \bar{x} \sim (\mathcal{X}_n | \mathbb{X}_n = \bar{x})$$

We let \mathbb{Y}_k be the first coordinate of the particle Gibbs–Glauber dynamics defined above (using the second sampling method). More formally, the elementary Markov transitions \mathbb{K}_n of the chain \mathbb{Y}_k are given for any bounded measurable function f on S_n and any path $x \in S_n$ by the formula:

$$\mathbb{K}_n(f)(x) := \mathbb{E}(f(\mathbb{Y}_1) | \mathbb{Y}_0 = x) = \mathbb{E}(m(\mathcal{X}_n)(f) | X_n = x) \quad \text{with} \quad m(\mathcal{X}_n) = \frac{1}{N} \sum_{1 \leq i \leq N} \delta_{\mathcal{X}_i^i}$$

To get one step further in our discussion, we consider π'_n the marginal of π_n on the state space $(S_n \times \mathcal{S}'_n)$. By Theorem 2.1, for any bounded measurable function f_n on $(S_n \times \mathcal{S}'_n)$ (symmetric on the product spaces \mathcal{S}'_k , with $0 \leq k \leq n$), we have:

$$\pi'_n(f_n) \otimes \mathbb{E} \left(f_n(\mathbb{X}_n^b, \mathcal{X}'_n) Z_n(\chi) \right) = \mathbb{E} (f_n(\mathbb{X}_n, \mathcal{X}'_n) Z_n(\chi))$$

In this situation, the first transition of the Gibbs–Glauber dynamics targeting π'_n reduces to the backward sampling of an ancestral line. Here again, by the duality formula (4), the second transition amounts to sampling a genetic particle model with a frozen ancestral line.

We let \mathbb{Y}_k^b be the first coordinate of this Gibbs–Glauber dynamics, and \mathbb{K}_n^b its elementary Markov transition. We let $\beta(M) := \sup \{ \text{osc}(M(f)); f \text{ s.t. } \text{osc}(f) \leq 1 \}$ be the Dobrushin coefficient of a Markov transition M on some measurable state space E , with $\text{osc}(f) := \sup_{x,y} |f(x) - f(y)|$. The next result shows the uniform ergodicity of the particle Gibbs–Glauber dynamics discussed above (we also refer to [6] for more refined estimates in terms of Feynman–Kac semigroups).

Corollary 3.1. *For any $n \geq 0$, we have \mathbb{K}_n and \mathbb{K}_n^b are reversible w.r.t. the Feynman–Kac measure η_n , and we have:*

$$\beta(\mathbb{K}_n) \vee \beta(\mathbb{K}_n^b) \leq 1 - \epsilon^n (1 - 1/N)^n \tag{8}$$

For sufficiently large population sizes, a more refined estimate is provided in (11), under some additional mild stability properties on the Feynman–Kac flow η'_n .

4. Stability properties

Recall the notion of the differential for sequences of measures introduced in [9]. We let μ^N be a uniformly bounded sequence of measures on some measurable state space S in the sense that $\sup_{N \geq 1} \|\mu^N\|_{TV} < \infty$, where $\|\cdot\|_{TV}$ stands for the total variation norm. The sequence μ^N is said to converge strongly to some measure μ , as $N \uparrow \infty$ if we have $\lim_{N \uparrow \infty} \mu^N(f) = \mu(f)$, for any bounded measurable function f . In this case, the discrete derivative of μ^N is defined by $\partial \mu^N := N (\mu^N - \mu)$. We say that μ^N is differentiable whenever $\partial \mu^N$ is uniformly bounded and it strongly converges to some signed measure $d^{(1)}\mu$, as $N \uparrow \infty$. When $\partial \mu^N$ is differentiable, with a discrete derivative written $\partial^{(2)}\mu^N$, we can define its derivative, denoted by $d^{(2)}\mu$, and so on. A mapping $N \mapsto \mu^N$ that is differentiable up to some order l can be written as

$$\mu^N = \sum_{0 \leq k \leq l} \frac{1}{N^k} d^{(k)}\mu + \frac{1}{N^{l+1}} \partial^{(l+1)}\mu^N$$

with the convention $d^{(0)}\mu = \mu$. We easily extend these definitions to a sequence of integral operators Q^N and a sequence of functions f^N . Here, we denote the corresponding differentials by $d^{(l)}Q$ and $d^{(l)}f$.

The sequence of measures η'_n satisfies a nonlinear updating-correction evolution equation (aka the filtering equation in signal processing, or the infinite population model in the scientific computing literature). We let $\eta'_{p,n,x}$ be the solution to these equations starting at the Dirac measure δ_x at time $p \leq n$, for some state $x \in S'_p$.

We further assume $\sup_{x,y} \|\eta'_{p,n,x} - \eta'_{p,n,y}\|_{TV} \leq a e^{-b(n-p)}$, for some finite constants $0 < a, b < \infty$. For time-homogeneous models, this condition is met as soon as the Markov transition M' satisfies the minorization condition $M^m(x, dz) \geq \epsilon M^m(y, dz)$ for some $m \geq 1$ and $\epsilon > 0$, and for any $x, y \in S'$.

Theorem 4.1. *The Markov transitions \mathbb{K}_n are differentiable at any order $l \geq 1$ with $d^{(0)}\mathbb{K}_n(f) = \eta_n(f)$, for any bounded measurable function f on S_n s.t. $\|f\| \leq 1$. In addition, we have the non-asymptotic estimates*

$$\forall 1 \leq k \leq l \quad \left\| d^{(k)}\mathbb{K}_n(f) \right\| \leq (cnk^2)^k \quad \text{and} \quad \left\| \partial^{(l+1)}\mathbb{K}_n(f) \right\| \leq (cn(l+1)^2)^{l+1} \quad (9)$$

as soon as $N > cn(l+1)^2$, for some finite constant $c < \infty$.

Corollary 4.2. *There exists some constant $c < \infty$ s.t. for any $1 \leq p \leq \infty$, any bounded measurable function f on S_n s.t. $\|f\| \leq 1$, and any $N > cn$, we have a sharp estimate of the $\mathbb{L}_p(\eta_n)$ -mean error norms*

$$\left| \left\| \mathbb{K}_n^m(f) - \eta_n(f) \right\|_{\mathbb{L}_p(\eta_n)} - N^{-m} \left\| \left[d^{(1)}\mathbb{K}_n \right]^m(f) \right\|_{\mathbb{L}_p(\eta_n)} \right| \leq (cn/N)^{m+1} \quad (10)$$

with the m -th iterates $\mathbb{K}_n^m = \mathbb{K}_n^{m-1}\mathbb{K}_n$ and $\left[d^{(1)}\mathbb{K}_n \right]^m := \left[d^{(1)}\mathbb{K}_n \right]^{m-1} d^{(1)}\mathbb{K}_n$ of \mathbb{K}_n and $d^{(1)}\mathbb{K}_n$.

Consequently, for any $m \geq 1$, $x \in S_n$, we have:

$$\left| \mathbb{E}(f(\mathbb{Y}_m) \mid \mathbb{Y}_0 = x) - \eta_n(f) \right| \leq \beta \left(\mathbb{K}_n^m \right) \leq (cn/N)^m \quad \left(\longrightarrow_{\min(N,m) \rightarrow \infty} 0 \right) \quad (11)$$

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