

Necessary criterion for distinguishing true superdiffusion from correlated random walk processes

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A difficulty in interpreting phenomena related to anomalous diffusion concerns how to identify scale invariant superdiffusive from Markovian correlated random walk processes. Here we propose a criterion that can distinguish between these two kinds of random walks and describe its usefulness in interpreting real data. To do so, we estimate the correlation time τ of the orientation persistence of a general correlated random walk. If the experimentally observed random walk appears diffusive on scales larger than τ , then the data cannot support the possibility of superdiffusion. We argue that the criterion is a necessary but not sufficient condition for establishing true superdiffusive behavior.

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I. INTRODUCTION

A classic problem in physics concerns the type of diffusion generated by the dynamics underlying random walks (RW)[1–3]. For large enough times t the root mean square (rms) displacement of the RW scales as t^α . Normal diffusion leads to $\alpha=1/2$ and super(sub)-diffusion corresponds to $\alpha>1/2$ ($<1/2$). In this respect, different processes can be associated to different classes of RW. For instance, correlated random walks (CRW) are characterized by retention of directional memory, finding applications [4] in problems as diverse as tracer diffusion in lattice gas systems [5], polymers chains [6,7], scattering [6,8], and animal motion [9]. But due to their Markovian nature, CRW tend asymptotically to Brownian diffusion for times beyond a correlation time τ . On the other hand, Lévy walks (or flights) (LW) [1,2] can give rise to genuine superdiffusive behavior ($\alpha>1/2$) in a number of phenomena [1,10–12]. In contrast with CRW, LW models use a broad class of move length distributions that renormalize to the Lévy-stable distribution [1]. For the steps ℓ_j , the long-range tails of such distributions follow the power law

$$P(\ell_j) \sim \ell_j^{-\mu}, \quad \ell_j \gg \ell_0, \quad (1)$$

where ℓ_0 is a typical lower cutoff distance for the power-law tail regime and the exponent $\alpha_L = \mu - 1$ (for $2 \leq \mu \leq 3$) is the Lévy index. For $2 \leq \mu < 3$, one obtains superdiffusion. Normal diffusion results for $\mu \geq 3$. The limit $\mu \rightarrow 1$ leads to ballistic motion.

The above two classes of RW models have a high degree of explanatory power in many concrete instances. But exactly which one to choose will depend on the distinct statistical and scaling properties of the system in hand (see, e.g.,

Ref. [13]). Consider animal movement for example. Taken as a whole, both CRW and LW can adequately account for animal motion [14,15]. However, in random foraging [11,16] there are certain ecological mechanisms which, in specific cases, can provide the necessary clues for the identification of the model class resulting in the best search strategies [17]. On the other hand, the absence of *a priori* extra information may pose great challenges in interpreting real data. For instance, in ecological studies the same data set can lead to apparent agreement with both kinds of RW [15]. Similar issues are important in classifying experimental data for cell motility [18,19], where both normal as well as anomalous diffusion can arise. Moreover, Gaussian as well as non-Gaussian velocity distributions do occur [19].

In fact, the necessity to better characterize experimentally the type of diffusion (i.e., normal versus anomalous) exists in contexts as diverse as surface growth, molecular dynamics, and nuclear spectra analysis [20]. Our aim here is to propose a general criterion that distinguishes more carefully between diffusive and scale invariant superdiffusive processes. Furthermore, we show how to apply it to experimental data, establishing whether the amount of information is sufficient to identify the type of diffusion.

In principle many methods can be used to detect correlations in time series. For example, usually it is not complicated to detect correlations in CRW models which are absent in Lévy walks and flights. However, the nature of experimental data creates extra difficulties to make such distinctions, since in practice one “slices” the observed trajectory into many small steps to generate a RW [9]. For example, the most commonly used standard procedures of trajectory discretization into step lengths assume that animal movement is a continuous process. So, the transformation of a recorded path into a discretized RW is somewhat arbitrary. In particular, the values of the “turning angles” between successive RW steps depend greatly on the values of the step lengths, which in turn, depend on different aspects of the discretization procedure (e.g., whether the step length are fixed or

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variable). Thus, intrinsically the discretization introduced by RW methods is an artefactual technicality. These procedures, used to digitize experimental data, typically lead to RW with a Gaussian-like distribution of step lengths but having correlations in the velocity vectors. A relevant parameter is the maximum tolerance for the deviation between the discretized random walk and the original trajectory. Smaller tolerances lead to smaller RW step sizes on average, i.e., one obtains a higher resolution for the RW.

For these reasons even a LW, after discretization, will appear to have a Gaussian-like distribution of step sizes with long-range (non-Markovian) correlations between successive step velocity vectors. The asymptotic power law distribution of step sizes in the original LW becomes lost in the discretization. To compensate this artefact, the discretized steps maintain directional memory for distances equal to the original LW step sizes. Hence, a major challenge in analyzing experimental data concerns how to distinguish LW from CRW processes. In this context, the criterion we propose may represent a different approach to study and analyze experimental data.

II. METHODS AND RESULTS

A. Markovian correlated random walks

Consider two-dimensional CRW models, in which persistence (or directional memory) is controlled by the probability distribution of the relative turning angles. CRW models cannot have scale invariance, presenting, instead, a characteristic scale (or time τ) associated with the exponentially decaying correlations typical of Markov processes. To obtain τ , we define an adimensional two-point correlation function in terms of the RW step vectors \mathbf{r}_j as $C(|j-i|) \equiv \langle \mathbf{r}_j \cdot \mathbf{r}_i \rangle / \langle r_j r_i \rangle$, where i, j are integer indices representing steps. We assume that a CRW process has mutually independent and identically distributed step lengths r_j (of finite variance) and turning angles θ_j . So, $C(1) = \langle \mathbf{r}_j \cdot \mathbf{r}_{j-1} \rangle / \langle r_j r_{j-1} \rangle$ reads

$$C(1) = \langle \cos[\theta] \rangle = \int_{-\pi}^{+\pi} d\theta \cos[\theta] f_w(\theta), \quad (2)$$

with f_w denoting the circular ‘‘wrapped’’ probability density function (PDF) of relative turning angles. In the above equation θ represents the angle between two successive step vectors, so only the relative orientations, but not the actual turning angles, have correlations. For circular statistics [21] the mean resultant length ρ and mean direction $\bar{\theta}$ are related to the first circular characteristic function by $\phi_1 \equiv \langle \exp[i\theta] \rangle = \rho \exp[i\bar{\theta}]$. Unless $\bar{\theta}=0$, the CRW will contain ‘‘loops’’ that prevent persistence. Therefore, we can restrict our attention to the case $\bar{\theta}=0$, so that $\rho = \alpha_1 = C(1)$. Note that $\rho=1$ for a δ distribution, and $\rho=0$ for a uniform distribution. The Markovian character of CRW implies $C(t/t_0) \sim [C(1)]^{t/t_0} = \exp[(t/t_0) \ln[\langle \cos[\theta] \rangle]]$, where t_0 is the typical time of one step. We thus have $\tau = -1/\ln[\langle \cos[\theta] \rangle]$ as the adimensional correlation time (or length) measured in step units. The validity of this general expression extends to all one-step Markovian CRW models. For any scale a few orders of mag-

nitude larger than τ , the CRW appears Brownian because the model cannot keep the orientations correlated at such relatively large scales.

B. Criterion for superdiffusion

The natural question is then whether a data set supports genuine superdiffusion (e.g., a LW) as opposed to a CRW that only appears superdiffusive at sufficiently small scales. Our results suggest a natural criterion for determining when a data set contains enough information to answer to this question. Since a CRW only converges to Brownian motion on scales much larger than τ , any data set spanning a period Δ not larger than the correlation time does not contain sufficient information to make such a distinction with any level of statistical significance. We can estimate $\tau_{\text{meas.}} \equiv -1/\ln[\langle \cos[\theta] \rangle_{\text{meas.}}]$, in which the expectation $\langle \cos[\theta] \rangle_{\text{meas.}}$ denotes the experimentally measured value of the first cosine moment. Since we can typically infer $\tau_{\text{meas.}}$ from only a relatively small stretch of data, we can practically always calculate an upper bound for τ . We thus propose a necessary but not sufficient condition for establishing superdiffusive behavior:

$$\Delta \gg \tau_{\text{meas.}} = -\frac{1}{\ln[\langle \cos[\theta] \rangle_{\text{meas.}}]}. \quad (3)$$

Specifically, if a given finite data set corresponds to a time scale Δ two orders of magnitude larger than the value of $\tau_{\text{meas.}}$, then we can in principle distinguish CRW from true superdiffusive RW. Indeed, a CRW process at this scale would contain 10^2 or more independent RW stretches, thereby providing adequate statistics.

A genuinely superdiffusive RW will have a correlation time that diverges, but the estimated value $\tau_{\text{meas.}}$ via $\langle \cos[\theta] \rangle_{\text{meas.}}$ can never diverge unless the turning angle distribution is a δ . If a given data set does not span over such a long period then only indirect methods of inferring genuine superdiffusion can be employed, such as tests of self-affinity or direct estimation of the correlation function to check for long range power law decay of the turning angle memory retention. On the other hand, if a given data set satisfies the criterion, then a direct test of superdiffusion on scales larger than $\tau_{\text{meas.}}$ can eliminate possible spurious false positives for shorter scales that arise due to Markovian turning angle persistence.

C. Applications and examples

To demonstrate how the criterion, Eq. (3), helps distinguishing between normal and anomalous diffusion we consider two distinct RW, but with identical turning angle PDF. The RW *model 1* is a genuine superdiffusive random walk, constructed as the following:

(i) First, we generate a preliminary LW with increments or step sizes ℓ_j ($j=1, 2, \dots, N$) given by Eq. (1). We choose $\mu=2$, $\ell_0=1$, and truncate the flights larger than 10% of the total RW length. Then, we use this LW as a blueprint or skeleton to create N small CRW. In these CRW the individual steps have length ℓ_0 and turning angles obtained from a

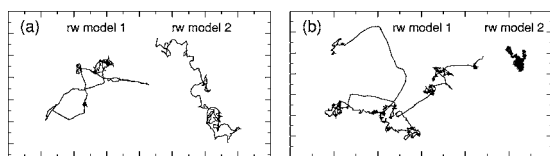


FIG. 1. Two random walks with identical turning angle distributions shown on a vertical \times horizontal scale of: (a) 165×400 units, with t not very much larger than $\tau_{\text{meas.}} \approx 10$; (b) 7000×12000 units with $t \gg \tau_{\text{meas.}} \approx 10$. Here $\ell_0 = 1$ unit.

wrapped Cauchy distribution (WCD; see Sec. II D below). For the j th set, the number of total steps N_j is given by the largest integer $\leq \ell_j / \ell_0$. Furthermore, the WCD width parameter, ρ_j , comes from $\rho_j = (e^{-1} - \exp[-\ell_0 / \ell_j]) / (e^{-1} - 1)$. The j th CRW will have a correlation length that increases as ℓ_j increases.

(ii) Next, we concatenate the N CRWs from (i), maintaining the ordering according to j . This resulting single RW with a turning angle sequence $\theta_i^{(a)}$ ($i=1, 2, \dots, N_c = N_1 + N_2 + \dots + N_N$) will appear locally as a CRW, but has Lévy-like global properties because we “tune” the local CRW correlation time according to the value of the original LW step size ℓ_j via ρ_j .

(iii) Last, we note that the concatenation introduces a nonstationarity in the turning angle distribution, because each segment j has a different WCD (i.e., a different ρ_j). Therefore, to compensate for the nonstationarity, we generate the set $\theta_i^{(b)}$ ($i=1, 2, \dots, N_c/2$) from a WCD with $\rho=0.9$. Then, we take as RW *model 1* the sequence $\theta_1^{(a)} + \theta_1^{(b)}, \theta_2^{(a)} - \theta_1^{(b)}, \dots, \theta_{2i-1}^{(a)} + \theta_i^{(b)}, \theta_{2i}^{(a)} - \theta_i^{(b)}, \dots, \theta_{N_c-1}^{(a)} + \theta_{N_c/2}^{(b)}, \theta_{N_c}^{(a)} - \theta_{N_c/2}^{(b)}$. The addition of pairwise perfectly anticorrelated turning angles will make the final distribution less nonstationary, since locally the distribution of the sums will equal the convolution of a $\rho = \rho_j$ WCD with a $\rho = 0.9$ WCD. Specifically, we obtain a series with perfectly stationary mean and sufficiently stationary variance ($\sim \rho = 0.9$), so that the beginning and end of segment j will no longer always be easily detectable without prior knowledge.

We construct the RW *model 2* by shuffling the sequence of turning angles of *model 1* in step (iii). By doing so we destroy any Lévy-like property arising from the ρ_j 's, and end up with a model very similar to a CRW with $\rho = 0.9$. The long range as well as short range (i.e., all) correlations become completely destroyed by this procedure.

In both models the measured $\tau_{\text{meas.}} \approx 10$ comes from the dominant $\rho = 0.9$ value of the set of anticorrelated turning angles $\theta^{(b)}$. The two cases have similar visual appearance on short scales [Fig. 1(a)], but differ quite considerably at larger scales [Fig. 1(b)]. Only the first model will also appear superdiffusive on scales larger than $\tau_{\text{meas.}}$. The point is that *model 2* maintains directional memory solely due to the turning angle distribution. On the other hand, *model 1* maintains directional memory by approximately following the underlying Lévy walk skeleton. Regarding the amount of data points, notice that Fig. 1(a) (with 800 points) shows approximately $800 / \tau_{\text{meas.}} = 80$ uncorrelated stretches of RW, whereas Fig. 1(b) (with 10^5 points) contains thousands of uncorrelated stretches. Whereas thousands of independent data

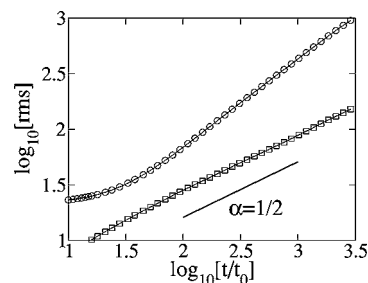


FIG. 2. Double log plot of rms displacement for the two data sets shown in Fig. 1 on the relevant range of scales $t \geq \tau_{\text{meas.}}$ ($t_0 = 1$). Circles (squares) represent *model 1* (2).

points [Fig. 1(b)] are sufficient to characterize the type of diffusion, note in contrast that 80 uncorrelated stretches of RW, equivalent to 80 independent data points, do not provide enough statistics [Fig. 1(a)]. Here we see why Δ must span at least two orders of magnitude of the correlation time.

Figure 2 shows the rms displacement for the two models on a double log plot. A slope of $\alpha = 1/2$ indicates diffusive behavior. We have performed the average by using a moving window over the single RW, rather than averaging over an ensemble of numerically generated walks, in order more closely to match the typical experimental scenario, in which large numbers of statistically similar RW cannot be easily obtained. Moving window methods are often used when one has limited amounts of experimental data. However, these methods demand some care because the results can strongly depend on the time separation of the different windows. If the separation is not large enough, the input may not be statistically independent. Thus, the ensemble average and the moving window average may not converge to the same value. *Model 2* has no correlations besides those arising from the nonuniform turning angle distributions, so there is no effect due to the moving window. On the other hand, *Model 1* is non-Markovian and has long-range correlations arising from the underlying LW skeleton, and it is not possible to obtain statistically independent windows. Nevertheless, since we are measuring only rms displacement within the windows as a function of the window size, therefore this procedure can correctly estimate the scaling for these models, which have no trends. Even with a moving window method, diffusive motion will give an exponent $\alpha = 1/2$ and a superdiffusive walk will give an exponent $\alpha > 1/2$ for both models. More sophisticated moving window methods for analyzing the scaling properties of RW include *Detrended Fluctuation Analysis* and wavelet based methods [22].

The two walks clearly differ in their scaling, confirming quantitatively the results observed in Figs. 1(a) and 1(b). It exemplifies the fact that two data sets representing the same system, but having distinct numbers of data points (i.e., “collected” at distinct scales), can appear qualitatively different, i.e., sets corresponding to the $t \lesssim \tau_{\text{meas.}}$ regime may not be relied on to come to clearcut conclusions about the type of diffusion.

D. Analytical results: τ dependence on the distributions parameters

The correlation time is a direct function of the parameters (through $\langle \cos[\theta] \rangle = \rho$) of the different probability distribu-

tions used to construct the CRW models. Thus, their variation towards $\rho=1$ leads to deterministic ballistic motion, since τ diverges as $1/(1-\rho)$ for $\rho \rightarrow 1$. Values for which $\rho < 1$ introduce stochasticity, giving rise to Markovian processes. Finally, parameter values giving $\rho=0$ result in pure Brownian RW. To illustrate such dependence explicitly we consider a CRW model based on a general class of circular PDF recently proposed by Jones and Pewsey [23], comprising the whole family of circular symmetric unimodal distributions ($\kappa \geq 0$ and γ real):

$$f_{\text{JP}}(\theta; \gamma, \kappa) = \frac{(\cosh[\kappa\gamma] + \sinh[\kappa\gamma]\cos[\theta])^{1/\gamma}}{2\pi P_{1/\gamma}^0(\cosh[\kappa\gamma])}. \quad (4)$$

Here, $P_{\mu}^n(\cdot)$ is the associated Legendre function of the first kind of order n and degree μ . The above distribution does reduce to some well known cases like the von Mises (vMD), cardioid (CD), and the quite studied WCD, $f_{\text{WCD}} = (2\pi)^{-1}(1 - \rho^2)/(1 + \rho^2 - 2\rho \cos[\theta])$, by setting, respectively, $\gamma=0$, $\gamma=-1$, and $\gamma=+1$.

For Eq. (4), we have that $\alpha_1 = \rho = \langle \cos[\theta] \rangle$ reads [23]:

$$\langle \cos[\theta] \rangle = \begin{cases} \tanh\left[\frac{\kappa}{2}\right], & \gamma = -1 (\text{WCD}) \\ \frac{I_1(\kappa)}{I_0(\kappa)}, & \gamma = 0 (\text{vMD}) \\ \frac{|\gamma| P_{1/\gamma}^1(\cosh[\kappa\gamma])}{(1 + \gamma) P_{1/\gamma}^0(\cosh[\kappa\gamma])}, & \text{otherwise.} \end{cases} \quad (5)$$

For the CD case ($\gamma=1$) the last expression in the above equation reduces to $\tanh[\kappa]/2$. So, it becomes clear from the expression for τ and from Eq. (5) that the correlation time is directly characterized by the parameters κ and γ of the CRW associated PDF, Eq. (4).

III. DISCUSSION

We now comment on why the criterion, Eq. (3), may represent a necessary but not sufficient condition for establishing superdiffusive behavior in certain instances. Indeed, it may happen that besides the directional persistence, the RW can also have additional correlations (or, more realistically, anticorrelations) in the turning angles themselves. So, for a given data set corresponding to such a RW, the calculation of $\tau_{\text{meas.}}$, based on the theoretical CRW τ , will give a minimum lower bound for the correlation time (thus leading to a necessary condition), but may not give the upper bound of the correlation time of the system. Thus, even if the data set satisfies the criterion and appears superdiffusive on scales much larger than $\tau_{\text{meas.}}$, yet this is not sufficient to rule out diffusive behavior at yet larger scales. The absence of loops in the movement patterns of some organisms is evidence of anticorrelated turning angles.

We also comment on how $\tau_{\text{meas.}}$, which is an average over a finite data set, fluctuates as a random variable. Note that for nonergodic processes, strong fluctuations in $\tau_{\text{meas.}}$ become a possibility. For a genuinely superdiffusive RW, such as a LW,

the measured expectation $\langle \cos[\theta] \rangle_{\text{meas.}}$ will increase inside the RW stretches corresponding to ultralong Lévy flight lengths, but decrease inside the regions of many short flights. Since the real correlation length of a LW diverges, for a finite data set $\langle \cos[\theta] \rangle_{\text{meas.}}$ will usually underestimate the true value $\langle \cos[\theta] \rangle$. For a genuinely superdiffusive RW, this will not pose a problem. For a true CRW, on the other hand, such fluctuations may lead to $\tau_{\text{meas.}}$ underestimating the CRW τ , which could in principle invalidate the criterion. However, recall that the criterion specifies that the data should span at least two orders of magnitude beyond $\tau_{\text{meas.}}$. To violate the criterion, a fluctuation would have to make $\tau_{\text{meas.}}$ change by (at least) one order of magnitude. For this to happen, the fluctuation $\delta\rho$ in the measured mean resultant $\rho_{\text{meas.}}$ would have to exceed $-\delta\rho \approx \rho - \rho^{10}$. For small ρ (i.e., small τ) this would mean $-\delta\rho \approx \rho$, which is plausible (e.g., a uniform distribution). However, the consequent reduction in $\tau_{\text{meas.}}$ would pose no problem, since it would already have had a relatively small value to begin with. As $\rho \rightarrow 1$, however, the criterion becomes more sensitive to fluctuations. In practice we expect such fluctuations not to cause serious problems. For instance, only rarely does one observe, say, $\rho \geq 0.99$, in experimental data, and even for $\rho=0.99$ the fluctuation would have to reach 8.5% to lead to a decrease in $\tau_{\text{meas.}}$ of one order of magnitude. We thus see that the criterion remains fairly robust in the experimentally relevant range of the observed values of ρ . On the other hand, if the fluctuation goes in the opposite direction, leading to an increase in $\tau_{\text{meas.}}$, then the criterion remains valid.

We also note that truncated Lévy distributions, i.e., where there are cutoffs for large ℓ in Eq. (1), lead to superdiffusion for a very long time, after which they crossover to Gaussian (i.e., Brownian) behavior [24]. In this sense, the CRW is nonunique, and has been chosen over other models mainly due to its relevance to experimental data and the procedures used to discretize RW trajectories.

Another important issue is that transitions between normal and anomalous diffusion typically lead to logarithmic corrections of the form $t^\alpha[\log(t)]^\beta$ in the time t (see, e.g., Ref. [25]). In the case of LW that follows Eq. (1), for instance, logarithmic corrections arise for $\mu=3$, which corresponds to the transition between diffusive and superdiffusive behavior. Since our results above do not consider logarithmic corrections to the algebraic decay for the rms displacement, therefore one may ask how the proposed criterion applies at such transition points. We note that in such cases, the rms displacement will grow linearly in time, but with a logarithmic correction that cannot easily be identified in the usual double log plots. However, further analysis would reveal their presence. The criterion on its own does not restrict the choice of data analysis methods for characterizing the scaling of the rms displacement. The criterion provides the necessary minimum scale which allows one in principle to tell the difference between the two kinds of diffusion.

How does the criterion apply for subdiffusive behavior? We note that if $\langle \cos[\theta] \rangle < 0$, then a CRW will have a dispersive transport regime for small scales, although their Markovian properties lead to normal diffusion at sufficiently large scales. Since

$$C(t/t_0) \sim [C(1)]^{t/t_0} = (-1)^{t/t_0} \exp[(t/t_0) \ln[-\langle \cos[\theta] \rangle]], \quad (6)$$

therefore the correlation time for such cases will be

$$\tau = -1/\ln[-\langle \cos[\theta] \rangle]. \quad (7)$$

More complicated behavior can be modeled using n -step Markovian CRW models instead of considering only one step Markov processes.

Finally, we observe that experimentally measured angular distributions can sometimes be multimodal and asymmetric. Our examples were based on unimodal and symmetric PDF. Nevertheless, the general result for τ is valid regardless the

type of PDF, provided $\bar{\theta}=0$. The circular variance ν is conventionally defined by $\nu \equiv 1 - \rho$, which, for the case $\bar{\theta}=0$, can be expressed as $\nu = 1 - \alpha_1$. So, to write $\tau = -1/\ln[1 - \nu]$ may have a more direct bearing on experimental studies, since ν is one of the most frequently studied parameters of turning angles.

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