Mean Field Simulation for Monte Carlo Integration

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Mean Field Simulation for Monte Carlo Integration

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A CHAPMAN & HALL BOOK

To Laurence, Tiffany, and Timothée

Contents

Preface

Monte Carlo integration

This book deals with the theoretical foundations and the applications of mean field simulation models for Monte Carlo integration.

In the last three decades, this topic has become one of the most active contact points between pure and applied probability theory, Bayesian inference, statistical machine learning, information theory, theoretical chemistry and quantum physics, financial mathematics, signal processing, risk analysis, and several other domains in engineering and computer sciences.

The origins of Monte Carlo simulation certainly start with the seminal paper of N. Metropolis and S. Ulam in the late 1940s [435]. Inspired by the interest of his colleague S.Ulam in the poker game N. Metropolis, coined, the term "Monte Carlo Method" in reference to the "capital" of Monaco well known as the European city for gambling.

The first systematic use of Monte Carlo integration was developed by these physicists in the Manhattan Project of Los Alamos National Laboratory, to compute ground state energies of Schödinger's operators arising in thermonuclear ignition models. It is also not surprising that the development of these methods goes back to these early days of computers. For a more thorough discussion on the beginnings of the Monte Carlo method, we refer to the article by N. Metropolis [436].

As its name indicates, Monte Carlo simulation is, in the first place, one of the largest, and most important, numerical techniques for the computer simulation of mathematical models with random ingredients. Nowadays, these simulation methods are of current use in computational physics, physical chemistry, and computational biology for simulating the complex behavior of systems in high dimension. To name a few, there are turbulent fluid models, disordered physical systems, quantum models, biological processes, population dynamics, and more recently financial stock market exchanges. In engineering sciences, they are also used to simulate the complex behaviors of telecommunication networks, queuing processes, speech, audio, or image signals, as well as radar and sonar sensors.

Note that in this context, the randomness reflects different sources of model uncertainties, including unknown initial conditions, misspecified kinetic parameters, as well as the external random effects on the system. The repeated random samples of the complex system are used for estimating some *averaging* type property of some phenomenon.

Monte Carlo integration theory, including Markov chain Monte Carlo algorithms (abbreviated MCMC), sequential Monte Carlo algorithms (abbreviated SMC), and mean field interacting particle methods (abbreviated IPS) are also used to sample complex probability distributions arising in numerical probability, and in Bayesian statistics. In this context, the random samples are used for computing deterministic multidimensional *integrals*.

In other situations, stochastic algorithms are also used for solving complex *estimation problems*, including inverse type problems, global optimization models, posterior distributions calculations, nonlinear estimation problems, as well as statistical learning questions (see for instance [77, 93, 163, 274, 521]). We underline that in this situation, the randomness depends on the design of the stochastic integration algorithm, or the random search algorithm.

In the last three decades, these extremely flexible Monte Carlo algorithms have been developed in various forms mainly in applied probability, Bayesian statistics, and in computational physics. Without any doubt, the most famous MCMC algorithm is the Metropolis-Hastings model presented in the mid-1960s by N. Metropolis, A. Rosenbluth, M. Rosenbluth, A. Teller, and E. Teller in their seminal article [437].

This rather elementary stochastic technique consists in designing a reversible Markov chain, with a prescribed target invariant measure, based on sequential acceptance-rejection moves. Besides its simplicity, this stochastic technique has been used with success in a variety of application domains. The Metropolis-Hastings model is cited in *Computing in Science and Engineering* as being in the top 10 algorithms having the "greatest influence on the development and practice of science and engineering in the 20th century."

As explained by N. Metropolis and S. Ulam in the introduction of their pioneering article [435], the Monte Carlo method is, "essentially, a statistical approach to the study of differential equations, or more generally, of integro-differential equations that occur in various branches of the natural sciences."

In this connection, we emphasize that any evolution model in the space of probability measures can always be interpreted as the distributions of random states of Markov processes. This key observation is rather well known for conventional Markov processes and related linear evolution models.

More interestingly, *nonlinear* evolution models in distribution spaces can also be seen as the laws of Markov processes, but their evolution interacts in a nonlinear way with the distribution of the random states. The random states of these Markov chains are governed by a flow of complex probability distributions with often unknown analytic solutions, or sometimes too complicated to compute in a reasonable time. In this context, Monte Carlo and mean field methods offer a catalog of rather simple and cheap tools to simulate and to analyze the behavior of these complex systems.

These two observations are the stepping stones of the mean field particle theory developed in this book.

Mean field simulation

The theory of mean field interacting particle models had certainly started by the mid-1960s, with the pioneering work of H.P. McKean Jr. on Markov interpretations of a class of nonlinear parabolic partial differential equations arising in fluid mechanics [428]. We also quote an earlier article by T.E. Harris and H. Kahn [322], published in 1951, using mean field type and heuristic-like splitting techniques for estimating particle transmission energies.

Since this period until the mid-1990s, these pioneering studies have been further developed by several mathematicians; to name a few, in alphabetical order, J. Gärtner [265], C. Graham [295, 296, 297, 298, 299, 300, 301, 302, 303, 304, 305, 306], B. Jourdain [348], K. Oelschläger [450, 451, 452], Ch. Léonard [394], S. Méléard [429, 430, 431], M. Métivier [434], S. Roelly-Coppoletta [431], T. Shiga and H. Tanaka [516], and A.S. Sznitman [538]. Most of these developments were centered around solving Martingale problems related to the existence of nonlinear Markov chain models, and the description of propagation of chaos type properties of continuous time IPS models, including McKean-Vlasov type diffusion models, reaction diffusion equations, as well as generalized Boltzmann type interacting jump processes. Their traditional applications were essentially restricted to fluid mechanics, chemistry, and condensed matter theory. Some of these application domains are discussed in some detail in the series of articles [111, 112, 126, 317, 402, 128, 423]. The book [360] provides a recent review on this class of nonlinear kinetic models.

Since the mid-1990s, there has been a virtual explosion in the use of mean field IPS methods as a powerful tool in real-word applications of Monte Carlo simulation in information theory, engineering sciences, numerical physics, and statistical machine learning problems. These sophisticated population type IPS algorithms are also ideally suited to parallel and distributed environment computation [65, 269, 272, 403]. As a result, over the past few years the popularity of these computationally intensive methods has dramatically increased thanks to the availability of cheap and powerful computers. These advanced Monte Carlo integration theories offer nowadays a complementary tool, and a powerful alternative to many standard deterministic function-based projections and deterministic grid-based algorithms, often restricted to low dimensional spaces and linear evolution models.

In contrast to traditional MCMC techniques (including Gibbs sampling techniques [270], which are a particular instance of Metropolis-Hasting models), another central advantage of these mean field IPS models is the fact that their precision parameter is not related to some stationary target measure, nor of some burning time period, but only to *the size of the population.* This precision parameter is more directly related to the computational power of parallel computers on which we are running the IPS algorithms.

In the last two decades, the numerical solving of concrete and complex nonlinear filtering problems, the computation of complex posterior Bayesian distribution, as well as the numerical solving of optimization problems in evolutionary computing, has been revolutionized by this new class of mean field IPS samplers [93, 163, 161, 186, 222, 513, 547]. Nowadays, their range of application is extending from the traditional fluid mechanics modeling towards a variety of nonlinear estimation problems arising in several scientific disciplines; to name a few, with some reference pointers: Advanced signal processing and nonlinear filtering [104, 151, 161, 154, 163, 225, 222, 223, 288, 366, 364], Bayesian analysis and information theory [93, 133, 163, 165, 222, 252, 403], queueing networks [33, 296, 297, 299, 300, 301], control theory [373, 337, 338, 575], combinatorial counting and evolutionary computing [7, 163, 186, 513, 547], image processing [8, 150, 251, 476], data mining [490], molecular and polymer simulation [163, 186, 309], rare events analysis [125, 122, 163, 175, 176, 282], quantum Monte Carlo methods [16, 91, 175, 176, 326, 433, 498], as well as evolutionary algorithms and interacting agent models [82, 157, 286, 327, 513, 547].

Applications on nonlinear filtering problems arising in turbulent fluid mechanics and weather forecasting predictions can also be found in the series of articles by Ch. Baehr and his co-authors [25, 26, 28, 29, 390, 487, 537]. More recent applications of mean field IPS models to spatial point processes, and multiple object filtering theory can be found in the series of articles [101, 102, 103, 137, 221, 459, 460, 461, 510, 564, 565, 566, 567]. These spatial point processes, and related estimation problems occur in a wide variety of scientific disciplines, such as environmental models, including forestry and plant ecology modeling, as well as biology and epidemiology, seismology, materials science, astronomy, queuing theory, and many others. For a detailed discussion on these applications areas we refer the reader to the book of D. Stoyan, W. Kendall, and J. Mecke [532] and the more recent books of P.J. Diggle [218] and A. Baddeley, P. Gregori, J. Mateu, R. Stoica, and D. Stoyan [24].

The use of mean field IPS models in mathematical finance is more recent. For instance, using the rare event interpretation of particle methods, R. Carmona, J. P. Fouque, and D. Vestal proposed in [98] an interacting particle algorithm for the computation of the probabilities of simultaneous defaults in large credit portfolios. These developments for credit risk computation were then improved in the recent developments by R. Carmona and S. Crépey [95] and by the author and F. Patras in [187]. Following the particle filtering approach which is already widely used to estimate hidden Markov models, V. Genon-Catalot, T. Jeantheau, and C. Laredo [271] introduced particle methods for the estimation of stochastic volatility models.

More generally, this approach has been applied for filtering nonlinear and non-Gaussian Models by R. Casarin [106], R. Casarin, and C. Trecroci [107]. More recently, M. S. Johannes, N. G. Polson, and J.R. Stroud [345] used a similar approach for filtering latent variables such as the jump times and sizes in jump diffusion price models. Particle techniques can also be used in financial mathematics to design stochastic optimization algorithms. This version of particle schemes was used by S. Ben Hamida and R. Cont in [47] for providing a new calibration algorithm allowing for the existence of multiple global minima. Finally, in [196, 197], interacting particle methods were used to estimate backward conditional expectations for American option pricing.

For a more thorough discussion on the use of mean field methods in mathematical finance, we refer the reader to the review article [96], in the book [97].

As their name indicates, branching and interacting particle systems are of course directly related to individual based population dynamics models arising in biology and natural evolution theory. A detailed discussion on these topics can be found in the articles [56, 108, 110, 315, 313, 314, 442, 445, 446, 455], and references therein.

In this connection, I also quote the more recent and rapidly developing mean field games theory introduced in the mid-2000s by J.M. Lasry and P.L. Lions in the series of pioneering articles [381, 382, 383, 384]. In this context, fluid particles are replaced by agents or companies that interact mutually in competitive social-economic environments so that to find optimal interacting strategies w.r.t. some reward function.

Applications of game theory with multiple agents systems in biology, economics, and finance are also discussed in the more recent studies by V. Kolokoltsov and his co-authors [361, 362, 363], in the series of articles [9, 48, 83, 84, 376, 395, 449, 548], the ones by P.E. Caines, M. Huang, and R.P. Malhamé [329, 330, 331, 332, 333, 334, 335], as well as in the pioneering article by R. J. Aumann [23]. Finite difference computational methods for solving mean field games Hamilton-Jacobi nonlinear equations can also be found in the recent article by Y. Achdou, F. Camilli, and I. Capuzzo Dolcetta [4].

For a more detailed account on this new branch of games theory, I refer to the seminal Bachelier lecture notes given in 2007-2008 by P.L. Lions at the Collège de France [401], as well as the series of articles [287, 329, 426] and references therein.

A need for interdisciplinary research

As attested by the rich literature of mean field simulation theory, many researchers from different disciplines have contributed to the development of this field. However, the communication between these different scientific domains often requires substantial efforts, and often a pretty longer time frame to acquire domain specific languages so as to understand the recent developments in these fields. As a result, the communication between different scientific domains is often very limited, and many mean field simulation methods developed in some domains have been rediscovered later by others researchers from different scientific fields. For instance, mean field Feynman-Kac models are also known under a great many names and guises. In physics, engineering sciences, as well as in Bayesian statistical analysis, *the same* interacting jump mean field model is known under several lively buzzwords; to name a few: pruning [403, 549], branching selection [170, 286, 484, 569], rejuvenation [8, 134, 275, 336, 490], condensation [339], look-ahead and pilot exploration resampling [263, 403, 405], Resampled Monte Carlo and RMC-methods [556], subset simulation [20, 21, 22, 396, 399], Rao-Blackwellized particle filters [280, 444, 457], spawning [138], cloning [310, 500, 501, 502], go-with-the-winner [7, 310], resampling [324, 522, 408], rejection and weighting [403], survival of the fittest [138], splitting [121, 124, 282], bootstrapping [43, 289, 290, 409], replenish [316, 408], enrichment [54, 336, 262, 374], and many other botanical names.

On the other hand, many lines of applied research seem to be developing in a blind way, with at least no visible connections with mathematical sides of the field. As a result, in applied science literature some mean field IPS models are presented as natural heuristic-like algorithms, without a single performance analysis, nor a discussion on the robustness and the stability of the algorithms.

In the reverse angle, there exists an avenue of mathematical open research problems related to the mathematical analysis of mean field IPS models. Researchers in mathematical statistics, as well as in pure and applied probability, must be aware of ongoing research in some more applied scientific domains. I believe that interdisciplinary research is one of the key factors to develop innovative research in applied mathematics, and in more applied sciences.

It is therefore essential to have a unified and rigorous mathematical treatment so that researchers in applied mathematics, and scientists from different application domains, can learn from one field to another. This book tries to fill the gap with providing a unifying mathematical framework, and a self-contained and up-to-date treatment, on mean field simulation techniques for Monte Carlo integration. I hope it will initiate more discussions between different application domains and help theoretical probabilist researchers, applied statisticians, biologists, statistical physicists, and computer scientists to better work across their own disciplinary boundaries.

On the other hand, besides the fact that there exists an extensive number of books on simulation and conventional Monte Carlo methods, and Markov chain Monte Carlo techniques, very few studies are related to the foundations and the application of mean field simulation theory. To guide the reader we name a few reference texbooks on these conventional Monte Carlo simulations. The series of books by E.H.L. Aarts and J.H.M. Korst [1, 2], R.Y. Rubinstein [503, 504, 505, 506], and G. Pflug [471] discuss simulation and randomized techniques to combinatorial optimization, and related problems in operation research. The books by W.R. Gilks, S. Richardson, and D.J. Spiegelhalter [276], the one by B. D. Ripley [491], and the one by C.P. Robert and G. Casella [493] are more centered around conventional Monte Carlo methods, and MCMC techniques with applications in Bayesian inference.

The books by G. Fishman [256], as well as the one by S. Asmussen and

P.W. Glynn [18], discuss standard stochastic algorithms including discretization techniques of diffusions, Metropolis-Hasting techniques, and Gibbs samplers, with several applications in operation research, queueing processes, and mathematical finance. The book by P. Glasserman [284] contains more practically oriented discussions on the applications of Monte Carlo methods in mathematical finance. Rare event Monte Carlo simulation using importance sampling techniques are discussed in the book by J.A. Bucklew [85]. The book by O. Cappé, E. Moulines, and T. Rydèn [93], as well as the book [222] edited by A. Doucet, J.F.G. de Freitas, and N.J. Gordon, are centered around applications of sequential Monte Carlo type methods to Bayesian statistics, and hidden Markov chain problems.

In this connection, the present book can be considered as a continuation of the monograph [163] and lecture notes [161] edited in 2000, and the more recent survey article [161, 186], dedicated to Feynman-Kac type models. These studies also discuss continuous time models, and uniform concentration inequalities. In the present volume, we present a more recent unifying mean field theory that applies to a variety of discrete generation IPS algorithms, including McKean-Vlasov type models, branching and interacting jump processes, as well as Feynman-Kac models, and their extended versions arising in multiple object nonlinear filtering, and stochastic optimal stopping problems.

I have also collected a series of new deeper studies on general evolution equations taking values in the space of nonnegative measures, as well as new exponential concentration properties of mean field models. Researchers and applied mathematicians will also find a collection of modern stochastic perturbations techniques, based on backward semigroup methods, and second order Taylor's type expansions in distribution spaces. Last, but not least, the unifying treatment presented in this book sheds some new light on interesting links between physical, engineering, statistical, and mathematical domains which may appear disconnected at first glance. I hope that this unifying point of view will help to develop fruitfully this field further.

Use and interpretations of mean field models

I have written this book in the desire that post-graduate students, researchers in probability and statistics, as well as practitioners will use it.

To accomplish this difficult task, I have tried to illustrate the use of mean field simulation theory in a systematic and accessible way, across a wide range of illustrations presented through models with increasing complexity in a variety of application areas. The illustrations I have chosen are very often at the crossroad of several seemingly disconnected scientific disciplines, including biology, physics, engineering sciences, probability, and statistics.

In this connection, I emphasize that most of the mean field IPS algorithms

I have discussed in this book are mathematically identical, but their interpretations strongly depend on the different application domains they are thought. Furthermore, different ways of interpreting a given mean field particle technique often guide researchers' and development engineers' intuition to design and to analyze a variety of consistent mean field stochastic algorithms for solving concrete estimation problems. This variety of interpretations is one of the threads that guide the development of this book, with constant interplays between the theory and the applications.

In fluid mechanics, and computational physics, mean field particle models represent the physical evolution of different kinds of macroscopic quantities interacting with the distribution of microscopic variables. These stochastic models includes physical systems such as gases, macroscopic fluid models, and other molecular chaotic systems. One central modeling idea is often to neglect second order fluctuation terms in complex systems so that to reduce the model to a closed nonlinear evolution equation in distribution spaces (see for instance [126, 526], and references therein). The mean field limit of these particle models represents the evolution of these physical quantities. They are often described by nonlinear integro-differential equations.

In computational biology and population dynamic theory, the mathematical description of mean field genetic type adaptive populations, and related spatial branching processes, is expressed in terms of birth and death and competitive selection type processes, as well as mutation transitions of individuals, also termed particles. The state space of these evolution models depends on the application domain. In genealogical evolution models, the ancestral line of individuals evolves in the space of random trajectories. In genetic population models, individuals are encoded by strings in finite or Euclidian product spaces. Traditionally, these strings represent the chromosomes or the genotypes of the genome. The mutation transitions represent the biological random changes of individuals. The selection process is associated with fitness functions that evaluate the adaptation level of individuals. In this context, the mean field limit of the particle models is sometimes called the infinite population model. For finite state space models, these evolutions are described by deterministic dynamical systems in some simplex. In more general situations, the limiting evolution belongs to the class of measure valued equations.

In computer sciences, mean field genetic type IPS algorithms (*abbreviated GA*) are also used as random search heuristics that mimic the process of evolution to generate useful solutions to complex optimization problems. In this context, the individuals represent candidate solutions in a problem dependent state space; and the mutation transition is analogous to the biological mutation so as to increase the variability and the diversity of the population of solutions. The selection process is associated with some fitness functions that evaluate the quality of a solution w.r.t. some criteria that depend on the problem at hand. In this context, the limiting mean field model is often given by some Boltzmann-Gibbs measures associated with some fitness potential functions.

In advanced signal processing as well as in statistical machine learning theory, mean field IPS evolution models are also termed Sequential Monte Carlo samplers. As their name indicates, the aim of these methodologies is to sample from a sequence of probability distributions with an increasing complexity on general state spaces, including excursion spaces in rare event level splitting models, transition state spaces in sequential importance sampling models, and path space models in filtering and smoothing problems. In signal processing these evolution algorithms are also called particle filters. In this context, the mutation-selection transitions are often expressed in terms of a prediction step, and the updating of the particle population scheme. In this case, the limiting mean field model coincides with the evolution of conditional distributions of some random process w.r.t. some conditioning event. For linear-Gaussian models, the optimal filter is given by Gaussian conditional distributions, with conditional means and error covariance matrices computed using the celebrated Kalman filter recursions. In this context, these evolution equations can also be interpreted as McKean-Vlasov diffusion type models. The resulting mean field model coincides with the Ensemble Kalman Filters (*abbreviated EKF*) currently used in meteorological forecasting and data assimilation problems.

In physics and molecular chemistry, mean field IPS evolution models are used to simulate quantum systems to estimate ground state energies of a many-body Schödinger evolution equation. In this context, the individuals are termed walkers to avoid confusion with the physical particle based models. These walkers evolve in the set of electronic or macromolecular configurations. These evolution stochastic models belong to the class of Quantum and Diffusion Monte Carlo methods (*abbreviated QMC and DMC*). These Monte Carlo methods are designed to approximate the path space integrals in many-dimensional state spaces. Here again these mean field genetic type techniques are based on a mutation and a selection style transition. During the mutation transition, the walkers evolve randomly and independently in a potential energy landscape on particle configurations. The selection process is associated with a fitness function that reflects the particle absorption in an energy well. In this context, the limiting mean field equation can be interpreted as a normalized Schrödinger type equation. The long time behavior of these nonlinear semigroups is related to top eigenvalues and ground state energies of Schrödinger's operators.

In probability theory, mean field IPS models can be interpreted into two ways. Firstly, the particle scheme can be seen as a step by step projection of the solution of an evolution equation in distribution spaces, into the space of empirical measures. More precisely, the empirical measures associated with a mean field IPS model evolve as a Markov chain in reduced finite dimensional state spaces. In contrast to conventional MCMC models based on the long time behavior of a single stochastic process, the mean field IPS Markov chain model is associated with a population of particles evolving in product state spaces. In this sense, mean field particle methods can be seen as a stochastic linearization of nonlinear equations. The second interpretation of these models relies on an original stochastic perturbation theory of nonlinear evolution equations in distribution spaces. More precisely, the local sampling transitions of the population of individuals induce some local sampling error, mainly because the transition of each individual depends on the occupation measure of the systems. In this context, the occupation measures of the IPS model evolve as the limiting equation, up to these local sampling errors.

A unifying theoretical framework

Most of the book is devoted to the applications of mean field theory to the analysis of discrete generation and nonlinear evolution equations in distribution spaces. Most of the models come from discrete time approximations of continuous time measure valued processes. Because of the importance of continuous time models in physical, finance, and biological modeling, as well as in other branches of applied mathematics, several parts of this book are concerned with the deep connections between discrete time models measure valued processes and their continuous time version, including linear and nonlinear integro-differential equations.

Our mathematical base strongly differs from the traditional convergence to equilibrium properties of conventional Markov chain Monte Carlo techniques. In addition, in contrast with traditional Monte Carlo samplers, mean field IPS models are not based on statistically independent particles, so that the law of large numbers cannot be used directly to analyze the performance of these interacting particle samplers.

The analysis of continuous time interacting particle systems developed in the last decades has been mainly centered around propagation of chaos properties, or asymptotic theorems, with very little information on the long time behavior of these particle models and on their exponential concentration properties.

To the best of my knowledge, the first studies on discrete generation mean field particle models, uniform quantitative estimates w.r.t. the time parameter, and their applications to nonlinear filtering problems and genetic type particle algorithms were started in the mid-1990s in [151, 152], as well as in the series of articles [154, 198, 169, 170]. In the last two decades, these studies have been further developed in various theoretical and more applied directions. For a detailed discussion on these developments, with a detailed bibliography, I refer to [161, 163, 186], and references therein. In this connection, I apologize in advance for any possible errors or omissions due to the lack of accurate information.

While exploring the convergence analysis of discrete generation mean field models, the reader will encounter a great variety of mathematical techniques, including nonlinear semigroup techniques in distribution spaces, interacting empirical process theory, exponential concentration inequalities, uniform convergence estimates w.r.t. the time horizon, as well as functional fluctuation theorems. These connections are remarkable in the sense that every probabilistic question related to the convergence analysis of IPS models requires to combine several mathematical techniques. For instance, the uniform exponential concentration inequalities developed in this book are the conjunction of backward nonlinear semigroup techniques, Taylor's type first order expansions in distribution spaces, $\mathbb{L}_m$-mean error estimates, and Orlicz norm analysis or Laplace estimates.

Uniform quantitative $\mathbb{L}_m$-mean error bounds, and uniform concentration estimates w.r.t. the time horizon rely on the stability properties of the limiting nonlinear semigroup. These connections between the long time behavior of mean field particle models and the stability properties of the limiting flow of measures are not new. We refer the reader to the articles [161, 163, 169, 170, 160, 182] published in the early 2000s in the context of Feynman-Kac models, and the more recent studies [166, 186] for more general classes of mean field models.

The analysis of discrete generation genetic type particle models is also deeply connected to several remarkable mathematical objects including complete ancestral trees models, historical and genealogical processes, partially observed branching processes, particle free energies, as well as backward Markov particle models. A large part of the book combines semigroup techniques with a stochastic perturbation analysis to study the convergence of interacting particle algorithms in very general contexts. I have developed, as systematically as I can, the application of this stochastic theory to applied models in numerical physics, dynamical population theory, signal processing, control systems, information theory, as well as in statistical machine learning research.

The mean field theory developed in this book also offers a rigorous and unifying framework to analyze the convergence of numerous heuristic-like algorithms currently used in physics, statistics, and engineering. It applies to any problem which can be translated in terms of nonlinear measure valued evolution equations.

At a first reading, the frustration some practitioners may get when analyzing abstract and general nonlinear evolution models in distribution state spaces will be rapidly released, since their mean field interacting particle approximations provide instantly a collection of powerful Monte Carlo simulation tools for the numerical solution of the problem at hand. Several illustrations of this mean field theory are provided in the context of McKean-Vlasov diffusion type models, Feynman-Kac distribution flows, as well as spatial branching evolution models, probability hypothesis density equations, and association tree based models arising in multiple object nonlinear filtering problems.

I also emphasize that the present book does not give a full complete treatment of the convergence analysis of mean field IPS models. To name a few missing topics, we do not discuss increasing and strong propagation of chaos properties, and we say nothing on Berry-Esseen theorems and asymptotic large deviation principles. In the context of Feynman-Kac models, the reader interested in these topics is recommended to consult the monograph [163], and references therein. To the best of our knowledge the fluctuation, and the large deviation analysis, of the intensity measure particle models and some of the extended Feynman-Kac models discussed in this book are still open research problems.

While some continuous time models are discussed in the first opening chapter, Chapter 2, and in Chapter 5, I did not hesitate to concentrate most of the exposition to discrete time models. The reasons are threefold:

Firstly, in the opening chapter I will discuss general state space Markov chain models that encapsulate without further work continuous time Markov processes by considering path spaces or excursion type continuous time models. The analysis of discrete time models only requires a smaller prerequisite on Markov chains, while the study of continuous time models would have required a different and specific knowledge on Markov infinitesimal generators and their stochastic analysis. In this opening chapter, I underline some connections between discrete generation and mean field IPS simulation and the numerical solving of nonlinear integro-differential equations. A more detailed and complete presentation of these continuous time models and their stochastic analysis techniques would have been too much digression.

The interested reader in continuous time models is recommended to consult the series of articles [295, 302, 303, 428, 429, 430, 451, 452, 538] and the more recent studies [57, 109, 295, 349, 418]. Interacting jumps processes and McKean-Vlasov diffusions are also discussed in the book [360] and the series of articles [161, 173, 176, 178, 498]. Uniform propagations of chaos for interacting Langevin type diffusions can also be found in the recent study [200]. For a discussion on sequential Monte Carlo continuous time particle models, we also refer the reader to the articles by A. Eberle, and his co-authors [237, 238, 239].

Uniform propagation of chaos for continuous time mean-field collision and jump-diffusion particle models can also be found in the more recent studies [440, 441]. The quantitative analysis developed in these studies is restricted to weak propagation of chaos estimates. It involves rather complex stochastic and functional analysis, but it also relies on backward semigroup expansions entering the stability properties of the limiting model, as the ones developed in [161, 163, 169, 170, 160, 182] in the early 2000s, and in the more recent studies [166, 186]. In this connection, an important research project is to extend the analysis developed in [440, 441] to obtain some useful quantitative uniform concentration inequalities for continuous time mean field, collision and interacting jump-diffusion models w.r.t. the time horizon.

The second reason is that, apart from some mathematical technicalities, the study of continuous time models often follows the same intuitions and the same semigroup analysis of discrete time models. On the other hand, to the best of my knowledge, various nonasymptotic convergence estimates developed in this book, such uniform concentration inequalities w.r.t. the time horizon, the convergence analysis at the level of the empirical process, as well as the analysis of backward Feynman-Kac particle models, remain nowadays open problems for continuous time mean field models.

Our third reason comes from two major practical and theoretical issues. Firstly, to get some feasible computer implementation of mean field IPS algorithms, continuous time models require introduction of additional levels of approximation. On the other hand, it is well known that at any time discretization schemes induce an additional and separate bias in the resulting discrete generation particle algorithm (see for instance [155] in the context of nonlinear filtering models).

Last, but not least, the convergence analysis of time discretization schemes is also based on different mathematical tools, with specific stochastic analysis techniques. In this connection, it is also well known that some techniques used to analyze continuous time models, such as the spectral analysis of Langevin type reversible diffusions, fail to describe the convergence properties of their discrete time versions.

A contents guide

One central theme of this book will be the applications of mean field simulation theory to the mathematical and numerical analysis of nonlinear evolution equations in distribution spaces.

To whet the appetite and to guide the different classes of users, the opening chapters, Chapter 1, and Chapter 2, provide an overview of the main topics that will be treated in greater detail in the further development of this book, with precise reference pointers to the corresponding chapters and sections.

These two chapters *should not be skipped* since they contain a detailed exposition of the mean field IPS models, and their limiting measure valued processes discussed in this book. To support this work, we also discuss some high points of the book, with a collection of selected convergence estimates, including contraction properties of nonlinear semigroups, nonasymptotic variance theorems, and uniform concentration inequalities.

Our basis is the theory of Markov processes. Discrete, and continuous time, Markov processes play a central role in the analysis of linear, and nonlinear evolution equations, taking values in the space probability measures. In this context, these evolution models in distribution spaces can always be interpreted as the distribution of the random states of a Markov process. In this interpretation, the theory of Markov processes offers a natural way to solve these measure valued equations, by simulating repeated samples of the random paths of the stochastic process. To provide a development of the area pertinent to each reader's specific interests, in the opening chapter, Chapter 1, we start with a rather detailed discussion on different classes of measure valued evolution models, and their linear, and nonlinear, Markov chain interpretation models.

In order to have a concrete basis for the further development of the book, in Chapter 2, we illustrate the mathematical models with a variety of McKean-Vlasov diffusion type models, and Feynman-Kac models, with concrete examples arising in particle physics, biology, dynamic population and branching processes, signal processing, Bayesian inference, information theory, statistical machine learning, molecular dynamics simulation, risk analysis, and rare event simulations.

In Chapter 3, we introduce the reader to Feynman-Kac models and their application domains, including spatial branching processes, particle absorption evolutions, nonlinear filtering, hidden Markov chain models, as well as sensitivity measure models arising in risk analysis, as well as in mathematical finance. We also provide some discussions on path space models, including terminal time conditioning principles and Markov chain bridge models.

It is assumed that the interpretation of mean field Feynman-Kac models strongly depends on the application area. Each interpretation is also a source of inspiration for researchers and development engineers to design stochastic particle algorithms equipped with some tuning parameters, adaptive particle criteria, and coarse grained techniques. To guide the reader's intuition, in Chapter 4, we present four equivalent particle interpretations of the Feynman-Kac mean field IPS models; namely the branching process interpretation and related genetic type algorithms (*abbreviated GA*), the sequential Monte Carlo methodology (*abbreviated SMC*), the interacting Markov chain Monte Carlo sampler (*abbreviated i-MCMC*), and the more abstract mean field interacting particle system interpretation (*abbreviated IPS*).

From the mathematical perspective, we recall that these four interpretation models are, of course, equivalent. Nevertheless, these different interpretations offer complementary perspectives that can be used to design and to analyze more sophisticated particle algorithms. These new classes of IPS models often combine branching techniques, genealogical tree samplers, forward-backward sampling, island type coarse graining models, adaptive MCMC methodologies, and adaptive selection type models [11, 186, 227, 279, 280]. More sophisticated mean field IPS algorithms include adaptive resampling rules [60, 158, 159], as well as particle MCMC strategies [11], particle SMC techniques and interacting Kalman filters [12, 132, 163, 225, 253, 444, 457], approximate Bayesian computation style methods [36, 154, 155, 156], adaptive temperature schedules [279, 280, 511], and convolution particle algorithms [497, 558].

We also emphasize that McKean-Vlasov diffusion type models can be also combined with mean field Feynman-Kac type models. This sophisticated class of mean field IPS filtering models has been used with success to solve nonlinear filtering problems arising in turbulent fluid mechanics and weather forecasting predictions [25, 26, 28, 29, 390, 487, 537]. Related, but different classes of coarse grained and branching type mean field IPS models are also discussed in the series of articles [135, 144, 161, 186].

In Chapter 5, we discuss some connections between discrete generation Feynman-Kac models and their continuous time version. We briefly recall some basic facts about Markov processes and their infinitesimal generators. For a more rigorous and detailed treatment, we refer to the reference textbooks on stochastic calculus [355, 375, 454, 488]. We also use these stochastic modeling techniques to design McKean jump type interpretations of Feynman-Kac models, and mean field particle interpretations of continuous time McKean models, in terms of infinitesimal generators.

Chapter 6 focuses on nonlinear evolution of intensity measure models arising in spatial branching processes and multiple object filtering theory. The analysis and the computation of these nonlinear equations are much more involved than the traditional single object nonlinear filtering equations. Because of their importance in practice, we have chosen to present a detailed derivation of these conditional density models. Of course these conditional density filters are not exact; they are based on some Poisson hypothesis at every updating step. The solving of the optimal filter associated with a spatial branching signal requires computing all the possible combinatorial structures between the branching particles and their noisy observations.

The second part of this book is dedicated to applications of the mean field IPS theory to two main scientific disciplines: namely, particle absorption type models arising in quantum physics and chemistry; and filtering and optimal control problems arising in advanced signal processing and stochastic optimal control. These two application areas are discussed, respectively, in Chapter 7 and in Chapter 8. Some application domains related to statistical machine learning, signal processing, and rare event simulation are also discussed in the first two opening chapters of the book, Chapter 1, and Chapter 2. The list of applications discussed in this book is by no means exhaustive. It only reflects some scientific interests of the author.

Chapter 9 is an intermediate as well as a pedagogical step towards the refined stochastic analysis of mean field particle models developed in the further development of the book, dedicated to the theoretical analysis of this class of models. We hope the rather elementary mathematical material presented in this opening chapter will help to make the more advanced stochastic analysis developed in the final part of the book more accessible to theoreticians and practitioners both. This chapter focuses on Feynman-Kac particle models. More general classes of particle models arising in fluid mechanics, spatial branching theory, and multiple object filtering literature are discussed in Chapter 10, as well as in Chapter 13.

Our main goals are to analyze in some more detail the theoretical structure of mean field interpretations of the Feynman-Kac models. This opening chapter, on the theoretical analysis of mean field models, does not pretend to have strong leanings towards applications. Our aim was just to provide some basic elements on the foundations of mean field IPS models in the context of Feynman-Kac measures. The applied value of Feynman-Kac particle models has already been illustrated in some details in Chapter 1, as well as in Chapter 7, and in Chapter 8, through a series of problems arising in rare event simulation, particle absorption models, advanced signal processing, stochastic optimization, financial mathematics, and optimal control problems.

In Chapter 10, we investigate the convergence analysis of a general and abstract class of mean field IPS model. We begin with a formal description of mean field IPS models associated with Markov-McKean interpretation models of nonlinear measure valued equations in the space of probability measures. Then, we present some rather weak regularity properties that allow development of stochastic perturbation techniques and a first order fluctuation analysis of mean field IPS models. We also present several illustrations, including Feynman-Kac models, interacting jump processes, simplified McKean models of gases, Gaussian mean field models, as well as generalized McKean-Vlasov type models with interacting jumps. Most of the material presented in this chapter is taken from the article [166]. Related approaches to the analysis of general mean field particle models can be found in the series of articles [144, 152, 168].

Chapter 11 is dedicated to the theory of empirical processes and measure concentration theory. These techniques are one of the most powerful mathematical tools to analyze the deviations of particle Monte Carlo algorithms. In the last two decades, these mathematical techniques have become some of the most important steps forward in infinite dimensional stochastic analysis and advanced machine learning techniques, as well as in the development of statistical nonasymptotic theory.

For an overview of these subjects, we refer the reader to the seminal books of D. Pollard [480], one of A.N. Van der Vaart and J.A. Wellner [559], and the remarkable articles by E. Giné [277], M. Ledoux [391], and M. Talagrand [542, 543, 544], and the article by R. Adamczak [6]. In this chapter, we have collected some more or less well known stochastic techniques for analyzing the concentration properties of empirical processes associated with independent random sequences on a measurable state space. We also present stochastic perturbation techniques for analyzing exponential concentration properties of functional empirical processes. Our stochastic analysis combines Orlicz's norm techniques, Kintchine's type inequalities, maximal inequalities, as well as Laplace-Cramèr-Chernov estimation methods.

Most of the mathematical material presented in this chapter is taken from a couple of articles [166, 186]. We also refer the reader to a couple of articles by the author, with M. Ledoux [160] and S. Tindel [199], for complementary material related to fluctuations, and Donsker's type theorems, and Berry-Esseen type inequalities for genetic type mean field models. Moderate deviations for general mean field models can also be found in the article of the author, with S. Hu and L.M. Wu [174].

Chapter 12 and Chapter 13 are concerned with the semigroup structure, and the weak regularity properties of Feynman-Kac distribution flows, and their extended version discussed in Chapter 6. Chapter 14 is dedicated to the convergence analysis of the particle density profiles associated. It covers

Feynman-Kac particle models, and their extended version discussed in Chapter 6, as well as more general classes of mean field particle models.

This chapter presents some key first order Taylor's type decompositions in distribution spaces, which are the progenitors for our other results. Further details on the origins and the applications on these expansions and their use in the bias and the fluctuation analysis of Feynman-Kac particle models can be found in [151, 161, 163, 169, 186].

In Chapter 15, we focus on genealogical tree based particle models. We present some equivalence principles that allow application without further work of most of the results presented in Chapter 14 dedicated to the stochastic analysis of particle density profiles.

The last two chapters of the book, Chapter 16 and Chapter 17, are dedicated to the convergence analysis of particle free energy models and backward particle Markov chains.

Lecture courses on advanced Monte Carlo methods

The format of the book is intended to serve three different audiences: researchers in pure and applied probability, who might be interested in specializing in mean field particle models; researchers in statistical machine learning, statistical physics, and computer sciences, who are interested in the foundations and the performance analysis of advanced mean field particle Monte Carlo methods; and post-graduate students in probability and statistics, who want to learn about mean field particle models and Monte Carlo simulation.

I assume that the reader has some familiarity with basic facts of Probability theory and Markov processes. The prerequisite texts in probability theory for understanding most of the mathematical material presented in this volume are the books by P. Billingsley [53], and the one by A. N. Shiryaev [518], as well as the book by S. N. Ethier and T. G. Kurtz [375], dedicated to continuous time Markov processes.

The material in this book can serve as a basis for different types of advanced courses in pure and applied probability. To this end, I have chosen to discuss several classes of mean field models with an increasing level of complexity, starting from the conventional McKean-Vlasov diffusion type models, and Feynman-Kac distribution flows, to more general classes of backward particle Markov models, interacting jump type models, and abstract evolution equations in the space of nonnegative measures.

The mathematical analysis developed in this book is also presented with increasing degrees of refinements, starting from simple inductive proofs of $\mathbb{L}_m$-mean error estimates, to more sophisticated functional fluctuations theorems, and exponential concentration inequalities expressed in terms of the bias and the variance of mean field approximation schemes.

To make the lecture easier, I did not try to avoid repetitions, and any chapter starts with an introduction connecting the results developed in earlier parts with the current analysis. On the other hand, with a very few exceptions, I gave my best to give a self-contained presentation with detailed proofs.

The first type of lectures, geared towards applications of mean field particle methods to Bayesian statistics, numerical physics, and signal processing, could be centered around one of the two opening chapters, and one on selected application domains, among the ones developed in the second part of the book.

The second type, geared towards applications of Feynman-Kac IPS models, could be centered around the Feynman-Kac modeling techniques presented in Chapter 3, and their four probabilistic interpretations discussed in Chapter 4.

The third type, geared towards applications of mean field particle methods to biology and dynamic population models, could also be centered around the material related to spatial branching processes and multiple object filtering problems presented in Chapter 2 and in Chapter 6.

There is also enough material to cover a course in signal processing on Kalman type filters, including quenched and annealed filters, forward-backward filters, interacting Kalman filters, and ensemble Kalman filters developed in Section 8.2 and in Section 8.3.

More theoretical types of courses could cover one selected application area and the stability properties of Feynman-Kac semigroups and their extended version developed in Chapter 13. A semester-long course could cover the stability properties of nonlinear semigroups and the theoretical aspects of mean field particle models developed in the last part of the book.

More specialized theoretical courses on advanced signal processing would cover multi-object nonlinear filtering models, the derivation of the probability hypothesis density equations, their stability properties, and data association tree models (Section 6.3 and Chapter 13).

There is also enough material to support three other sequences of mathematical courses. These lectures could cover the concentration properties of general classes of mean field particle models (Chapter 1 and Chapter 10), concentration inequalities of Feynman-Kac particle algorithms (Chapter 14, Chapter 15, Chapter 16, and Chapter 17), and the concentration analysis of extended Feynman-Kac particle schemes (Chapter 6, Section 14.7, and Section 14.8).

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Most of the text also proposes many new contributions to the subject. The reader will also find a series of new deeper studies of topics such as uniform concentration inequalities w.r.t. the time parameter and functional fluctuation theorems, as well as a fairly new class of application modeling areas.

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