Non-Gaussian fluctuations in stochastic models with absorbing barriers

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received 22 July 2011; accepted in final form 22 October 2011
published online 24 November 2011

PACS 02.50.-r – Probability theory, stochastic processes, and statistics
PACS 05.10.Gg – Stochastic analysis methods (Fokker-Planck, Langevin, etc.)
PACS 05.40.-a – Fluctuation phenomena, random processes, noise, and Brownian motion

Abstract – The dynamics of a one-dimensional stochastic model is studied in the presence of an absorbing boundary. The distribution of fluctuations is analytically characterized within the generalized van Kampen expansion, accounting for higher-order corrections beyond the conventional Gaussian approximation. The theory is shown to successfully capture the non-Gaussian traits of the sought distribution returning an excellent agreement with the simulations, for all times and arbitrarily close to the absorbing barrier. At large times, a compact analytical solution for the distribution of fluctuations is also obtained, bridging the gap with previous investigations, within the van Kampen picture and without resorting to alternative strategies, as elsewhere hypothesized.

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Studying the dynamics of a large ensemble of interacting entities is a fascinating field of investigations of broad applied and fundamental interest. Atom and nuclei result for instance in extended systems of mutually interacting discrete elements. Similarly, proteins can be ideally imagined as a coherent sea of microscopic actors that e.g. densely populate the inside of the cells. Social and human communities are also examples of systems that display rather intricate dynamics, microscopically governed by the very complex network of interlaced connections among individuals. Surprisingly, and as follows a widespread observation of cross-disciplinary breath, regular collective modes can spontaneously emerge at the macroscopic level, as resulting from the erratic dynamics of the microscopic discrete constituents [1–4].

The time evolution of such inherent stochastic system is generally described in terms of a master equation [5], a differential equation for the probability of observing the scrutinized system in a certain configuration at given time. In practically all cases of interest, solving the master equation proves to be a task of formidable complexity, and approximated strategies need to be implemented to gain analytical insight into the system being examined. The celebrated van Kampen expansion [6] represents a viable technique to enable one for analytical progress. It is customarily believed that such a method works efficiently well provided the system is defined in an open domain or, conversely, if it evolves sufficiently far from any existing boundaries [1]. As an emblematic example, when the system has to face an asymptotic extinction, thus evolving towards an attractive absorbing state, the van Kampen perturbative scheme is only assumed appropriate for short times. Recently, and to eventually bypass these supposedly stringent limitations, a different perturbative approach has been pioneered in [7] that suites for large times, when the system is feeling the absorbing barrier. Working within this generalized setting, and operating with reference to a paradigmatic model of systems with an absorbing state, the voter model, a closed expression for the distribution of fluctuations was obtained which agrees with direct

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simulations. The derivation rests however on speculative grounds, which, despite the a posteriori validation, seem to lack of a solid physical interpretation, fully justified from first principles.

The purposes of this letter are twofold. On the one side, and with reference to the same version of the voter model as considered in [7], we will analytically demonstrate that by extending the van Kampen expansion to include higher-orders corrections [8], beyond the classical approximation, allows us to accurately reproduce the observed distribution of fluctuations at any time. Non-Gaussian traits reflecting the presence of the absorbing barrier are nicely captured by the method, which proves therefore accurate also close to the boundary. Even more interesting, the van Kampen solution is shown to converge at late times to the distribution calculated in [7], this latter being hence explained within a sound and universal descriptive picture. It is worth emphasizing that the voter model is assumed as a mere case study. Our aim is in fact to elaborate on the methodological aspects and so provide a proof of principle on the adequacy of the generalized van Kampen system size expansion\footnote{As already remarked the voter model has been advocated in [7] to propose a perturbative scheme alternative to the van Kampen expansion. It seems therefore natural to operate within exactly the same setting when arguing, on the contrary, on the relevance of the van Kampen ansatz beyond the routinely adopted Gaussian approximation.}.

Let us start by introducing the stochastic discrete voter model. As in the spirit of [7], we consider a system made of \( N \) elements in mutual interactions, possibly organized in different species. Label with \( X_i \) the elements of a specific species and with \( X_0 \) all the other entities. The following chemical equations are proposed to rule the microscopic dynamics:

\[
\begin{align*}
X_1 + X_0 & \xrightarrow{1} 2X_0, \\
X_0 + X_1 & \xrightarrow{1-\nu} 2X_1, \\
X_1 + X_1 & \xrightarrow{\nu} X_1 + X_0
\end{align*}
\]

The master equation which stems from the above system reads

\[
\frac{d}{dt} P_n(t) = (\epsilon_n^+ - 1)[T(n+1|n)P_n(t)] + (\epsilon_n^- - 1)[T(n-1|n)P_n(t)],
\]

where \( P_n(t) \) is the probability of photographing the system at time \( t \) in a configuration with \( n \) individuals belonging to the population of \( X_1 \). The symbols \( \epsilon_n^\pm \) denote the so-called step operators [6], which act on a generic function \( f(n) \) as \( \epsilon_n^\pm f(n) = f(n \pm 1) \). The transition rates are given by

\[
\begin{align*}
T(n+1|n) &= (1-\nu) \frac{(N-n) \ n}{N} , \\
T(n-1|n) &= \nu \frac{N-n}{N} \ n + \epsilon_n^- \frac{n}{N} .
\end{align*}
\]

where the initial states are the right entries and the final states the left ones. As follows the above, \( n = 0 \) is an absorbing state while \( n = N \) corresponds to a reflecting barrier. The van Kampen approach requires imposing:

\[
\frac{n}{N} = \phi(t) + \frac{\xi}{\sqrt{N}},
\]

where \( 1/\sqrt{N} \) plays the role of a small parameter and paves the way to the perturbative expansion hereafter discussed. By inserting the working ansatz (2) into the master equation (1), and hierarchically organizing the resulting terms with respect to their \( N \)-dependence (see appendix), one obtains at the first order the mean-field deterministic equation for the continuum concentration \( \phi(\tau) \) (\( \tau \) being the rescaled time \( t/N \)), namely \( d\phi/d\tau = -\nu \phi \), whose solution reads \( \phi(\tau) = \phi_0 \exp(-\nu \tau) \). Higher-order contributions results in a generalized Fokker-Planck equation for the new probability \( \Pi(\xi, \tau) = P(\phi(k) + \xi/\sqrt{N}, \tau) \). By truncating the expansion at the second order yields the standard Fokker-Planck equation, which predicts Gaussian fluctuations. Allowing instead for higher-order corrections, generates a cascade of terms whose relative weights are controlled by the finite size \( N \). Through a lengthy but straightforward derivation that is described in the appendix one eventually ends up with

\[
\frac{\partial \Pi}{\partial \tau} = \sum_{k=1}^{\infty} \frac{1}{(k+1)!} \frac{1}{N^{(k-1)/2}} \frac{\partial^{k+1}}{\partial \xi^{k+1}} [f(\phi, k+1)\Pi] + \sum_{k=1}^{\infty} \frac{1}{k!} \frac{1}{N^{(k-1)/2}} \frac{\partial^{k}}{\partial \xi^{k}} [g(\phi, \xi, k)\Pi] + \sum_{k=1}^{\infty} \frac{1}{(k-1)!} \frac{1}{N^{(k-1)/2}} \frac{\partial^{k-1}}{\partial \xi^{k-1}} [q(\xi^2, k-1)\Pi],
\]

where

\[
\begin{align*}
f(\phi, k) &= \begin{cases} 2\phi - 2\phi^2 - \nu \phi + 2\nu \phi^2 & \text{for } k \text{ even}, \\
\nu \phi & \text{for } k \text{ odd},\end{cases} \\
g(\xi, \phi, k) &= \begin{cases} 2\xi - 4\phi \xi + 4\nu \phi \xi - \nu \xi^2 & \text{for } k \text{ even}, \\
\nu \xi^2 & \text{for } k \text{ odd},\end{cases} \\
q(\xi^2, k^2) &= \begin{cases} 2\xi^2(\nu - 1) & \text{for } k \text{ even}, \\
0 & \text{for } k \text{ odd}.\end{cases}
\end{align*}
\]

Formally, the positiveness of the probability \( \Pi(\cdot) \) is not guaranteed a priori under the (truncated) generalized Fokker-Planck evolution, an observation that was made rigorous in [9,10]. However, with reference to specific case studies [11], it was shown that unphysical negative values are just occasionally attained by \( \Pi(\xi, \tau) \), and punctually localized in the tails of the distribution. The phenomenon fades off when including a sufficiently large number of terms in the development. The adequacy of the prediction
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can be a posteriori evaluated via a direct comparison with the numerical experiments\(^2\).

To progress with the calculation, we set off to estimate the moments of the sought distribution \(\Pi(\xi, \tau)\). Let us recall that the moment of order \(h\) is defined as

\[
\langle \xi^h \rangle = \int_{-\infty}^{\infty} \Pi(\xi) \xi^h \, d\xi.
\]

Multiply both sides of the generalized Fokker-Planck equation by the factor \(\xi^h\) and integrate over \(\mathbb{R}\) in \(d\xi\). A straightforward manipulation yields

\[
\frac{d}{d\tau}(\langle \xi^h \rangle) = \\
+ \sum_{k=1}^{h-2} \frac{1}{(k+1)!} f(\phi, k+1) \frac{h!}{N^{(k-1)/2}} (h-(k+1+1)) \langle \xi^{k+1} \rangle \\
+ \sum_{k=1}^{h+2} \frac{1}{k!} \frac{h!}{N^{(k-1)/2}} (h-k+1) \langle \xi^{h-k+1} \rangle \\
+ \sum_{k=3}^{h+2} \frac{1}{(k-1)!} \frac{h!}{N^{(k-1)/2}} (h-(k-1)+2) \langle \xi^{h-(k-1)+2} \rangle,
\]

where use has been made of the supposed regularity of the distribution \(\Pi(\xi, \tau)\) to drop out the boundary terms resulting from integrating by parts\(^3\).

We therefore deal with a closed system of first-order differential equations for the moments of the distribution \(\Pi(\xi, \tau)\). We can integrate it numerically and so estimate the quantities \(\langle \xi^h \rangle\), for all \(h\), at any time \(\tau\). The knowledge of the moments enables us to immediately reconstruct the characteristic function, and so recover, upon Fourier transform inversion, the distribution \(\Pi(\xi, \tau)\). The predicted profiles are displayed in fig. 1 (solid line) for different times. A comparison is drawn with the outcome of direct stochastic simulations based on the exact

\[\text{Gillespie algorithm} [13] \text{ (symbols), returning excellent agreement. The distribution of fluctuations displays clear non-Gaussian traits. It gets in fact more and more skewed as time progresses, reflecting the non-trivial interplay with the absorbing boundary.} \]

Surprisingly, and at odds with what customarily believed, the van Kampen ansatz proves accurate well beyond the Gaussian approximation that is often invoked to justify its intrinsic validity. As a corollary, it seems tempting to argue that the transformation (2) from discrete to continuum variables is an exact one, and not just an approximation that presumably descends from the central-limit theorem, as occasionally speculated.

It is also very instructive to analyze the asymptotic fate of the distribution of fluctuations, as predicted within the realm of the van Kampen theory. Based on intuition, we expect that when time goes to infinity, the distribution \(\Pi(\xi, \tau)\) converges to a Dirac delta centred in zero. Indeed, plugging into the moments’ equations (3), the asymptotic mean-field solution \(\phi = 0\), and looking for stationary solutions of the obtained system (i.e. setting the derivatives to zero), one readily gets \(\langle \xi^h \rangle \rightarrow 0 \forall h\), the moments of a delta function. However, for times large enough that \(\phi \approx 0\), but before the system has relaxed to its stationary state, the generalized Fokker-Planck equation (3) reads

\[
\frac{d}{d\tau}(\Pi) = \nu \frac{d}{d\xi}(\Pi) + \frac{2-\nu}{2\sqrt{N}} \frac{d^2}{d\xi^2}(\Pi) + \nu \frac{d}{d\xi}(\Pi) + \frac{2-\nu}{2\sqrt{N}} \frac{d^2}{d\xi^2}(\Pi),
\]

where we have only retained the term in \(1/\sqrt{N}\) dropping higher-orders corrections. Perform now the scaling \(\xi \rightarrow \xi/\sqrt{N}\). Equation (6) can be cast in the form

\[
\frac{d}{d\tau}(\Pi) = \nu \frac{d}{d\xi}(\Pi) + \frac{2-\nu}{2\sqrt{N}} \frac{d^2}{d\xi^2}(\Pi).
\]

The large time distribution \(\Pi(\xi', \tau)\) is therefore insensitive to the system size \(N\) and bears consequently universal traits. Equation (7) can be solved analytically (see also [7]) to give

\[
\Pi(\xi', \tau) = \frac{2\nu}{2-\nu} \frac{1}{1-e^{\nu\tau}} \exp \left[ \frac{2\nu(\xi' + \xi_0 e^{-\nu\tau})}{(2-\nu)(1-e^{-\nu\tau})} \right] \\
\times \frac{\xi'}{\xi_0 e^{\nu\tau}} \frac{1}{I_1 \left( \frac{4\nu \sqrt{\xi_0^2 e^{2\nu\tau}}}{(2-\nu)(e^{\nu\tau} - 1)} \right)},
\]

where \(I_1(\cdot)\) is the modified Bessel function of the first kind. For large \(\tau\), recalling that \(I_1(x) \approx x/2\) when \(x\) is small, one can approximate eq. (8) as

\[
\Pi(\xi', \tau) \propto \xi_0^2 \left( \frac{2\nu}{2-\nu} \right) \exp \left[ \frac{-2\nu}{2-\nu} \xi' \right] \exp(-\nu\tau).
\]

Operating with the rescaled variable \(\xi'\), which it is worth emphasizing, emerges naturally within the van Kampen expansion, when the large time limit is being considered, it is equivalent to inserting into the governing master equation the modified ansatz \(n = N \phi + \xi'\). This

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Fig. 1: (Colour on-line) The distribution of fluctuations at distinct rescaled times \( \tau \). The snapshots refer to: (a) \( \tau = 5 \), (b) \( \tau = 36 \), (c) \( \tau = 41 \) and (d) \( \tau = 50 \). The symbols stand for direct stochastic simulations. The solid lines represent the theoretical predictions as obtained within the generalized Fokker Planck scenario. We have in particular truncated the sums in the Fokker-Planck (3) to \( k = 3 \) (\( 1/N^{3/2} \) corrections) and included 200 moments in the final estimates of the generating function. The dashed lines refer to the Gaussian solutions obtained working within the van Kampen expansion at the, conventional, next-to-leading approximation (\( 1/N^{1/2} \) terms). Here \( \nu = 0.01 \) and the distributions are normalized so to have the maximum equal to one.

Fig. 2: (Colour on-line) The distribution of fluctuations at large times. Left panel: the distribution \( \Pi(\xi, \tau) \) is plotted vs. \( \xi \) at \( \tau = 388 \). Symbols refer to the simulations (\( N = 1000 \)), while the solid line stands for the (normalized) solution (9) after the change of variable \( \xi' \rightarrow \xi \sqrt{(N)} \) is performed. Right panel: the distribution \( \Pi(\xi', \tau) \) is plotted as a function of the rescaled \( \xi' \). Symbols refer to numerical simulations relative to distinct \( N \). In particular, \( N = 500 \) (circles) and \( N = 1000 \) (triangles). The solid line stands for the (normalized) solution (9). Here \( \nu = 0.01 \) and the distributions are normalized to unit.

latter corresponds to the strategy adopted in [7] for the specific choice \( \alpha = 0 \). In other words, and interestingly enough, the expected fluctuations \( \xi' \) are comparable to the discrete population size \( n \), when the absorbing boundary is being approached. We have therefore recovered exactly the same solution as obtained in [7], while working within the generalized, but conventional, van Kampen approach. The adequacy of (9) is challenged in fig. 2 vs. numerical
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The work is partially supported by Ente Cassa di Risparmio di Firenze. Financial support from the program PRIN2009 is also acknowledged. DF acknowledges financial support from the EU 7th Framework Programme project Recognition.

Appendix

This appendix is devoted to reporting the details of the calculations that yield to the generalized Fokker-Planck equation (3) starting from the master equation (1).

\footnote{This is equivalent, in Fourier space, to the transformation \( \xi \to \xi'/\sqrt{N} \) of the original fluctuation \( \xi \).}

The first step in the perturbative approach requires to make explicit in the stochastic variable \( n \) the role of the fluctuations \( \xi \). Following the van Kampen prescription we impose

\[ n = N\phi(t) + \sqrt{N}\xi, \quad (A.1) \]

where \( \phi(t) \) stands for the deterministic variable and \( 1/\sqrt{N} \) plays the role of a small parameter in the expansion that we shall implement below. Let us notice first that a new probability distribution \( \Pi \) can be defined as \( \Pi(\xi, t) = P(n, t) \). A simple manipulation of the left-hand side of the master equation (1) yields hence

\[ \frac{\partial P}{\partial t} = -\sqrt{N}\frac{\partial \Pi}{\partial \xi} \frac{d\phi}{dt} + \frac{\partial \Pi}{\partial \xi}, \quad (A.2) \]

For large \( N \), the steps operators \( \epsilon^\pm_n \) that appear in the master equation (1) can be expanded:

\[ \epsilon^\pm_n = 1 \pm \frac{1}{\sqrt{N}} \frac{\partial}{\partial \xi} + \frac{1}{2N} \frac{\partial^2}{\partial \xi^2} + \ldots. \quad (A.3) \]

We then proceed by substituting (A.1) and (A.3) into the right-hand side of eq. (1) and rearranging the term so to bring together the contributions that display a homogeneous scaling \( \xi, N \). Consider the first of the two terms on the right-hand side of equation (1):

\[ (\epsilon^-_n - 1)[T(n + 1|n)P_n(t)] = \]

\[ (1 - \nu) \left[ \sum_{k=1}^{\infty} (-1)^k \frac{1}{k! N^{k/2}} \frac{\partial^k}{\partial \xi^k} [(\phi - \phi^2)\Pi] \right. \]

\[ + \sum_{k=1}^{\infty} (-1)^k \frac{1}{k! N^{k/2+1/2}} \frac{\partial^k}{\partial \xi^k} [(-2\xi\phi)\Pi] \]

\[ + \sum_{k=1}^{\infty} (-1)^k \frac{1}{k! N^{k/2+1}} \frac{\partial^k}{\partial \xi^k} [(-\xi^2)\Pi]] \quad (A.4) \]

The second term gives instead:

\[ (\epsilon^+_n - 1)[T(n - 1|n)P_n(t)] = \]

\[ + \sum_{k=1}^{\infty} \frac{1}{k! N^{k/2}} \frac{\partial^k}{\partial \xi^k} [(-\phi^2 + \phi + \nu^2\phi)\Pi] \]

\[ + \sum_{k=1}^{\infty} \frac{1}{k! N^{k/2+1/2}} \frac{\partial^k}{\partial \xi^k} [(2\nu^2\phi + \xi - 2\xi\phi)\Pi] \]

\[ + \sum_{k=1}^{\infty} \frac{1}{k! N^{k/2+1}} \frac{\partial^k}{\partial \xi^k} [(\nu\xi^2 - \xi^4)\Pi]. \quad (A.5) \]

Making explicit the terms corresponding to \( k = 1 \) in the first sum of eqs. (A.5) and (A.4) one isolates the contributions proportional to \( 1/\sqrt{N} \). Combining these terms
with the contribution \(-\sqrt{N} \cdot \partial \Pi / \partial \xi \cdot d\phi / dt\) in (A.2), expression:

we obtain

\[
- \frac{1}{\sqrt{N}} \frac{\partial \Pi}{\partial \xi} \frac{d\phi}{dt} = \frac{1}{\sqrt{N}} \frac{\partial}{\partial \xi} \left[ ((1-\nu)(-\phi + \phi^2) + \phi - \phi^2 + \nu \phi^2) \Pi \right],
\]

where the rescaled time \(\tau\) is defined as \(\tau = t/N\). Thus the following system of differential equations holds for the concentration amount \(\phi\):

\[
\frac{d\phi}{d\tau} = -\nu \phi, \quad (A.6)
\]

that in turn corresponds to working within the so-called mean-field approximation and eventually disregarding the finite-size (demographic) corrections. It is worth emphasizing that eq. (A.6) is here obtained by elaborating on the exact stochastic chemical model and exploring the infinite system size (\(N \to \infty\)) limit.

Higher-order contributions read

\[
\frac{\partial \Pi}{\partial \tau} = (1-\nu) \left[ \sum_{k=2}^{\infty} \frac{(-1)^k}{k!} \frac{1}{N^{k/2-1}} \frac{\partial^k}{\partial \xi^k} \left[ ((1-\nu)(-\phi + \phi^2) + \phi - \phi^2 + \nu \phi^2) \Pi \right] 
+ \sum_{k=1}^{\infty} \frac{(-1)^k}{k!} \frac{1}{N^{k/2+1/2}} \frac{\partial^k}{\partial \xi^k} \left[ \xi^2 \Pi \right] \right] 
+ \sum_{k=2}^{\infty} \frac{1}{k!} \frac{1}{N^{k/2-1}} \frac{\partial^k}{\partial \xi^k} \left[ (2\nu \phi \xi + \xi - 2\xi \phi) \Pi \right] 
+ \sum_{k=1}^{\infty} \frac{1}{k!} \frac{1}{N^{k/2+1/2}} \frac{\partial^k}{\partial \xi^k} \left[ (\nu \xi^2 - \xi^2) \Pi \right].
\]

By reorganizing the above terms according to their respective powers in \(N\), one obtains the equivalent

\[
\frac{\partial \Pi}{\partial \tau} = \sum_{k=2}^{\infty} \frac{1}{k!} \frac{1}{N^{k/2-1}} \frac{\partial^k}{\partial \xi^k} \left[ ((1-\nu)(-\phi + \phi^2) + (-\phi^2 + \phi + \nu \phi^2)) \Pi \right] + \left[ (2\nu \phi \xi + \xi - 2\xi \phi) \Pi \right] + \left[ (\nu \xi^2 - \xi^2) \Pi \right].
\]

Introducing the auxiliary functions \(f(\phi, k), g(\xi, \phi, k)\) and \(q(\xi, k^2)\) as defined by eqs. (4), we recover the generalized Fokker Planck equation (3).

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