A SPATIAL STRUCTURAL DERIVATIVE MODEL FOR ULTRASLOW DIFFUSION

by

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This study investigates the ultraslow diffusion by a spatial structural derivative, in which the exponential function e^x is selected as the structural function to construct the local structural derivative diffusion equation model. The analytical solution of the diffusion equation is a form of Biexponential distribution. Its corresponding mean squared displacement is numerically calculated, and increases more slowly than the logarithmic function of time. The local structural derivative diffusion equation with the structural function e^x in space is an alternative physical and mathematical modeling model to characterize a kind of ultraslow diffusion.

Key words: *ultraslow diffusion, spatial structural derivative, structural function, exponential function, Biexponential distribution*

Introduction

Anomalous diffusion [1, 2] has attracted great attention in diverse fields, such as fractal porous media [3], polymer materials [4], and biomedical engineering [5], just to mention a few. The mean squared displacement (MSD) of anomalous function is a power law function of time [6, 7]:

$$\left\langle x^2\left(t\right)\right\rangle \propto t^\eta \tag{1}$$

when $\eta > 1$ characterizes super-diffusion, when $\eta < 1$ is a sub-diffusion, and it is a Brownian motion when $\eta = 1$ [8]. Anomalous diffusion is non-Markovian non-locality movement, so it must consider the temporal correlation and spatial correlation of the motion process, which can be used to introduce fractional calculus and deal with it by the fractional differential equation [9, 10].

Unlike the aforementioned anomalous diffusion, ultraslow diffusion also behaves in a dramatically different way from the normal Brownian motion and is widely observed in nature and engineering. As an important branch of mathematics, fractional calculus has been widely studied [11] and applied in many fields [12], but it is incapable of ultraslow diffusion which diffuses even far slower than the sub-diffusion [13], the MSD of ultraslow diffusion is often characterized by a logarithmic function of time in literature:

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$$\left\langle x^2(t)\right\rangle \propto (\ln t)^\alpha, \quad \alpha > 0 \tag{2}$$

when $\alpha = 4$ the MSD (2) reduces to the classical Sinai diffusion law [14]. When $\alpha = 0.5$, it is correlated with the well-known Harris law [15].

In order to provide more generalized description of ultraslow diffusion, the structural derivative modeling methodology was proposed [16], in which the structural function is chosen as the inverse Mittag-Leffler function of time. Its corresponding diffusion MSD is $\left\langle x^2(t)\right\rangle \propto [E_\alpha^{-1}(t)]^\lambda$, $\lambda > 0$, where $E_\alpha^{-1}(t)$ is the inverse of Mittag-Leffler. Instead of time inverse Mittag-Leffler function ultraslow diffusion model, this study proposes a spatial structural derivative ultraslow diffusion model via the structural derivative in space, in which the exponential function e^x is chosen as the structural function. The analytical solution of the diffusion model is derived by the scaling transform, and the features of its MSD are further analyzed.

Methodologies

Structural derivative

The structural derivative is an extension of the Hausdorff derivative. According to scaling transforms, the definition of the Hausdorff fractal distance in 1-D can be given [17]:

$$\begin{cases} \Delta\hat{t} = \Delta t^\alpha \\ \Delta\hat{x} = \Delta x^\beta \end{cases} \tag{3}$$

Suppose a particle moves uniformly along a curve, the displacement l in Hausdorff fractal time can be redefined [18]:

$$l = v(t - t_0)^\alpha \tag{4}$$

The corresponding derivative of displacement in eq. (4) can be obtained:

$$v = \frac{\mathrm{d}l}{\mathrm{d}\left[(t - t^0)^\alpha\right]} \tag{5}$$

Then the Hausdorff derivative on time is given:

$$\frac{\mathrm{d}l}{\mathrm{d}t^\alpha} = \lim_{t^{'} - t} \frac{l(t) - l(t^{'})}{(t - t_0)^\alpha - (t^{'} - t_0)^\alpha} \tag{6}$$

The derivative of displacement l under structural time metric is given [18]:

$$\mathrm{d}l = v\mathrm{d}\left[s(t)\right], \quad t_0 = 0 \tag{7}$$

In analogy with the above structural time derivative, the structural derivative in space can be defined [19]:

$$\frac{\mathrm{d}p}{\mathrm{d}_s x} = \lim_{x^{'} \to x} \frac{p(x,t) - p(x^{'},t)}{s(x) - s(x^{'})}, \quad x_0 = 0 \tag{8}$$

where S denotes the structural derivative, and $f(x)$ is the structural function.

The definition of the global structural derivative in space can be derived from the global structural derivative in time [19]:

$$\frac{\delta p(x,t)}{\delta_s x} = \frac{\partial}{\partial x}\int_{x_1}^{x} f(x-\tau)p(\tau,t)\mathrm{d}\tau \tag{9}$$

which degenerates into the Riemann-Liouville fractional derivative when $f(x) = x^{-\alpha}/\Gamma(1-\alpha)$ [20].

The classical derivative modeling strategy depicts the particular factors on the rate of the change of time or space variables, but less considers the important influence of the mesoscopic structure of time-space fabric of the complex system on its physical behaviors. While in the structural derivative, the structure function depicts the time-space inherent property of the system, which is a space-time transformation [21]. Consequently, the structural derivatives can describe the causal relationship between the mesoscopic space-time structure and the specific physical quantity.

Spatial structural derivative equation model for ultraslow diffusion

According to the local structural derivative, we establish the spatial structural derivative model for ultraslow diffusion:

$$\frac{\mathrm{d}p}{\mathrm{d}t} = K\frac{\mathrm{d}}{\mathrm{d}_s x}\left(\frac{\mathrm{d}p}{\mathrm{d}_s x}\right) \tag{10}$$

where K is the diffusion coefficient. When the structural function $f(x) = x$, eq. (10) yields a Gaussian distribution [22]:

$$p(x,t) = \frac{1}{\sqrt{4\pi Kt}}\exp\left(-\frac{x^2}{4Kt}\right) \tag{11}$$

When $f(x) = x^\beta$, the solution of eq. (10) is a stretched Gaussian distribution:

$$p(x,t) = \frac{1}{\sqrt{4\pi Kt}}\exp\left(-\frac{x^{2\beta}}{4Kt}\right) \tag{12}$$

When $f(x) = e^x$, the corresponding structural derivative is stated:

$$\frac{\mathrm{d}p}{\mathrm{d}_s x} = \lim_{x_1\to x}\frac{p(x_1,t)-p(x,t)}{e^{x_1}-e^x} \tag{13}$$

and the corresponding solution of eq. (10) can be derived:

$$p(x,t) = \frac{1}{\sqrt{4\pi Kt}}\exp\left(-\frac{e^{2x}}{4Kt}\right) \tag{14}$$

Substituting the eq. (14) into eq. (10) can easily verify:

$$\frac{\mathrm{d}}{\mathrm{d}e^x}\left[\frac{\mathrm{d}p(x,t)}{\mathrm{d}e^x}\right] = -p(x,t)\left(\frac{1}{2Kt}-\frac{e^{2x}}{4K^2t^2}\right) = \frac{1}{K}\frac{\mathrm{d}}{\mathrm{d}t} \tag{15}$$

Namely, eq. (14) is the solution of eq. (10), in which the structural function is an exponential function. Equation (14) is a new kind of distribution, called the Biexponential distribution in this paper. The relationship between the structural function and the solution of structural derivative diffusion equation in space is derived:

$$p(x,t)=\frac{1}{\sqrt{4\pi Kt}}\exp\left\{-\frac{\left[f(x)\right]^2}{4Kt}\right\} \tag{16}$$

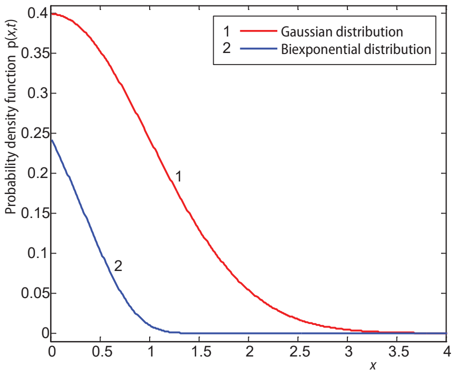

Figure 1. The probability density function $t=1$, $K=0.5$

Generally speaking, the spatial structural derivative is a modeling strategy and can be employed in modeling ultraslow diffusion phenomena in complex fluids. It is solution of the corresponding structural derivative diffusion equation constructed by the arbitrary structural function in the local structural derivative in space is statistical distribution, *i. e.*, the probability density function.

Figure 1 is the probability density function described of Gaussian and Biexponential distribution with $x>0, t=1, K=0.5$. From the simulation results, we can see that the Biexponential distribution decreases more rapidly than Gaussian distribution in a short time. That means that compared with the probability of specify random variables falling in a specific range, the Biexponential distribution of tailing phenomenon is more evident.

Results and discussions

In this section, we numerically compute the MSD of the proposed ultraslow diffusion model, and then explore the transient diffusion behavior by comparing with the normal diffusion, sub-diffusion, super-diffusion, and the proposed ultraslow diffusions. Figure 2 shows the differences of various diffusion processes.

In fig. 2, the yellow (1) area represents the super-diffusion process, the corresponding MSD is $\left\langle x^2(t)\right\rangle=(t+1)^{\beta}$, $\beta>1$. The blue (3) and the green (2) areas, respectively, belong to the ultraslow diffusion and sub-diffusion.

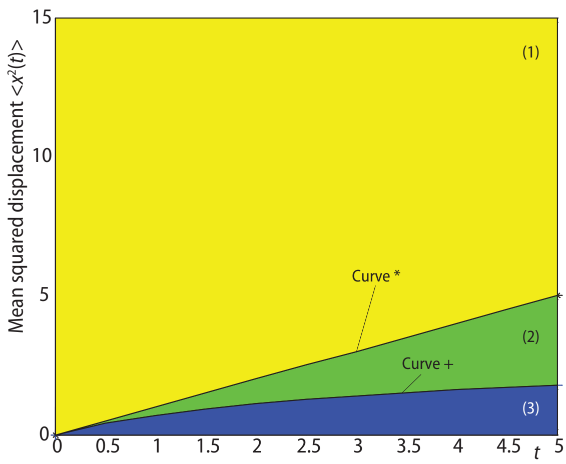

Figure 2. Schematic diagram of normal diffusion, sub-diffusion, super-diffusion, and the exponential structural derivative ultraslow diffusion, in which the proposed ultraslow diffusion and sub-diffusion is separated by the logarithm ultraslow diffusion $\left\langle x^2(t)\right\rangle=\ln(1+t)$ dotted with +, and the normal diffusion $\left\langle x^2(t)\right\rangle=t$ curve divides sub-diffusion and super-diffusion dotted with *

The MSD of the proposed exponential function ultraslow diffusion can be derived from eq. (14):

$$\left\langle x^2(t)\right\rangle = \int_{-\infty}^{\infty} x^2 p(x,t)\mathrm{d}x = \frac{1}{\sqrt{4Kt\pi}}\int_{-\infty}^{\infty} x^2 \exp\left(-\frac{e^{2x}}{4Kt}\right)\mathrm{d}x \tag{17}$$

Its analytical solution can not directly be obtained, instead we define the MSD in $(0, +\infty)$ and calculate the following integral form:

$$\left\langle x^2(t)\right\rangle = \int_{0}^{\infty} x^2 p(x,t)\mathrm{d}x = \frac{1}{\sqrt{4Kt\pi}}\int_{0}^{\infty} x^2 \exp\left(-\frac{e^{2x}}{4Kt}\right)\mathrm{d}x \tag{18}$$

Figure 3 shows the MSD of normal diffusion, logarithm ultraslow diffusion and the present exponential structural function ultraslow diffusion. We can observe from fig. 3 that the MSD of the proposed ultraslow diffusion increases slower with time than that of the logarithmic diffusion. Thus, the local structural derivative diffusion equation with the structural function $f(x) = e^x$ in space is a mathematical modeling method to characterize a kind of ultraslow diffusion.

It is worthy of noting that the exponential function $f(x) = e^x$ is a special case of the popular Mittage-Leffler function:

$$E_\alpha\left(x\right) = \sum_{k=0}^{\infty}\frac{x^k}{\Gamma\left(\alpha k+1\right)} \tag{19}$$

when $\alpha = 1$, it degenerates into the exponential function.

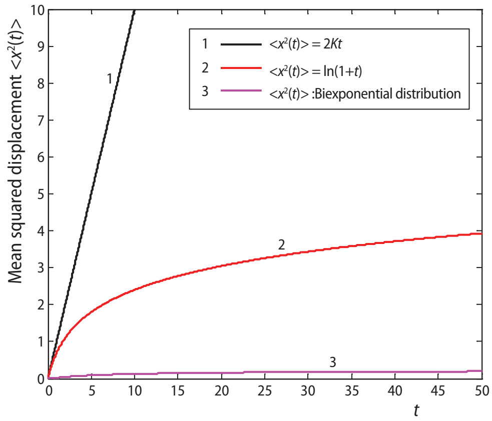

Figure 3. Mean squared displacement of normal diffusion, logarithm ultraslow diffusion and exponential function ultraslow diffusion with $K = 0.5$

In recent years, the Mittage-Leffler function has widely been used in the fractal dynamics, anomalous diffusion and fractal random field [23-25]. In addition, the inverse Mittage-Leffler function as has also been applied to describe ultraslow diffusion [21]. In further study, we will try to investigate different structural functions with clear physical mechanism, such as Mittag-Leffler function and its inverse function, to construct both local and global structural derivative diffusion equation in modeling non-Gaussian motion.

Conclusions

In this paper, we present a local spatial structural derivative diffusion model to depict the ultraslow diffusion, in which the exponential function e^x is selected as the structural function. Based on the foregoing results and discussions, the following conclusions can be drawn.

- The analytical solution of the proposed ultraslow diffusion equation is a form of Biexponential distribution.
- The corresponding mean squared displacement is numerically calculated, and increases more slowly with than that of the logarithmic ultraslow diffusion.
- The local structural derivative diffusion equation with the structural function e^x in space is an alternative mathematical modeling method to characterize a kind of ultraslow diffusion.

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Nomenclature

$E_\alpha(t)$– Mittag-Leffler function

$E_\alpha^{-1}(t)$ – inverse Mittag-Leffler function

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