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Fluctuations in Markov Processes

Time Symmetry and Martingale Approximation

Springer

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To Raghu Varadhan, a continuous source of inspiration

Preface

In statistical mechanics as in many other fields, diffusion phenomena may arise from Markovian stochastic modeling. This has motivated, since the early investigations of Kolmogorov and Doeblin's seminal paper (Doeblin, 1938), an increasing interest in central limit theorems for Markov processes. Doeblin made a close connection between the validity of such theorems and the time mixing properties of the Markov process. Such mixing conditions, nowadays called Doeblin's conditions, are sometimes difficult to verify. In particular many problems in statistical mechanics are intrinsically infinite dimensional, and in that case the Doeblin mixing assumption typically does not hold.

In the 1960s Gordin (1969) introduced another more analytical approach, based on martingale approximation of additive functionals of Markov processes. Consider a Markov process $\{X_t,\ t \geq 0\}$ with an ergodic stationary probability measure $\pi(dx)$, and let $V(x)$ be a function on the state space of the process with mean zero with respect to π. Let L be the generator of the corresponding Markovian semigroup $P_t u(x) = \mathbb{E}_x[u(X_t)]$. Then if u is a function in the domain of L, the process $u(X_t) - u(X_0) - \int_0^t Lu(X_s)ds$ is a martingale. Solving the Poisson equation $Lu = V$ with a *nice* function u in the domain of L, one can express $\int_0^t V(X_s)ds$ as a martingale plus a boundary term, and reduce the problem to proving a central limit theorem for martingales. As we will explain in Chaps. 1 and 2, central limit theorems for martingales requires only ergodicity of the process and a global control of the corresponding quadratic variation.

Of course the possibility of inverting the generator L is related to the mixing properties of the process, but it permits to tailor the conditions to the particular function V we are studying. If L possesses a spectral gap, then the corresponding Poisson equation can be solved for any function V with mean zero.

However in many applications in statistical mechanics, the generator L does not have a spectral gap. The typical infinite dimensional situation deals with a dynamics that has conservation laws and there is an entire family of stationary ergodic measures. The classical example is given by the problem of the macroscopic diffusive behavior of a *tagged particle* in a system of interacting particles. The dynamics of the interacting particles may conserve the density and eventually some other quantities.

The problem of the tagged particle in exclusion processes (studied in detail in Part II of this book) motivated Kipnis and Varadhan to develop a general central limit theorem that exploits the time symmetries of the process. The idea in the article (Kipnis and Varadhan, 1986) can be summarized as follows: the asymptotic variance for $t^{-1/2}\int_0^t V(X_s)ds$ is given by

$$\sigma^2(V) = 2\int_0^\infty \mathbb{E}_\pi\big[V(X_t)V(X_0)\big]\,dt,$$

where $\mathbb{E}_\pi$ is the expectation with respect to the path measure of the process starting from the stationary measure π. If the measure is time-reversible, i.e. the generator L is self-adjoint in $L^2(\pi)$, then $\mathbb{E}_\pi[V(X_t)V(X_0)] \geq 0$ for all $t \geq 0$ and $\sigma^2(V)$ will be finite if this time correlation decays sufficiently fast. The condition $\sigma^2(V) < +\infty$ is much weaker than asking that V belongs to the range of L, and it translates to an integrability condition on the corresponding spectral measure (supported on the real line) around zero that is relatively easy to verify. A simple argument using this spectral measure shows that the martingale approximation can be done using the resolvent solution $u_\lambda = (\lambda - L)^{-1}V$, even when V is outside the range of L. In the introductory Chap. 1 we will explain this approach in detail for a simple example of a reversible (discrete time) Markov chain.

Some of the ideas discussed above were already present in the literature dealing with the problem of homogenization of diffusions in stationary ergodic random environments (cf. Kozlov 1979; Papanicolaou and Varadhan 1981), but it is in the aforementioned work of Kipnis and Varadhan (1986) that the connection with reversibility has been exploited fully and the finiteness of the variance $\sigma^2(V)$ has been formulated as a sufficient condition for the central limit theorems for reversible Markov processes.

Later on the theory has been extended to certain classes of *non-reversible* Markov processes, i.e. Markov processes with a stationary ergodic (but non-reversible) probability measure π. When this measure is explicitly known, the generator can be decomposed as the sum of a symmetric and an anti-symmetric operator in $L^2(\pi)$, $L = S + A$. If for a sufficiently large set C, that is a common core of L and S, there exists a finite constant K such that

$$\left(\int f L g\, d\pi\right)^2 \leq K \int f(-S)f\, d\pi \int g(-S)g\, d\pi, \qquad f, g \in C$$

then we say that L satisfies a *sector condition*. The name illustrates the fact that the spectrum of L, in general a subset of the complex plane, is contained now in a cone around the negative reals touching the imaginary axis only at 0, where the constant K is the tangent of the corresponding semiangle of the cone. There are many interesting examples of Markov processes that satisfy the sector condition: asymmetric exclusion processes with null average jump rate (studied in Sect. 5.3), *cyclic* random walks in random environment (Sect. 3.3), doubly stochastic random walks in one dimension (Sect. 3.6), diffusions with the random generator in a divergence form (Chap. 9).

Another class of processes where the theory can be extended is provided by Markov processes with *normal* generators L and their bounded perturbations (Sect. 2.7.5). This condition allows to deal with examples like random walks, or diffusions in time dependent random environment (Sect. 9.9).

A further extension concerns processes where the generator L satisfies a *graded sector condition*: this is the case where the space $L^2(\pi)$ can be decomposed into a direct sum of orthogonal subspaces, $L^2(\pi) = \bigoplus_{n\geq 0} \mathscr{A}_n$, and L satisfies a sector condition on each subspace with a constant K_n eventually growing to infinity not too fast (see Sect. 2.7.4 for the precise formulation of this condition). Examples include asymmetric exclusion processes in dimension $d \geq 3$ (Sect. 5.5, this example motivated the extension), and diffusions with Gaussian drifts (Chap. 12).

We also present some examples that go beyond sector type conditions:

- *diffusions in divergence free fields* with the stream matrix that is square integrable (i.e. finite Péclet number), can be dealt with by an approximation procedure (Chap. 11);
- *doubly stochastic random walks* in space-mixing environment in dimension 3 or higher, where an approximation procedure can be implemented (Sect. 3.5);
- *Ornstein–Uhlenbeck process in a random potential* (position-velocity Langevin diffusion). This is a very degenerate diffusion (noise acting only on the velocity), but time symmetry of the Gibbs measure can be exploited by changing sign of the velocity in the reversed process (see Chap. 13).

All these examples of the central limit theorem for processes with the generator not satisfying any sector condition exploit particular features of the dynamics. What is missing is a general theorem for non-reversible Markov processes. We expected the validity of the central limit theorem for any Markov process with stationary, ergodic measure π and a function V such that $(-S)^{-1/2}V$ belongs to $L^2(\pi)$. We are not aware of any counterexamples to this statement.

Description of the Content of This Book Part I concerns the general theory, and could be used as the base for a graduate course. Only some basic probability is required, in particular ergodic theorems and martingales. In the first chapter we expose the central limit theorem for a countable state space, discrete time, reversible Markov chains. This is the most elementary, non-trivial set-up where we can illustrate the basic ideas without spending much time on technicalities. In Chap. 2 we develop the theory for general continuous time Markov processes, and introduce the various sector conditions. In Chap. 3 we apply the theory to random walks in random environment on $\mathbb{Z}^d$, that are nice and relatively simple, although at the same time quite non-trivial examples of the general theory. We conclude this part of the book with Chap. 4 that contains estimates and variational formulas for the asymptotic variance $\sigma^2(V)$, which turn out to be quite useful in applications. In fact in some examples the central limit theorem follows by the application of the general theory, while proving strict positivity of the variance requires some extra effort.

Part II is completely dedicated to central limit theorems for exclusion processes, the problem which motivated the development of the theory presented in this book.

In Chap. 5, we introduce the simple exclusion process, prove the main properties of its generator, and examine central limit theorems for additive functionals. In the case where the jump rates of the particles are symmetric, this result is a straightforward consequence of the first part of the book since the generator is self-adjoint. If the jump rates have mean zero, the generator of the exclusion process satisfies a sector condition and we may still apply the general theory.

In the asymmetric case, the picture is different. The duality introduces an orthogonal decomposition of the L^2 space which permits to consider the central limit theorem from the perspective of the graded sector condition. However, one needs to assume that the dimension is larger than or equal to three to prove that the asymmetric part of the generator which changes the degree of a function satisfies hypothesis (2.45) assumed in the general theory. Moreover, the asymmetric part of the generator which keeps the degrees of the functions does not satisfy condition (2.50). To overcome this obstacle a method, known as the removal of the hard core interaction, has been developed and is presented in Theorem 5.19.

To proceed step by step, increasing progressively the level of difficulty, we first present a central limit theorem for additive functionals of asymmetric exclusion processes in dimension $d \geq 3$ when the density of particles is equal to $1/2$, in which case the asymmetric part of the generator which keeps the degree of the functions does not appear. In the following section we examine the full asymmetric case in $d \geq 3$. In the last section of this chapter we present some results on transient Markov chains needed in the chapter and which have intrinsic interest.

In the following two chapters, we extend the central limit theorem to the case of a tagged particle, deriving the self-diffusion coefficient of exclusion processes, and to the case of a second class particle which is connected to the equilibrium fluctuations from the hydrodynamic limit of the empirical measure, Kipnis and Landim (1999).

In the last chapter of this second part of the book we prove that the asymptotic variance depends smoothly on the density of particles. In particular, we show that the self-diffusion and the bulk diffusion coefficients are smooth functions, a property which has important consequences in the theory of hydrodynamic limits.

Part III deals entirely with diffusions in random environments. Chapter 9 contains the main applications of the general theory. It starts with the periodic environments, where a spectral gap is present in the dynamics. In the quasi-periodic case we illustrate the loss of compactness and of the spectral gap property. This motivates the study of general ergodic random environments. Chapter 10 contains variational principles for the *homogenized diffusion matrix*, while the following chapters contain some other applications and extensions: divergence free drifts (Chap. 11, where the homogenized diffusion is enhanced by the microscopic convection), Gaussian drifts (see Chap. 12), where we have included also the discussion on superdiffusion effect due to large convection. Chapter 13 deals with the Ornstein–Uhlenbeck process in a random potential. The final Chap. 14 is dedicated to the relation of this probabilistic approach with the classical analytic homogenization theory and the notions of G-convergence of operators and Γ-convergence of quadratic forms.

There are many problems and results related to this theory that we have not included:

- The theory is about Markov processes in a stationary, ergodic state, and is tailor made for situations where there can be many ergodic measures. So the central limit theorem obtained refers to the particular ergodic measure chosen, the diffusion coefficient may depend on it, and the convergence of the laws are *in probability* with respect to the initial chosen ergodic measure. There are many *almost sure* results for diffusions in random environments, and it remains an open problem in the case of interacting particles systems, like for the self-diffusion of the tagged particles (Part II), even in the reversible case.
- For the same reason we do not deal with non-stationary problems, or locally ergodic environments etc. Some limited results in these directions do exist in the literature.

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