Fractional Brownian Motion Versus the Continuous-Time Random Walk: A Simple Test for Subdiffusive Dynamics

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Fractional Brownian motion with Hurst index less then 1/2 and continuous-time random walk with heavy tailed waiting times (and the corresponding fractional Fokker-Planck equation) are two different processes that lead to a subdiffusive behavior widespread in complex systems. We propose a simple test, based on the analysis of the so-called p variations, which allows distinguishing between the two models on the basis of one realization of the unknown process. We apply the test to the data of Golding and Cox [Phys. Rev. Lett. **96**, 098102 (2006)], describing the motion of individual fluorescently labeled mRNA molecules inside live *E. coli* cells. It is found that the data does not follow heavy tailed continuous-time random walk. The test shows that it is likely that fractional Brownian motion is the underlying process.

Distinguishing between normal and anomalous diffusion is usually based on the analysis of the mean-squared displacement (MSD) of the diffusing particles. In the case of classical diffusion, the second moment is linear in time, whereas anomalous diffusion processes exhibit distinct deviations from this fundamental property. In particular, subdiffusive systems are characterized by the sublinear pattern $\langle x^2(t)\rangle \sim t^\alpha$, $0 < \alpha < 1$, [1]. The origin of subdiffusive dynamics in a given system is often unknown. It is not always clear which model applies to a particular system [2,3], an information which is essential when diffusion-controlled processes are considered. Therefore, determining the appropriate model of subdiffusive dynamics is an important and timely problem; see [2–6] for discussion on the origins of anomaly in the case of single protein fluctuations and intracellular diffusion.

Two distinct processes have been proposed to account for subdiffusion. The first one is the fractional Brownian motion (FBM), [7]. FBM is a generalization of the classical Brownian motion. The MSD of FBM satisfies $\langle x^2(t)\rangle \sim t^{2H}$, where $0 < H < 1$ is the Hurst exponent. Thus, for $H < 1/2$ we obtain the subdiffusive dynamics, [8,9].

The second model of subdiffusion is the continuous-time random walk (CTRW) and the corresponding fractional Fokker-Planck equation (FFPE) [1]. In this model, a particle performs random jumps whose length is given by the probability density function (PDF) with finite second moment. The waiting times between consecutive jumps are assumed to follow a power law $t^{-\alpha-1}$ with $0 < \alpha < 1$. These heavy tailed waiting times correspond to nonstationary increments and give rise to sublinear MSD of the particle. As a consequence, the CTRW model exhibits ergodicity breaking and aging. The MSD can be obtained either by performing an average over an ensemble of particles, or by taking the temporal average over a single trajectory [10–12]. Recent advances in single molecule spectroscopy enabled single particle tracking experiments following individual particle trajectories [3,4]. These require temporal, moving averages. Although temporal averages of heavy tailed CTRW and FBM have been shown to differ [10,12–14], the issue of determining the underlying process is still open.

Motivated by growing interest in single molecule spectroscopy, in particular, by single particle tracking, we propose a method to distinguish between mechanisms leading to subdiffusion. Introducing such a method is timely and goes beyond the very basic claims of "normal" vs "anomalous" diffusion by seeking an origin for the anomalous. We apply our theoretical approach to experimental data (random motion of an individual molecule inside the cell by tracking fluorescently labeled mRNA molecules in *E. coli* in the experiment described in details in [3]) and resolve a recent controversy on the origin of the Golding-Cox subdiffusion [12,13]. We clearly demonstrate that, unlike some claims, the observed subdiffusion cannot stem from a broad distribution of waiting times. It is likely that fractional Brownian motion is the underlying process.

Subdiffusive dynamics.—We begin with recalling the two models of subdiffusion, namely, FBM and CTRW.

For $0 < H < 1$, FBM of index H is the mean-zero Gaussian process $B_H(t)$ whose covariance function is given by $E(B_H(s)B_H(t)) = (\sigma^2/2)(s^{2H} + t^{2H} - |t - s|^{2H})$, t, $s > 0$. Here, $\sigma^2 = E(B_H^2(1))$. For $H = 1/2$, $B_H(t)$ reduces to the standard Brownian motion $B(t)$. FBM is self-similar

with respect to H [9], i.e., for every $c > 0$ we have $B_H(ct) \stackrel{d}{=} c^H B_H(t)$. Here, $\stackrel{d}{=}$ stands for "equal in distribution." Moreover, FBM has stationary increments. The stationary sequence of FBM increments $b_H(j) = B_H(j + 1) - B_H(j)$ is very strongly correlated. One can show that the autocovariance function of $b_H(\cdot)$ satisfies $r(j) = E(b_H(j)b_H(0)) \sim \sigma^2 H(2H - 1)j^{2H-2}$ as $j \to \infty$.

For the second moment of the FBM we have $E(B_H^2(t)) = \sigma^2 t^{2H}$, which for $H < 1/2$ gives the subdiffusive dynamics. We assume that $\sigma^2 = 1$. Note that one can always normalize the process in such a manner by dividing it by $\sigma > 0$. The parameter σ can be estimated using the property $B_H(t + s) - B_H(t) \sim N(0, \sigma^2 s^{2H})$.

The second fundamental model of subdiffusive dynamics is the CTRW and the corresponding FFPE. A force-free FFPE has the form [1]:

$$\frac{\partial w(x, t)}{\partial t} = {}_0D_t^{1-\alpha}\left[\frac{1}{2}\frac{\partial^2}{\partial x^2}\right]w(x, t) \qquad (1)$$

with the initial condition $w(x, 0) = \delta(x)$. Here, the operator ${}_0D_t^{1-\alpha}$, $0 < \alpha < 1$, is the fractional derivative of the Riemann-Liouville type. The derivation of the above equation is based on the CTRW scheme with heavy tailed waiting times. It is easy to verify [1] that the MSD corresponding to $w(x, t)$ is equal to $\frac{t^\alpha}{\Gamma(\alpha+1)}$.

In Eq. (1), $w(x, t)$ denotes the PDF of a subdiffusive stochastic process $Z_\alpha(t)$. The process $Z_\alpha(t)$ can be equivalently written in the form of subordination [15–17]

$$Z_\alpha(t) = B(S_\alpha(t)), \qquad (2)$$

where $B(t)$ is the standard Brownian motion and $S_\alpha(t)$ is the inverse α-stable subordinator independent of $B(t)$. The inverse α-stable subordinator is defined as

$$S_\alpha(t) = \inf\{\tau > 0: U_\alpha(\tau) > t\}, \qquad (3)$$

$0 < \alpha < 1$, where $U_\alpha(\tau)$ is the α-stable subordinator [18] with Laplace transform $E(e^{-uU_\alpha(\tau)}) = e^{-\tau u^\alpha}$. The process $S_\alpha(t)$ is α-self-similar, and therefore $Z_\alpha(t)$ is $\alpha/2$-self-similar. For every jump of $U_\alpha(\tau)$ there is a corresponding flat period of its inverse. These flat periods of $S_\alpha(t)$ are characteristic for the subdiffusive dynamics and correspond to the heavy tailed waiting times in the underlying CTRW scenario. The Langevin-type process (2) corresponding to FFPE (1) gives insight into the structure of trajectories. Therefore, it allows to detect differences between single trajectories of FBM $B_H(t)$ and CTRW-based model $Z_\alpha(t)$.

p Variation.—Let us now discuss the idea of p variation, $p > 0$, which will be our main tool in a procedure of identifying the type of subdiffusion. The concept of p variation generalizes the well-known notion of total variation, which has found applications in various branches of mathematics, physics and engineering, like optimal control, numerical analysis of differential equations, and calculus of variations [19]. Let $X(t)$ be a stochastic process

observed on time interval $[0, T]$. Then, for $t \in [0, T]$, the p variation corresponding to $X(t)$ is defined as

$$V^{(p)}(t) = \lim_{n \to \infty} V_n^{(p)}(t), \qquad (4)$$

where $V_n^{(p)}(t)$ is the partial sum of increments of the process $X(t)$ given by

$$V_n^{(p)}(t) = \sum_{j=0}^{2^n-1}\left| X\left(\frac{(j + 1)T}{2^n} \wedge t\right) - X\left(\frac{jT}{2^n} \wedge t\right)\right|^p \qquad (5)$$

with $a \wedge b = \min\{a, b\}$. Let us underline that $V_n^{(p)}(t)$ is very easy to calculate, since it is just the finite sum of pth powers of the increments of $X(t)$. For large enough n, $V_n^{(p)}(t)$ approximates nicely p variation $V^{(p)}(t)$. When $p = 1$, $V^{(1)}(t)$ reduces to the total variation.

As an example let us recall the variational properties of the standard Brownian motion. It is a well known fact that the total variation of Brownian motion is infinite, which is not very surprising given the "wild" behavior of the trajectories of $B(t)$. However, the quadratic variation of $B(t)$ is finite and equals $V^{(2)}(t) = t$ [18].

It is well known that the p variation of the FBM $B_H(t)$ satisfies [20]

$$V^{(p)}(t) = \begin{cases} +\infty & \text{if } p < \frac{1}{H}, \\ tE(|B_H(1)|^{1/H}) & \text{if } p = \frac{1}{H}, \\ 0 & \text{if } p > \frac{1}{H}, \end{cases} \qquad (6)$$

The expected value in the above expression is given by $E(|B_H(1)|^{1/H}) = \frac{2^{\frac{1}{2H}}}{\sqrt{\pi}}\Gamma(\frac{1}{2H} + \frac{1}{2})$. Let us note that for the considered here subdiffusive case $H < 1/2$, the quadratic variation $V^{(2)}(t)$ of $B_H(t)$ is infinite.

The p variation of the Langevin process $Z_\alpha(t) = B(S_\alpha(t))$ satisfies [21]

$$V^{(p)}(t) = \begin{cases} +\infty & \text{if } p < 2, \\ S_\alpha(t) & \text{if } p = 2, \\ 0 & \text{if } p > 2. \end{cases} \qquad (7)$$

The above formula confirms that the quadratic variation of $Z_\alpha(t)$ is finite and equal to the inverse subordinator $S_\alpha(t)$, [22]. We underline that in this case $V^{(2)}(t)$ is a stochastic process and not the deterministic function as in (6). Moreover, $V^{(2)}(t) = S_\alpha(t)$ is an α-self-similar process.

Test.—Suppose we are given one realization (time series) of some subdiffusive process $X(t)$ observed on the time interval $[0, T]$. If not known, estimate the index of self-similarity of the process $X(t)$, [10,12,23,24]. Recall that the estimated self-similarity index will give us the approximate value of H or $\alpha/2$ depending on the type of subdiffusion. Our goal is to verify if the subdiffusive dynamics originates from the FBM process $B_H(t)$ or the CTRW-based model $Z_\alpha(t)$. Using Eqs. (6) and (7) we propose the following procedure:

p variation test.—Calculate the partial sums $V_n^{(1/H)}(t)$ and $V_n^{(2)}(t)$, which approximate $1/H$ variation and 2 variation of $X(t)$, respectively. Here, H is the previously estimated self-similarity index. (i) If the process $X(t)$ is the FBM, then $V_n^{(1/H)}(t) \approx tE(|B_H(1)|^{1/H})$ and $V_n^{(2)}(t)$ should increase with increasing n. (ii) If the process $X(t)$ originates from the CTRW model $Z_\alpha(t)$, then $V_n^{(1/H)}(t)$ should tend to zero with increasing n, whereas $V_n^{(2)}(t)$ should stabilize [recall that for $Z_\alpha(t)$ we have $V^{(2)}(t) = S_\alpha(t)$].

The implementation of the above test is based on the computation of the finite sums $V_n^{(p)}(t)$ (5), which is rather straightforward for analytical models as well as for empirical data.

For H very close to $1/2$ it is necessary to take large enough n while calculating the partial sum $V_n^{(p)}(t)$. Otherwise, one can not practically distinguish the properties of p variation corresponding to B_H and Z_α.

In practice an analyzed empirical trajectory is given as a time series $X(t_1), X(t_2), \ldots, X(t_{2^N})$. The sequence $t_1 < t_2 < \ldots < t_{2^N}$ represents the time points, in which position of the test particle is observed. In such setting, N is the largest value for which the sum $V_N^{(p)}(t)$ can be calculated. Then, for fixed $t = t_i$, we have $V_N^{(p)}(t) = \sum_{k=1}^{i-1} |X(t_{k+1}) - X(t_k)|^p$. Similarly, to determine $V_{N-1}^{(p)}(t)$, one has to sum up the pth powers of the increments $|X(t_3) - X(t_1)|$, $|X(t_5) - X(t_3)|, \ldots, |X(t_{2^N-1}) - X(t_{2^N-3})|$. Then, for fixed $t = t_i$, with $i = 2j + 1$, we have $V_{N-1}^{(p)}(t) = \sum_{k=1}^{j} |X(t_{2k+1}) - X(t_{2k-1})|^p$. Consequently, to determine $V_{N-2}^{(p)}(t)$, one sums up the pth powers of the increments $|X(t_5) - X(t_1)|$, $|X(t_9) - X(t_5)|, \ldots$, etc. Finally, plotting $V_n^{(p)}(t)$

for different values of n and observing how it behaves while n increases/decreases, one can draw conclusions on the origins of subdiffusion.

First, we tested the algorithm on simulated data. We simulated one trajectory of FBM $B_H(t)$ and one trajectory of $Z_\alpha(t)$. We demonstrate the results in Fig. 1. The quadratic variation of $B_H(t)$ diverges, whereas the quadratic variation of $Z_\alpha(t)$ is equal to $S_\alpha(t)$. Moreover, the $1/H$ variation of $B_H(t)$ is a linear function, while the $1/H$ variation of $Z_\alpha(t)$ vanishes. These differences in the behavior of variations of both subdiffusive processes $B_H(t)$ and $Z_\alpha(t)$ allow to distinguish between mechanisms leading to subdiffusion.

Next, we applied the test to the Golding-Cox experimental data [3]. We analyzed six two-dimensional sample paths (all those having more than $2^9 = 512$ points, which seems reasonable for the p variation test) from their set of 27 trajectories. We examined X and Y coordinates as well as the two-dimensional trajectories separately. The test clearly demonstrated (see the supplementary material in Ref. [25] for the details, and Fig. 2 for the analysis of one sample trajectory) that the subdiffusion cannot stem from the CTRW model. Moreover, the test also shows that there is no reason to reject the hypothesis that the data follows FBM. This resolves a recent controversy over the underlying reason for the Golding-Cox subdiffusion [12,13]. However, to reach a more conclusive statement on the FBM origins of the experimental data, longer trajectories and extended statistical analysis are necessary.

The conclusion also concurs with the result of [10] contrasting temporal average of heavy tailed CTRW with that of FBM. We strongly believe that our approach pro-
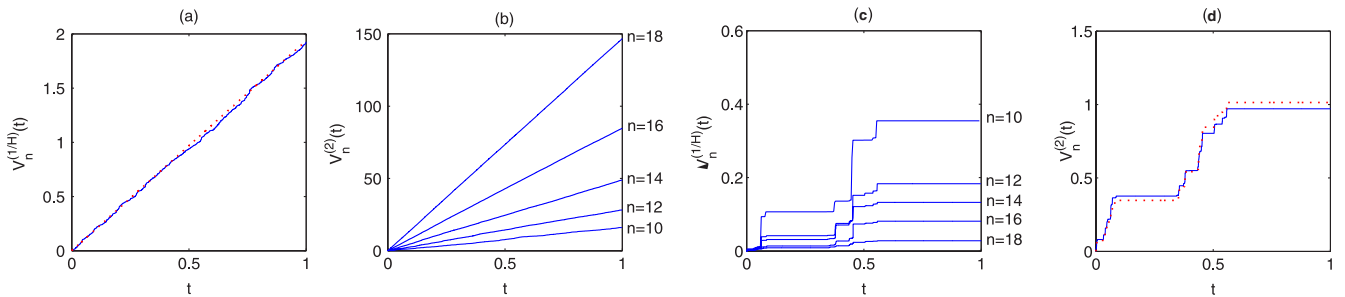

FIG. 1 (color online). In panels (a)–(b) the analysis of a simulated trajectory of FBM $B_H(t)$, with Hurst index $H = 0.3$, is presented. Panel (a) shows the value of $V_n^{(1/H)}(t)$, $n = 12$, corresponding to the sample path of $B_H(t)$ (solid blue line). The dotted red line is the theoretical $1/H$ variation of FBM given in Eq. (6). We observe excellent agreement between the two lines. The approximation gets even better for larger n. Panel (b) depicts the value of $V_n^{(2)}(t)$ corresponding to the simulated trajectory of $B_H(t)$, calculated for different $n = 10, 12, \ldots, 18$. We observe the rapidly increasing values of $V_n^{(2)}(t)$ while n increases. This demonstrates the fact that the quadratic variation of $B_H(t)$ is infinite for $H < 1/2$. Panels (c)–(d) depict the analysis of a simulated trajectory of the process $Z_\alpha(t)$ with $\alpha = 0.6$. In panel (c) we see the value of $V_n^{(1/H)}(t)$ corresponding to the sample path of $Z_\alpha(t)$ calculated for different $n = 10, 12, \ldots, 18$. We observe that $V_n^{(1/H)}(t)$ tends to zero while n increases. This confirms the fact that the $1/H$ variation of $Z_\alpha(t)$ is equal to zero. Panel (d) shows the value of $V_n^{(2)}(t)$, $n = 12$, calculated for the simulated trajectory of $Z_\alpha(t)$ (solid blue line). The dotted red line is the trajectory of the inverse subordinator $S_\alpha(t)$. We observe excellent agreement between the two lines, which confirms that the quadratic variation of $Z_\alpha(t)$ is equal to $S_\alpha(t)$. For larger n the approximation is even better. The observed differences in the behavior of quadratic and $1/H$ variations corresponding to $B_H(t)$ and $Z_\alpha(t)$ allow to distinguish between mechanisms leading to subdiffusion.
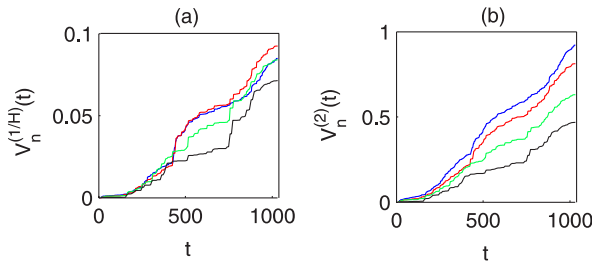
FIG. 2 (color online). Panel (a) shows the $1/H$ variation $V_n^{(1/H)}(t)$ of one sample trajectory taken from Golding-Cox empirical data (with $H = 0.35$ as in [3]). Parameters: $n = 10$ (blue line); $n = 9$ (red line); $n = 8$ (green line); $n = 7$ (black line). We observe that the $1/H$ variation does not exhibit any trend, meaning that $V_n^{(1/H)}(t)$ neither increases nor decreases with increasing n. Similar behavior is observed for simulated trajectories of the FBM with the same number of points. In panel (b) the 2 variation $V_n^{(2)}(t)$ of the analyzed trajectory is presented. Parameters as in panel (a). The 2 variation increases with increasing n, which confirms that the 2 variation is not finite. Thus, the data does not follow CTRW model.

vides a way, missing up to now, to look deeper into processes leading to single particle diffusion.

Finally, we note that the same methodology based on p variations can be applied to analyze another model of subdiffusion—random walks on fractal structures. Our preliminary results show that the quadratic variation of a random walk on a Sierpinski gasket embedded in two dimensions is infinite (similar to the FBM and different from the CTRW). The p variation is finite for $p = d_w$, where $d_w = \log 5/\log 2 = 2.32193\ldots$ is the walk dimension, which corresponds to the self-similarity index of the Sierpinski gasket.

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