Non-stationary Markovian Replication Process causing Diverse Diffusions

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We introduce a single generative mechanism with which it is able to describe diverse non-stationary diffusions. A non-stationary Markovian replication process for steps is considered, for which we analytically derive time-evolution of the probability distribution of the walker’s displacement and the generalized telegrapher equation with time-varying coefficients, and find that diffusivity can be determined by temporal changes of replication of a immediate step. By controlling the replications, we realize the diverse diffusions such as alternating diffusions, superdiffusions, subdiffusions, and marginal diffusions which are originated from oscillating, increasing, decreasing, and slowly increasing or decreasing replications with time, respectively.

I. INTRODUCTION

Starting with the purpose of understanding the random motion of Brownian particles, diffusive phenomena have been received great attention for a long time in the statistical physics as well as in recent various fields such as human geographical [1–4], hydrological [5, 6], biophysical [7–12], economic systems [13, 14], and so on. The Brownian motion follows the Fokker-Planck equation (FPE) well known as the diffusion equation for the probability density function (PDF) from which the mean-squared displacement (MSD) is linearly dependent on time, $\langle x_2^2 \rangle = 2D_0t$ where $D_0$ is the constant diffusion coefficient. This Brownian process is well described by a stationary Markovian model known as random walk [15, 16]. However recent studies report that MSD shows the nonlinear behavior rather than the linear behavior for time $[17–22]$. The MSD following the power-law behavior, $\langle x_2^2(t) \rangle \sim t^{2H}$ characterizes anomalous diffusion, where $H$ is called as the Hurst exponent which classifies superdiffusion ($H > 1/2$) in which the past and future random variables are positively correlated and thus persistence is exhibited, and subdiffusion ($0 < H < 1/2$) which behaves in the opposite way, showing antipersistence.

Efforts to describe mechanisms underlying anomalous diffusions have been tried through representative stochastic models such as fractional Brownian motion (fBM) where long-ranged temporal correlation between steps is given and the Hurst exponent ranges from 0 to 1 [23, 24], Lévy walk model that describes well superdiffusions by drawing a step length from the distribution with a heavy power-law tail and keeping a constant speed for a random time [24–26], continuous time random walks (CTRW) with the power-law distribution of time intervals for a step showing subdiffusions [15, 27], and scaled Brownian motion (sBM) which is described by a diffusion equation with explicitly time-dependent diffusion coefficient $[28, 29]$. These models show the non-stationarity or non-Markovianity which are responsible for the anomalous diffusive behaviors. The IBM is non-Markovian but stationary, and the Lévy walk, the CTRW and the sBM are semi-Markovian but non-stationary.

In addition, the stochastic models with the memory of whole previous trajectory in a walk process mimicking the movements of animals such as elephants [30] and monkeys [31], has been introduced and it is known that memorizing the history of a process which make a process be non-Markovian and non-stationary plays a key role in generating the long-term correlations between steps resulting in anomalous diffusions [30, 33]. However, memorizing whole history of previous steps is not easy and plausible except for some specific cases, rather it is much more acceptable to consider short-term memory like remembering just the immediate step. Although it did not start from the perspective of the short-term memory, it was already considered in the persistent random walk model [34] in which a step follows the previous step with a constant probability, resulting in a movement to the same direction that the walker was moving. Also it is known that such a process does not follow the diffusion equation but the telegrapher equation (TE) [35] which has an additional second order time derivative term of the PDF to the diffusion equation which introduces wave equation property and is related to ballistic motion of the diffusion particles, but asymptotically reduces to normal diffusive behavior [33, 36]. That is, although the telegrapher process has advantages in describing ballistic motion in early stages and is applicable to the diverse diffusion and transport phenomena [37, 38], eventually, it is a stationary normal diffusive process and not sufficient to explain property of nonstationary movements resulting in diverse diffusions appeared in nature.

In physical reality, nonstationary movements of living organisms are natural in making a adaptation for the various types of temporal stimuli coming from their natural environment [39]. In particular, in kinetics of eukaryotic cells under temporal chemotactic or mechanotactic signaling, it has been studied that cells response directly by changing their motion depending on temporal stimuli.
That is, to respond to such complex temporal stimuli a walker may move to the opposite direction to a previous step in a moment, or conversely, strengthen movements to the same direction. Thus memorizing previous steps can change with time and we modelize it with a time-varying replication probability which controls the degree of following the immediate step at the next step. Namely, a non-stationary persistent random walk model is introduced and a generalized TE with time-dependent coefficients is derived. We also calculate the relations between the time-dependent coefficients and the replication probability and thus show that explicit time dependence of the probability could produces long-term correlation between steps which results in diverse diffusions deviated from a normal diffusive behavior.

II. NON-STATIONARY MARKOVIAN REPLICAION MODEL

We consider a walker on a one dimensional homogeneous lattice with the uniform spacing \( l \) between the neighboring sites. With a regular time interval denoted as \( \tau \), the walker moves to one of the two neighboring sites. We denote the walker’s position at time \( t \) as \( x_t \), and the step walker takes as \( \sigma_t \), which is defined by the relation

\[
x_t = x_{t-\tau} + \sigma_t.
\]

The walker is initially at the origin. Details of the model is determined by a time-varying probability \( \alpha(t) \) which controls the dynamics of the process,

\[
\sigma_t = \begin{cases} 
\sigma_{t-\tau}, & \text{with a probability } \alpha(t) \\
-\sigma_{t-\tau}, & \text{with a probability } 1 - \alpha(t).
\end{cases}
\]

The first step(\( \sigma_{\tau} \)) is randomly chosen between the two possibilities \( \pm l \) with the equal probabilities \( 1/2 \). Successive steps and positions at \( t \geq 2\tau \) are determined by Eq. [1] and Eq. [2]. We note that the process defined as above is symmetric about the origin.

At each time \( t \), a step \( \sigma_t \) replicates or anti-replicates the latest step \( \sigma_{t-\tau} \). Since the next step is completely determined by the immediate step, this replication process is Markovian, while the probability of replication, \( \alpha(t) \), varies with time in general. Even if such a non-stationary nature is present, Markovianity of the step process makes the process analytically tractable. In terms of kinematics, anti-replication of the latest step corresponds to change of direction of motion, and when \( \alpha(t) \) is constant, the model reduces to the persistent random walk model [3]. From the perspective of memorizing a trajectory and concerning possible applications of the model not only to the diffusion processes in real space but also to the analysis of general two states time series, we prefer looking Eq. [2] as a replication-antireplication process rather than just alternating direction of motion. Thus, we call \( \alpha(t) \) and the process [3] the replication probability and the non-stationary Markovian replication process (NMRP), respectively.

III. TIME EVOLUTION OF THE PDF AND THE MSD

Now, we derive the time evolution of the probability distribution of the displacement \( P(x,t) \) for the NMRP model, which is the probability that the walker’s position is \( x \) at time \( t \), starting from the relation

\[
P(x,t) = \sum_{x_{\tau},x_{\tau-2\tau}} P(x,t|x_{\tau-\tau},x_{\tau-2\tau})P(x_{\tau-\tau},x_{\tau-2\tau}).
\]

Here, \( P(x_{t-\tau},x_{t-2\tau}) \) is the probability that the walker’s positions at times \( t-\tau \) and \( t-2\tau \) are \( x_{t-\tau} \) and \( x_{t-2\tau} \), respectively, and \( P(x,t|x_{t-\tau},x_{t-2\tau}) \) is the second order transition probability, which is a conditional probability that the walker’s position is \( x \) at time \( t \) given the two previous positions. The summation runs over all lattice sites. Because of the Markovianity of the step process [3], it is possible to use the second order transition probability which is determined in terms of only \( \sigma_t \) and \( \sigma_{t-\tau} \) at time \( t \) and is expressed by

\[
P(x,t|x_{t-\tau},x_{t-2\tau}) = \{\delta_{\sigma_{t-\tau},l} + \delta_{\sigma_{t-\tau},-l}\}
\times\{\alpha(t)\delta_{\sigma_t,\sigma_{t-\tau}} + [1 - \alpha(t)]\delta_{\sigma_t,\sigma_{t-\tau}}\}.
\]

Terms in the first bracket depict the two possible choices for the step \( \sigma_{t-\tau} \), and the other two terms in the second bracket indicate the probabilities that the replication or anti-replication occur at time \( t \), respectively.

By substituting the Eq. [4] into the Eq. [3], the time evolution of \( P(x,t) \) is described by the following master equation,

\[
P(x,t) = \alpha(t)\{P(x+l,t-\tau) + P(x-l,t-\tau)\}
+ \{1 - 2\alpha(t)\}P(x,t-2\tau),
\]

which is valid for \( t \geq 2\tau \). If \( \alpha(t) = 1/2 \), the last term on the right hand side vanishes, and Eq. [5] reduces to that of the normal random walk with symmetric probabilities.

Next, we take the continuum limit, considering the position and the time approximately as continuous variables. Expanding the master equation Eq. [5] into a Taylor series keeping the lowest non-vanishing order terms, the time evolution of the PDF \( \rho(x,t) \) in the continuum limit is obtained as follows,

\[
\frac{\partial \rho(x,t)}{\partial t} + R(t) \frac{\partial^2 \rho(x,t)}{\partial t^2} = D(t) \frac{\partial^2 \rho(x,t)}{\partial x^2},
\]

where

\[
R(t) = \frac{\tau}{2} \left[ \frac{3\alpha(t) - 2}{1 - \alpha(t)} \right]
\]

[1] [2]
and
\[ D(t) = D_0 \left[ \frac{\alpha(t)}{1 - \alpha(t)} \right] \tag{8} \]
with \( D_0 = l^2/2\tau \) being the diffusion coefficient for the normal diffusion. Eq. (8) becomes a generalized TE with the persistent coefficient \( R(t) \) and the diffusion coefficient \( D(t) \) depending on time. The relation between the coefficients \( R(t) \) and \( D(t) \) and the replication probability \( \alpha(t) \) are given by the Eq. (7) and the Eq. (6), respectively, which indicates that the larger \( \alpha(t) \), the larger coefficients. Note that when \( \alpha(t) \) approaches to 1, two coefficients \( R(t) \) and \( D(t) \) diverge, whereas the coefficient of the first term on the left hand side of Eq. (6) remains constant. Therefore, if the divergence is fast enough, a contribution from the first term on the left hand side of Eq. (6) becomes negligible. In this case, Eq. (6) evolves into the wave equation with the speed \( v = l/\tau \), which implies the occurrence of the ballistic motion of the walker. In the telegraph process, initial ballistic motion is transient as mentioned already. However, in the NMRP, ballistic motion appears whenever the replication is more dominant than the anti-replication, namely, \( \alpha(t) \) becomes close to 1. In more usual cases where \( \alpha(t) \) does not tend to 1 so fast, because of the relatively small value of the \( \tau \) in the continuum limit and the asymptotically small nature of the second order derivative of the PDF in \( t \) compared to the first order one, the second term on the left hand side of Eq. (6) can be neglected. In this case, Eq. (6) reduces to the diffusion equation for the PDF \( \rho(x,t) \) with the time dependent diffusion coefficient \( D(t) \) \cite{28,29,30},
\[ \frac{\partial \rho(x,t)}{\partial t} = D(t) \frac{\partial^2 \rho(x,t)}{\partial x^2} \tag{9} \]
and the solution is given by the Gaussian distribution provided zero mean of displacement,
\[ \rho(x,t) = \frac{1}{\sqrt{2\pi\langle x(t)^2 \rangle}} \exp \left[ -\frac{x^2}{2\langle x(t)^2 \rangle} \right]. \tag{10} \]

Now, we show that there is a unique relation between the MSD of NMRP and the replication probability, and by manipulating the replication probability, nearly any form of the MSD can be generated if the MSD does not exceed the ballistic limit set by the finite and constant maximum speed of the process, \( v = l/\tau \). By multiplying \( x^2 \) to both side of the Eq. (6) and then integrating with respect to \( x \) over all space, the following relation between \( \alpha(t) \) and the MSD is obtained,
\[ \alpha(t) = \frac{\langle x^2(t) \rangle - \tau \langle x(t)^2 \rangle}{l^2 + \langle x^2(t) \rangle - 3\tau \langle x(t)^2 \rangle}. \tag{11} \]
When the Eq. (9) could be considered, \( \langle x^2(t) \rangle \) in Eq. (11) is removed and the MSD is calculated for general \( \alpha(t) \) as
\[ \langle x^2(t) \rangle = 2D_0 \int_t^\infty \frac{\alpha(s)}{1 - \alpha(s)} ds. \tag{12} \]

If \( \alpha(t) \) does not change in time, the process reduces to normal diffusion. Thus, a stationary replication process can not make a deviation from the normal diffusive behavior in the asymptotic limit. The time-varying property in the replication process becomes the key point inducing diverse diffusions.

IV. DIFFUSIONS USING SEVERAL SPECIFIC REPLICATION PROBABILITIES

A. Alternating diffusions

In the experiments for the cellular motion, external temporal stimuli have been simply imposed by a step-function change in chemo-effector concentration \cite{40} or mechanotactic signaling of repeating step-like type \cite{41} and exponentiated sine-waves for more complex fluctuating signaling in time \cite{42}. For the responding movements to periodic temporal stimuli we can consider the periodic replication probability and if the value of probability changes from 0 to 1, we can also study the motion alternating from totally anti-persistent phase to persistent phase. As such an example, we have chosen the replication probability of \( \alpha(t) = \sin^2(\pi t/T) \), with the period \( T = N/5 \) where \( N \) is the total number of steps.

FIG. 1: Time evolution of \( P(x,t) \) for the oscillatory replication process, \( \alpha(t) = \sin^2(\pi t/T) \), with the period \( T = 2 \times 10^4 \). For the time interval between 0.4T and 0.8T, the exact \( P(x,t) \) obtained from solving Eq. (6) numerically (the black dashed lines) shows the perfect coincidence with the data obtained by simulating the model (the green lines). The inset (a) shows the simulation result of \( P(x,t) \) for two periods, in which periodic swelling and freezing of \( P(x,t) \) is observed. The inset (b) shows the simulated (the red circles) and numerically solved (the black solid line) MSD which shows a stair-like shape having periodic plateaus and sudden jumps. In this study, all simulations for the models have been done with the fixed values \( \tau = l = 1 \).

Overall, \( P(x,t) \) is composed of periodically repeating
swelling regions in which $\alpha(t)$ is around the maximum value and thus almost perfect replication happens, and freezing regions in which $\alpha(t)$ deviates from the maximum and the nature of anti-persistent is realized, (the inset (a) of Fig. 1). $P(x,t)$ around $\alpha(t) = 1$ is enlarged in the main panel of Fig. 1 in which a single peak of $P(x,t)$ at the origin at $t = 0.4T$ splits into two peaks away from the center after $t = 0.6T$. It shows that the walkers around the center is divided to the two opposite directions due to the almost perfect replications around $\alpha(t) = 1$ and then decreasing $\alpha(t)$ results in freezing walkers and the peaks are maintained until the next swelling point. However, after a several period such peaks disappear because repeating of the perfect replications makes much more small peaks and then a peak at the center is restored.

Characteristics of the periodic oscillation in the replication process directly propagate into the probability and the MSD shows a interesting behavior with the periodical stair-like shape in which plateaus of the MSD correspond to the freezing regions of $P(x,t)$, while sudden jumps appear in the swelling regions of $P(x,t)$ (the inset (b) of Fig. 1). Such an stepwise increasing MSD has been reported in [13] where there are two alternating waiting time distributions, one of which centered around zero and the other centered around some finite waiting time, where the standard deviations of both distributions are small. Such a setup leads to a movement in which the walker periodically repeats two sudden jumps and waitings where the waiting time is nearly a constant, thus making step-wise increasing MSD. On the other hand, in this case such a feature in the MSD does not occur because of the repetition of moving and stopping but continuous and periodic change from ultraslow ($\alpha(t) \sim 0$) to ballistic diffusion ($\alpha(t) \sim 1$).

The oscillating replication probability implies periodic and continuous alternation of the phase of the process between superdiffusion and subdiffusion. It can be compared to a dynamic system of intermittent locomotion which have been importantly studied by intermittent search models where discontinuous transition between explicitely defined two different diffusion phases are considered [14]. Pauses, along with changes in the duration and speed of motion form different intermittent locomotions which happens in contexts where animals adjust their motion to changing circumstances and thus the cumulant distances over time show step-like picture as well as another oscillatory pictures with increasing and pausing intervals [15].

So we consider another oscillatory motion with the MSD which has increasing and pausing intervals, $\langle x_t^2 \rangle \sim t/2 - \sin(2at)/4a$. $a$ is a constant and the MSDs with $a = 10^{-5}$ and $a = 5 \times 10^{-5}$ are shown in the Fig. 2 (a) and (b), respectively. Corresponding $\alpha(t)$’s by Eq. 11 with the MSDs oscillates from 0 to 0.5 (the insets of Fig. 2). The MSD is composed of periodically repeating plateaus and smoothly increasing regions, which correspond to the regions with the dominant anti-replication and the normal diffusive regions where $\alpha(t) \sim 1/2$, respectively. The shape of the MSD is similar to that of the Fig. 1 but the sudden increases have been smoothened due to the smaller maximum value of $\alpha(t)$.

We have shown that different diffusive phases can be alternated by an oscillatory replication probability, which implies that it may be a generative mechanism to be able to describe changes of diffusion phase with time shown in the kinetics of cells in external stimuli and intermittent locomotions of animals. However, what we have shown here is not about a specific system but about generic changes of diffusive phases, and it needs to be more closely analyzed to find which specific $\alpha(t)$ is appropriate to describe a specific system.

B. Superdiffusion with $H = 0.9$

To compare the early behaviors of two cases where $\alpha(t)$ of Eq. 11 and $\alpha_D(t)$ obtained by ignoring $\langle x_t^2 \rangle$ in Eq. 11 are used, respectively, we have used the MSD, $\langle x_t^2 \rangle = t^{2H}$ with $H = 0.9$. Fig. 3 (a) shows the MSD obtained through the simulation using the $\alpha(t)$, which shows excellent agreement with the given MSD. In Fig. 3 (b), we also plotted the simulation result using $\alpha_D(t)$. It shows that the data slightly deviate from the expected line. Taking the second derivative in Eq. 11 into account gives more accurate MSD. Although there is just a slight difference in the two MSDs, note that at the early times, $P(x,t)$ obtained by $\alpha(t)$ is distinguished from the
However, at large times $\alpha t$ is maintained by the left hand side of Eq. (6) at early times. (e) The PDF at time $t = 10^4$ is Gaussian, indicating the effect of the second term on the left side of Eq. (6) for the model (a). The solid line represents the Gaussian distribution showing the peaks at the possible maximum distances (Fig. 3 (c)), while $P(x, t)$ obtained by $\alpha_D(t)$ relatively follows the Gaussian (Fig. 3 (d)). However, at large times $P(x, t)$ obtained by $\alpha(t)$ also converges to the Gaussian distribution (Fig. 3 (c) and (d)) and thus it is sufficient to take just $\alpha_D(t)$ for the most of asymptotic behaviors (see Figure 3). The peaks of $P(x, t)$ at early times which resembles that of the Lévy walks [24] is because the divergence of $\mathcal{R}(t)$ is not so fast enough to make the second order derivative term in $t$ in Eq. (6) dominant, but significantly slows the convergence of $P(x, t)$ to the Gaussian distribution. In such cases, the effect survives in early dynamics of stochastic processes. Analysis of early dynamics is important in real and experimental environments in which it is difficult to take a sufficiently long time and thus the second term on the left hand side of Eq. (6) could play an important role in such contexts.

![Graphs showing MSD and PDFs](image)

**FIG. 3:** Simulation results of models created by the replication probabilities related to the given MSD $\langle x^2(t) \rangle = t^{2H}$ with $H = 0.9$. (a) The MSD data obtained using the $\alpha(t)$ in Eq. (11). The solid line represents the given MSD. (b) The MSD data obtained using $\alpha_D(t)$ which ignores the second order derivative of the MSD in Eq. (11). Results show that the models generate the MSD expected, while $\alpha(t)$ gives slightly more accurate coincidence with the MSD than $\alpha_D(t)$. Figure (c) and (d) show the PDFs corresponding to (a) and (b), respectively. Shape of the PDF is strikingly different from the Gaussian distribution after a sufficiently long time.

![Graphs showing plots of MSDs](image)

**FIG. 4:** Plots of the MSDs for anomalous diffusions with various $H$ induced by $\alpha_D(t)$ obtained from $\langle x^2(t) \rangle = t^{2H}$. In the inset, the corresponding $\alpha_D(t)$’s are plotted. The symbols representing the simulation data fall excellently on the solid lines of $t^{2H}$.

### C. Anomalous diffusions

We have also considered anomalous diffusions induced by the NMRP model. In Fig. 4, the MSDs for the anomalous diffusions with the Hurst exponents ranging from 0.1 to 0.9 are shown. Models have been generated with $\alpha_D(t)$ obtained by setting $\langle x^2(t) \rangle = t^{2H}$. For $H > 0.5$, $\alpha_D(t)$ increases with time, which induces the persistence in the process over time, resulting in the superdiffusions. While for $H < 0.5$, $\alpha_D(t)$ decreases with time, which invokes the anti-persistence showing the subdiffusions. Similar conclusion has been reported using the latest memory enhancement model [32] which can be thought of as a special case of the NMRP model. For instance, the positive latest memory enhancement model can be reproduced in the framework of the NMRP if we use $\alpha(t) = 1 - 1/2tp$ with $p$ being the memory parameter.

### D. Marginal diffusions

Fig. 5 shows simulation results for logarithmic MSDs which are generated by $\alpha(t)$’s using (a) $\langle x^2(t) \rangle \sim \ln t$, and (b) $\langle x^2(t) \rangle \sim \ln \ln t$. In each figures, excellent agreements between the given MSDs and the simulation results are shown. In the NMRP model, logarithmically slow subdiffusion is achieved by fast decreasing replication probability from the value of 0.5 (the inset of Fig. 5 (a)), that is, the probability that the walker escapes away from a position decreases more rapidly than that of subdiffusions with time and the anti-persistence is strongly developed. Such ultra-slow diffusions have been reported in various contexts [31, 46–50], and often arise as a marginal behavior of the subdiffusion with $H = 0$.

The MSD of the type of $\ln \ln t$ also appears in the
FIG. 5: The plot of the simulated MSDs using (a) $\langle x^2(t) \rangle = \ln t + 1$ and (b) $\langle x^2(t) \rangle = t \ln t + 1$. The insets show the corresponding $\alpha(t)$ calculated from Eq. (11), respectively. Stars and circles represent the data obtained from the simulation and the solid lines in each plots represent the analytic functions of the MSD.

Marginal behaviors of the superdiffusions [30, 32, 51], while in the NMRP model it is embodied with $\alpha(t)$ increasing slowly compared to the cases of superdiffusions as shown in the Fig. 5 (b). Thus the marginal behaviors of anomalous diffusions can be also induced by a single origin, the NMRP with appropriate replication probabilities.

V. CONCLUSION

In conclusion, we have proposed a non-stationary random walk model in which the steps are given by a Markov process replicating the immediate step with a time-varying probability. The master equation for the probability has been analytically acquired and the generalized TE for the PDF has been derived, from which we have obtained the general relation between the time-varying replication probability and the MSD with accuracy up to the second order. We realized several interesting cases such as alternating diffusions, anomalous diffusions, and marginal diffusions. Although the stepping process is Markovian, the time-varying nature of replication develops the long-term correlation between steps and the corresponding diffusive behaviors, i.e. ballistic, super, sub, slow-sub, and ultraslow diffusive phases as well as normal diffusion have been induced depending on the values of the replication probability changing in time. For oscillatory replication probability, alternating diffusions of different diffusion phases have been induced, increasing (decreasing) replication probability with the value larger (smaller) than 0.5 have caused superdiffusions (subdiffusions). This single mechanism inducing diverse diffusions may provide a theoretical guide to experimental results of various types of diffusions and furthermore, non-stationary stochastic processes shown in diverse fields.

We also remark that the further studies of the relation between a general replication probability and the auto-correlation function of steps will be helpful to elucidate the actual mechanism generating these long-term correlations. Non-stationarity of the model would invoke the ergodicity breaking [52, 53] and the characteristics represented by the time average should be dealt separately from the results in this study which are obtained from the ensemble averages.

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