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Simulation and calibration between parameters of continuous time random walks and subdifusive model [1]

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Abstract. We address the problem of subdiffusion or normal diffusion to perform a calibration between the parameters used in simulation and the parameters of a subdifusive model. The theoretical model is written as a generalized diffusion equation with fractional derivatives in time. The data is generated by simulations consisting of continuous-time random walks with controlled mean waiting time and jump length variance to provide a full range of cases between subdiffusion and normal diffusion. From the simulations, we compare the accuracy of two methods to obtain the diffusion constant, the order of fractional derivatives: the analysis of the dispersion of the variance in time and the optimization fitting of theoretical model solutions to histogram of positions. We highlight the connection between the parameters of the simulations the parameters of the theoretical models.

keywords. Anomalous diffusion, fractional diffusion equation, calibration

1. Introduction

Anomalous diffusion has been attracting the attention of the scientific community due the large plethora of natural systems which display large deviations from normal diffusion, as plasma diffusion [3], fluid flow in porous media [22, 7], diffusion

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in fractal structures [23], turbulence [8] etc. Differently to the normal diffusion, associated to local, short range correlations, the presence of long range correlations lead to non-Gaussian probability density functions (PDF).

In some anomalous Brownian motions, the microscopic kinetics is characterized by higher probabilities of having large steps or large waiting times elapsed between steps, causing the system to differ from the classical Brownian motion and leading to non-Gaussian PDF. Such class of problems are generically called anomalous diffusion. From a macroscopic point-of-view, those anomalous diffusion processes do not fit in the classical diffusion description by a classical Fokker-Planck equation for the evolution of the PDF $u(x,t)$ in space and time by means of classical linear diffusion equations [11, 24].

As a direct consequence of the central limit theorem, Markov processes displays a linear evolution of the mean square displacement with time, $\langle x^2(t)\rangle \propto Dt$, featuring the normal, or Brownian, diffusion [25]. According to that theorem, the cumulative density functions (CDF) of the sums are gaussian when the single variable probability density function (PDF) has finite second moment.

On the other hand, if the PDF has long-range tails, determining the divergence of the second moment, the Lévy-Gnedenko limit theorem states that the CDF is Lévy distributed [9]. Alternatively, the q-central limit theorem states that, for the case of PDF exhibits heavy tails, a q-Gaussian with $1 < q < 3$ is obtained [27]. Those process are generally characterized by a non-linear dependence of the mean square displacement in time, with $\langle x^2(t)\rangle \propto Dt^\alpha$ [17]. According to the value of the exponent α, the anomalous processes can be classified as sub-diffusive $(0 < \alpha < 1)$ or super-diffusive $(1 < \alpha < 2)$ [17]. A relation between the diffusion exponent α and the q parameter was proposed by Bukman and Tsallis [26] and recently verified experimentally [6].

Thus, the generalization of the random walk, the *continuous time random walk* (CTRW), is able to simulate processes which display anomalous diffusion. In particular, considering a random distribution of step lengths as well a random distribution on waiting times, it is possible to control the process in order to simulate both sub-diffusion or super-diffusion regimes[19, 17, 18].

The description of the macroscopic behaviour of $u(x,t)$ for anomalous diffusion process can be modelled by means of generalized diffusion equations with fractional derivatives in time as well as in space[15, 14, 13, 2, 1]. Another class of generalizations of diffusion equations is obtained by the inclusion of nonlinearity in the partial differential equation [4, 13, 25]. Those complementary approaches have motivated this study, which aims understanding the phenomena of anomalous diffusion in complex dynamic systems [14, 20, 18, 16].

From one side, there is the general interest in simulating anomalous diffusion systems in order to reproduce some observable macroscopic behaviour with associated variables. By another side, there lies the interest to provide macroscopic anomalous diffusion models to explain microscopic with detailed dynamics not easily observable. Thus, a question arises naturally: is there a systemic relation between microscopic model parameters and macroscopic anomalous diffusion behavior? In the case of a positive answer, which is this relation? Moreover, one can wonder which is the best method to compare models to simulations as well as which models are more appropriate to fit simulations.

In the present work, we address the problem of subdiffusion and normal diffusion to perform a calibration between simulation microscopic parameters and macroscopic theoretical model parameters of a generalized anomalous diffusion (subdiffusion) model. The data is generated by simulations of CTRW with controlled mean waiting time and jump length variance to provide a full range of cases between subdiffusion and normal diffusion. The theoretical model consists in a contour value problem with boundary conditions having a fractional partial differential equation (FPDE) as an subdiffusion equation, with fractional derivatives in time. From the simulations, we obtain the diffusion constant and the order of fractional derivatives by two different approaches: optimization fitting of theoretical model solutions to the histogram of positions of the particles and by analysis of the dispersion in time of the variance of the particles position. The microscopic parameters of the simulations are then associated to the theoretical macroscopic parameters. We then highlight the connection between the parameters of the simulations the parameters of the theoretical models for the cases of fractional derivatives in time. In Section (2.), we present the generalized model and solutions. The long range behaviour of the solutions is discussed in Section (3.). Section (4.) comprises the aspects of the simulations which is followed by the Section (5.) of results and Section (6.) for the conclusions.

2. Subdiffusion equation and contour value problem

To theoretically describe the subdiffusion, the Fokker-Planck equation for the probability density function $u(x,t)$ of finding a particle between x and $x+\delta x$ at the time t is written by means of a generalized diffusion equation with fractional derivatives in time. Hence, a uni-dimensional open contour value problem (CVP) subject to asymptotic contour conditions and appropriated initial conditions can be written as

$$\begin{aligned}
&{}^{C}\mathcal{D}_t^{\alpha} u(x,t) = D_\alpha \frac{\partial^2 u(x,t)}{\partial x^2}, \\
&u(\pm\infty,t)=0, \quad u(x,0)=N\delta(x-x_0)\,, \quad u_t(x,0)=0, \\
&-\infty < x < \infty \qquad t>0\,,
\end{aligned} \tag{2.1}$$

where D_α is the subdiffusion coefficient, N stands for the number of particles. The fractional derivative operator in time ${}^{C}\mathcal{D}_t$ is defined in the Caputo sense in order to allow the statement of initial conditions with physically meaningful derivatives of integer order in time [21],

$${}^{C}\mathcal{D}_t f = \frac{1}{\Gamma(\alpha-1)} \int_0^t f'(\tau) \frac{1}{(t-\tau)^\alpha} d\tau, \qquad 0<\alpha<1\,. \tag{2.2}$$

For $\alpha = 1$ in 2.1, the classical diffusion equation is recovered. The linear case with varying the fractional order of the derivatives, $0 < \alpha < 1$, one can describe subdiffusive processes [17].

The fractional derivative in time has the solution

$$u(x,t) = G_\alpha(x,t) = \frac{N}{2\sqrt{D_\alpha} t^{\frac{\alpha}{2}}} \sum_{k=0}^{\infty} \frac{(-z)^k}{k!\Gamma(-\frac{\alpha}{2}k + (1-\frac{\alpha}{2})}, \qquad z = \frac{|x-x_0|}{\sqrt{D_\alpha} t^{\frac{\alpha}{2}}}, \tag{2.3}$$

where $G_\alpha(x,t)$ is a Mittag-Leffler function [10]. Such solutions describe subdiffusive process. By using 2.1 and 2.2, one can obtain the following expression for the mean square displacement:

$$\langle x^2(t) \rangle_G = \frac{2D_\alpha}{\Gamma(\alpha+1)} t^\alpha \,, \qquad 0 < \alpha < 1 \,. \tag{2.4}$$

We use these case to fit the histogram of displacements of CTRW simulations to produce subdiffusive processes.

3. Long range behaviour of the model

By means of the the Laplace transform in the Caputo sense on the time variable $\mathcal{L}\{u(x,t);s\} = \tilde{u}(x,s)$ and the Fourier transform on space variable, $\mathcal{F}\{u(x,t);k\} = \widehat{u}(k,t)$, one obtains from 2.1 its Laplace-Fourier transform [21, 18],

$$\widehat{\tilde{u}}(k,s) = \frac{s^\alpha \widehat{u}(k,0)}{s(s^\alpha + D_\alpha |k|^\mu)}. \tag{3.5}$$

For a CTRW, the probability distribution function of a walk to the a given position x in a time t is given by the length of jump as well as the waiting time between successive jumps are well described by a function $\Psi(x,t)$, whose the marginal probabilities in the space and time are respectively given by $\lambda(x)$ and $\psi(t)$ [17]. It is possible to show that the Fourier-Laplace transform of the PDF $u(x,t)$ of finding the particle in the time t , between x and $x + dx$ is given by

$$\widehat{\tilde{u}}(k,s) = \frac{1-\tilde{\psi}(s)}{s} \frac{\tilde{\widehat{u}}(k,0)}{(1-\tilde{\psi}(s)\widehat{\lambda}(k))} \,, \tag{3.6}$$

which is known as the Montroll-Weiss formula [19, 12]. The long range behaviour of above equation is accessed in the infrared limit of the Fourier-Laplace transform, $s \to 0$, $k \to 0$, for which the moment expansions can be read as

$$\begin{aligned} \psi(s) &= e^{-(\tau s)^\alpha} \approx 1 - \tau^\alpha s^\alpha, && 0 < \alpha \leq 1, \\ \lambda(k) &= e^{-\sigma^2 |k|^\sigma} \approx 1 - \sigma^2 k^2, && . \end{aligned} \tag{3.7}$$

where, τ and σ are scale constants such that τ^α and σ^2 are identified to the first and second moments when $\alpha = 1$. To the first order in 3.7, equation 3.6 reduces to

$$\widehat{\tilde{u}}(k,s) = \frac{s^\alpha \widehat{\tilde{u}}(k,0)}{s(s^\alpha + \frac{\sigma^2}{(2\tau)^\alpha}k^2 + \cdots)} \,. \tag{3.8}$$

The comparison between D_α of equation 3.5 and the scales σ and τ above allows us to obtain the equation

$$\log(2D_\alpha) = \log(\sigma^2) - \alpha \log(\tau). \tag{3.9}$$

These equation exhibits a scale relation between the moments arising from the simulation and macroscopic parameters of the theoretical model.

Let the distributions of jump length δx and waiting times δt be, respectively, $\lambda'(\delta x)$ and $\psi'(\delta t)$. Then, the type of anomalous diffusion simulated by CTRW is also determined also by the long range behaviour of first moment $\langle \delta t \rangle_{\psi'}$ and the second moment $\langle (\delta x)^2 \rangle_{\lambda'}$ by the following rule [19]:

Case 1. If $\langle \delta t \rangle_{\psi'} \to \infty$ and $\langle (\delta x)^2 \rangle_{\lambda'}$ is finite, the process is subdifusive.

Case 2. If $\langle \delta t \rangle_{\psi'}$ is finite and $\langle (\delta x)^2 \rangle_{\lambda'} \to \infty$, the process is superdifusive.

Case 3. If $\langle \delta t \rangle_{\psi'}$ and $\langle (\delta x)^2 \rangle_{\lambda'} \to \infty$ are both finite, the process is a normal diffusion.

Such cases can be read as prescriptions to produce CTRWs with the desired types of anomalous diffusions. In this work, we restrict ourselves to the cases 1 and 3, subdifusive and normal diffusion.

4. Simulation of anomalous random walks

Let a power law PDF in the form $D(\xi) = \frac{a}{(\xi+\varepsilon)^p}$ with a as a normalization constant, $\xi \geq 0$, $p > 1$ and $0 < \varepsilon << 1$ in order to avoid a singularity in $\xi = 0$. After determining a, the m-th moment reads

$$\langle \xi^m \rangle = \frac{p-1}{p-(m+1)} \varepsilon^m \left[\frac{1 - \left(\frac{\varepsilon}{\Lambda+\varepsilon}\right)^{p-(m+1)}}{1 - \left(\frac{\varepsilon}{\Lambda+\varepsilon}\right)^{p-1}} \right] . \tag{4.10}$$

Formally, if $p > m+1$, $\langle \xi^m \rangle$ is divergent in the limit $\Lambda \to \infty$.

By defining power laws PDFs for δx and waiting time δt,

$$\lambda'(\delta x) = \frac{A}{(|\delta x| + \varepsilon)^r} \,, \qquad \text{and} \qquad \psi'(\delta t) = \frac{B}{(\delta t + \varepsilon)^s} \,, \tag{4.11}$$

By setting the power dependencies r and s with the criterion of the divergence $p > m + 1$ from equation 4.10, and consequently, determing the convergence or divergence of the first moment $\langle \delta t \rangle_{\psi'}$ or of the second moment $\langle (\delta x)^2 \rangle_{\lambda'}$, it is possible to fulfill the cases 1 to 3 in Section 3., controlling the anomalous diffusion processes ranging from subdiffusion to superdiffusion.

Simulated processes consisted of unidimensional CTRW composed by a population of $N = 10.000$ particles with step lengths and waiting times randomly determined by a Monte Carlo algorithm from power law PDFs 4.11. The time stop criterion was chosen to be so that $\sum \delta t \geq 2^{10}$. Figure 1 shows the time evolution of the population variance, $\log_2(t) \times \log_2(\langle x^2(t) \rangle)$ for cases of subdiffusion and normal diffusion. The histogram of positions of the particles is depicted in Figure 2 for the subdiffusion case.

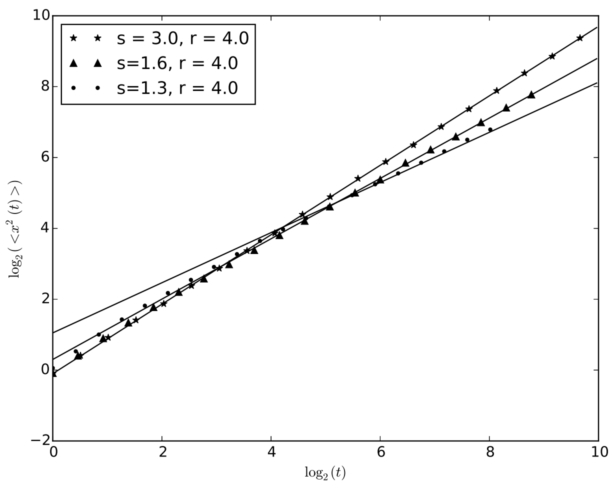

Figura 1: Time evolution of $\log_2(\langle x^2(t) \rangle)$ generated by CTRW of a population of $N = 10.000$ particles over a time $t \geq 2^{10}$ with random jump lengths and random waiting times, both obtained by power law PDF with $r = 4$ and different values powers s. According to the parameters, the process is set to be normal or subdiffusive. The lines are fitted by linear regression in order to determine the model parameters. Case $s = 3$ and $r = 4$ correspond to a normal diffusion process.

5. Results

Simulations were conducted by defining the parameters of the power laws PDF for jump length and waiting times. According to the definition of the parameters and, as the aforementioned cases 1 and 3 (section 3.), the processes were set to be subdiffusive or normal. The assessment of the macroscopic parameters from

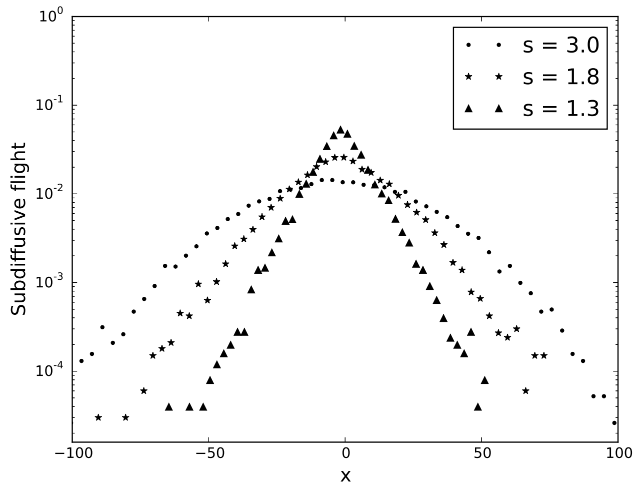

Figura 2: Histogram of positions of a population of of $N = 10.000$ particles generated by simulation over a time $t \geq 2^{10}$ of a CTRW with random jump lengths and random waiting times, both obtained by power law PDF. According to the simulation parameters r and s, the process is set to be normal or superdiffusive.

the simulated microscopic data which was acquired by two different approaches. Firstly, we analyzed the dispersion of the particles population by applying linear regression over the data in the space $\log_2(t) \times \log_2(\langle x^2(t) \rangle)$ according to the equation 2.4. The parameters α and D_α are achieved from subdiffusive processes simulations and their are given respectively by the slope and ordinate intercept of the linear regression plots (see Fig. 1). Since those parameters are obtained by the simulated data without any reference to the theoretical model, they receive the subscript S assigning for 'simulation'. The results of analysis of studied cases can be seen in table 1.

The second method to obtain the macroscopic parameters comprises the optimization fitting of the model solution $G_\alpha(x,t)$ 2.3 to the histogram of position of the processes according to the subdiffusion. Hence, $G_\alpha(x,t)$ is fitted to subdiffusion processes to asses the parameters α and D_α. The adopted optimization method was the Broyden-Fletcher-Goldfarb-Shanno (BFGS) [5]. The parameters obtained by that approach receive the subscript T in mention to the theoretical solutions. Results of such analysis are depicted in figure 3 and the parameters and mean squared deviations (MSD) are listed in table 1.

From the Table (1) one can notice that in the method which the macroscopic parameters were obtained from fitting the histogram by the respective models via the optimization, the MSD showed to be equal or smaller up to two orders of magnitude than those parameters obtained from the method of linear regression

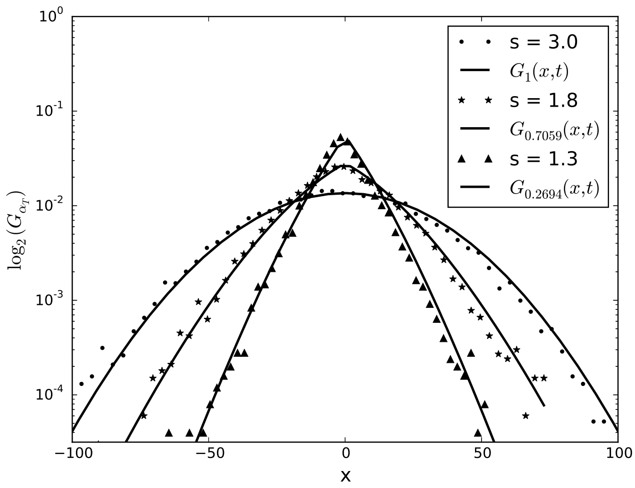

Figura 3: Model solutions $G_{\alpha_T}(x,t)$ (2.3) with parameters assessed by optimization fitting to the histogram of positions generated by simulation over a time $t \geq 2^{10}$ of a CTRW for a population of $N = 10.000$ particles.

Tabela 1: Simulation data generated by power law PDFs for random jump sizes with $r = 4$ and for waiting time varying s in order to provide subdiffusion processes and the respective values of the parameters α and D_α. The parameters assigned by 'S' are obtained by linear regression over the time evolution of the variance and those assigned by 'T' are obtained by fitting the model solution $G_\alpha(x,t)$ (2.3) by BFGS optimization technique. The mean squared deviations MSDs are also calculated in both cases.

s	α_S	D_{α_S}	α_T	D_{α_T}	MDS_S	MDS_T
3.0	0.9999	0.4202	1.0000	0.7217	10^{-9}	10^{-9}
1.9	0.8566	0.5934	0.8566	0.5991	10^{-8}	10^{-8}
1.8	0.7884	0.7612	0.7884	0.7612	10^{-8}	10^{-8}
1.7	0.7076	0.9699	0.7076	0.9699	10^{-8}	10^{-8}
1.6	0.5949	1.3328	0.5847	1.3316	10^{-7}	10^{-7}
1.5	0.4951	1.8141	0.4951	1.8141	10^{-6}	10^{-6}
1.4	0.3976	2.3669	0.3963	2.3668	10^{-6}	10^{-6}
1.3	0.3199	3.1402	0.2785	3.1383	10^{-7}	10^{-7}
1.2	0.2908	3.5099	0.2908	3.5099	10^{-7}	10^{-7}
1.1	0.2855	3.4311	0.2855	3.4311	10^{-6}	10^{-6}

from the time evolution of the variance. The simulations have produced processes with the expected behaviour as subdiffusion or normal diffusion in accord to the prescriptions given in cases 1 and 3 (section 3.) and to the criterion criterion $p < m+1$ ($r < 3$, $s < 2$).

6. Conclusion

The comparison between the methods for determining the parameters of the models indicated that, the optimization fitting of the model solutions to the histogram of position of the anomalous random walk showed a lower mean squared deviations than the fitting of the dispersion by the time evolution of the variance. The result was important to define the method which the study should be conducted.

The definition of the power laws is not uniquely dependent of the power parameter p, (r, s), but it also demands the choose of two additional cutoffs; the first ϵ to avoid the singularity at zero and the upper limit cutoff Λ to provide integrability when a given moment of interest $(\sigma^2, \ \tau)$ is divergent. In order to avoid excessive arbitrariness, we make a prescription which is to set a constraint between both cutoffs. Under such condition, the divergent factor of the moment of interest becomes near the unit.

It was possible to determine a set of equations and prescriptions to estimate which are the powers of the power law distributions for the jumps and waiting time would produce the macroscopic parameters of the linear model written in terms of partial differential equations with fractional derivatives. However, not all cases of fractional derivatives in time were explored. We restricted ourselves to the case which have one of the derivatives being of integer order: the second order derivative in space was fixed and the time derivative remained fractional. Although we could generate a table with those values. We found a strong correlation between the values of the simulation parameters and those of the theoretical parameters.

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