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ESTIMATION OF THE REDISTRIBUTION BEHAVIOR IN THE BIFLUX ANOMALOUS DIFFUSION PROBLEM

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Abstract. *Diffusion, a widespread phenomenon in nature, is commonly used to model various processes. This study focuses on complex anomalous diffusion processes involving temporary retention. We propose an inverse problem approach to estimate the redistribution behavior using synthetic experimental data. By assuming a polynomial of degree N, we determine both N and its coefficients to best match the experimental data. Additionally, we explore the use of Machine Learning for faster direct problem solving compared to traditional methods. Metaheuristics assist in searching for the optimal polynomial degree and coefficients. Our approach yields accurate predictions, making it a potential solution for applying the biux anomalous diffusion model without prior knowledge of the redistribution behavior.*
Keywords: *Biflux Diffusion Equation, Fourth Order Diffusion, BG Model, Inverse Problem, Differential Evolution*

1. INTRODUCTION

The phenomenon of diffusion, which usually refers to the scattering of particles in a medium, is widely observed in nature and everyday life. It is utilized to model various phenomena such as disease transmission, population dynamics, fluid and particle transport, heat transfer, financial markets, and others. In the conventional diffusion model, particles move randomly and uniformly within the medium, resulting in a linear increase in the mean square displacement with time, and displaying a Gaussian behavior. Anomalous diffusion, on the other hand, refers to a type of diffusion that deviates from the norm, where the mean square displacement increases at a non-linear rate. This deviation can be caused by several factors, such as structural heterogeneity, particle interactions, or complex physical processes .

Bevilacqua, Galeão and coworkers Bevilacqua *et al.* (2011, 2013) have developed an analytical formulation for diffusion with retention effects. In this particle spreading process, a portion (α) of the particles is retained and the non-retained portion ($\beta(x)$) is redistributed into neighboring cells. This implies that in order to predict the spreading process we must have knowledge about the redistribution behavior, i.e, $\beta(x)$. In real-case scenarios it is possible that no knowledge is available. To overcome this problem we aim to estimate $\beta(x)$ by using an inverse problem approach, given the registered particle spreading pattern at an arbitrary time t, i.e, the collected experimental data, here syntethic experimental data.

We begin with the assumption that $\beta(x)$ is a polynomial of degree N and our objective is to estimate both N and its coefficients that best generates the behavior of the spreading process according to the experimental data following the biflux anomalous diffusion equation with the help of a population-based approach, chosen because it brings the possibility to generate a collection of doable solutionsRaoui *et al.* (2021) that describes the redistribution behavior, which is precisely our goal.

Our research endeavors to eliminate the prerequisite of prior familiarity with $\beta(x)$ and even though we use concentration to refer to the diffusion process the analogy can be extended to several other physical processes. It is our aspiration that this study shall pave the way for further empirical examinations of the Bevilacqua and Galeão Model in instances where the pre-existing acquaintance with $\beta(x)$ is absent.

2. BIFLUX ANOMALOUS DIFFUSION (BG MODEL)

Considering a region in space that contains a high concentration of particles, represented by cell i in Fig. 1 and, a particle spreading process with retention, a portion (α) of the particles is retained, and the non-retained portion (β) is redistributed into neighboring cells. This process is represented in Fig. 1, where $\beta = 1 - \alpha$.

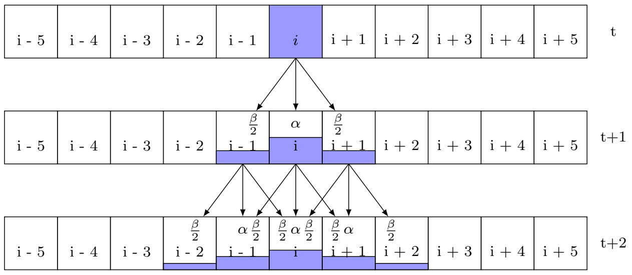

Figure 1. The discrete distribution as a function of time in the BG model for biflux anomalous diffusion with constant β.

This phenomenon in a continuous medium and with the possibility that the redistribution has a spatial dependence is governed by the following partial differential equationBevilacqua *et al.* (2011):

$$\frac{\partial p(x,t)}{\partial t} = K_2 \frac{\partial}{\partial x}\left[\beta(x)\frac{\partial p(x,t)}{\partial x}\right] - K_4 \frac{\partial}{\partial x}\left[\beta(x)(1-\beta(x))\frac{\partial^3 p(x,t)}{\partial x^3}\right] \tag{1}$$

where $p(x,t)$ represents the concentration, K_2 is the diffusion coefficient and K_4 is the reactivity coefficient.

Equation (1) is called the Biflux Anomalous Diffusion Equation, or BG Model for anomalous diffusion. For a review of how Eq. (1) was obtained we recommend reading the analytical development of this model in Refs. Bevilacqua *et al.* (2011, 2013). With the product rule, Eq. (1) can be written as

$$\frac{\partial p(x,t)}{\partial t} = A_1 \frac{\partial p(x,t)}{\partial x} + A_2 \frac{\partial^2 p(x,t)}{\partial x^2} - A_3 \frac{\partial^3 p(x,t)}{\partial x^3} - A_4 \frac{\partial^4 p(x,t)}{\partial x^4} \tag{2}$$

where

$$A_1(x) = K_2 \frac{d\beta(x)}{dx} \tag{3}$$

$$A_2(x) = K_2 \beta(x) \tag{4}$$

$$A_3(x) = K_4 (1 - 2\beta(x)) \frac{d\beta(x)}{dx} \tag{5}$$

$$A_4(x) = K_4 \beta(x)(1 - \beta(x)) \tag{6}$$

When K_2, K_4, $\beta(x)$, its derivative, along with the initial and four boundary conditions, are known, then the problem can be solved numerically using, for example, the Finite Difference Method.

3. DIRECT PROBLEM

3.1 Finite Difference Method

In order to generate a numerical solution for the BG Model, the well-established Finite Difference Method was employed. The system of algebraic linear equations generated by the discretization was solved with the Gauss Elimination Method followed by the Backward Substitution approach.

The following discretizations were used in a Forward-Time Centered-Space implicit approach, first for the time derivative

$$\frac{\partial p(x,t)}{\partial t} \approx \frac{\phi_i^{n+1} - \phi_i^n}{\Delta t} \tag{7}$$

where ϕ_i^n is the concentration at the i-th spatial node and the n-th time node. For the spatial derivatives, the scheme used is given as follows

$$\frac{\partial p(x,t)}{\partial x} \approx \frac{\phi_{i-2}^{n+1} - 8\phi_{i-1}^{n+1} + 8\phi_{i+1}^{n+1} - \phi_{i+2}^{n+1}}{12\Delta x} \tag{8}$$

$$\frac{\partial^2 p(x,t)}{\partial x^2} \approx \frac{-\phi_{i-2}^{n+1} + 16\phi_{i-1}^{n+1} - 30\phi_i^{n+1} + 16\phi_{i+1}^{n+1} - \phi_{i+2}^{n+1}}{12\Delta x^2} \tag{9}$$

$$\frac{\partial^3 p(x,t)}{\partial x^3} \approx \frac{-\phi_{i-2}^{n+1} + 2\phi_{i-1}^{n+1} - 2\phi_{i+1}^{n+1} + \phi_{i+2}^{n+1}}{2\Delta x^3} \tag{10}$$

$$\frac{\partial^4 p(x,t)}{\partial x^4} \approx \frac{\phi_{i-2}^{n+1} - 4\phi_{i-1}^{n+1} + 6\phi_i^{n+1} - 4\phi_{i+1}^{n+1} + \phi_{i+2}^{n+1}}{\Delta x^4} \tag{11}$$

With a substitution of the above equations in Eq. (1), we get the following algebraic linear system of equations

$$\begin{aligned} [-\Gamma_{1,i} + \Gamma_{2,i} - \Gamma_{3,i} + \Gamma_{4,i}]\phi_{i-2}^{n+1} \quad &+ \quad [8\Gamma_{1,i} - 16\Gamma_{2,i} + 2\Gamma_{3,i} - 4\Gamma_{4,i}]\phi_{i-1}^{n+1} + \\ [1 + 30\Gamma_{2,i} + 6\Gamma_{4,i}]\phi_i^{n+1} \quad &+ \quad [-8\Gamma_{1,i} - 16\Gamma_{2,i} - 2\Gamma_{3,i} - 4\Gamma_{4,i}]\phi_{i+1}^{n+1} + \\ [\Gamma_{1,i} + \Gamma_{2,i} + \Gamma_{3,i} + \Gamma_{4,i}]\phi_{i+2}^{n+1} \quad &= \quad \phi_i^n,\ i = 1, 2, \ldots, Nx \text{ and } n = 1, 2, \ldots, Nt \end{aligned} \tag{12}$$

where Nx represents the total number of spatial nodes, and Nt denotes the total number of nodes in time. $\Gamma_{1,i}$, $\Gamma_{2,i}$, $\Gamma_{3,i}$ and $\Gamma_{4,i}$ are defined as

$$\Gamma_{1,i} = \frac{A_{1,i}\Delta t}{12\Delta x} \tag{13}$$

$$\Gamma_{2,i} = \frac{A_{2,i}\Delta t}{12\Delta x^2} \tag{14}$$

$$\Gamma_{3,i} = \frac{A_{3,i}\Delta t}{2\Delta x^3} \tag{15}$$

$$\Gamma_{4,i} = \frac{A_{4,i}\Delta t}{\Delta x^4} \tag{16}$$

in our simulations, since this scheme in this particular case is unconditionally stable due to the implicit formulation, we arbitrarily defined Nt=$10,001$ and Nx = 501.

4. INVERSE PROBLEM FORMULATION

As the aim of this paper is to estimate the coefficients of the polynomial used to represent the function $\beta(x)$, our first goal is to solve the inverse problem that in this case is formulated as an optimization problem of minimizing a cost function in order to estimate the coefficients. In this scenario $\beta(x)$ is given by

$$\beta(x) = \sum_{i=0}^{N} A_i x^i \tag{17}$$

and the objective function to be minimized is defined as

$$F_{obj}(\phi) = \sum_{i=0}^{N_{meas}} [(\phi_i^*(\mathbf{Z}) - \Phi_i)^2 + G_i] \tag{18}$$

where

$$\mathbf{Z} = [A_0^*, A_1^*, A_2^*, \cdots, A_N^*]$$

is a vector of coefficients candidates, $\phi_i^*(\mathbf{Z})$ is the solution of the BG Model with $\mathbf{Z}$, and Φ_i is the experimental data, both at the same location and time instant. In Eq. 18, G_i is a penalization for when $\beta(x)$, with $\mathbf{Z}$, generates values bigger than 1 or smaller than 0. That is necessary because, according to the biflux theory, $\beta(x)$ must be constrained to the interval [0,1]. G_i is defined as

$$G_i = \begin{cases} 0, \text{if } 0 \leq \beta_i^Z \leq 1 \\ (\beta_i^Z)^2, \text{otherwise} \end{cases} \tag{19}$$

The inverse problem solution is then the vector $\mathbf{Z}$, namely the coefficients of $\beta(x)$, given by Eq. (17), that minimizes the cost function, see Eq. (18), in which Φ represents the experimental value that has been observed. In this study, we have generated synthetic data using $\beta_{exact}(x) = \log(x + 1)$ and adding random noise from a gaussian distribution with zero mean and 0.01 standard deviation in order to simulate real experimental data that always has measurement errors. The polynomial we are searching for is intended to approximate the observed data generated with $\beta_{exact}(x)$ in the BG model.

In order to find the vector $\mathbf{Z}$, in the present work we make use of a Differential Evolution algorithm as described in the previous section.

4.1 Differential Evolution

The Differential Evolution is a heuristic optimization method, proposed by Storn and Price Storn and Price (1997), based on vector operations where the weighted difference between two vectors is added to a third vector that generates potential candidates for the optimal solution of the problem. We can summarize our implemented version of this method as follows

1. Generation of an initial random population

   $$x_{k,j}^{t=0} = x_{L,k} + rand_{k,j}(x_{U,k} - x_{L,k}), \;\; j = 1, 2, \ldots, N_{pop}$$

   where $x_{U,k}$ and $x_{L,k}$ are the upper and lower bounds of the k-th variable, $rand_{k,j}$ is a random number between 0 and 1, and N_{pop} is the size of the population.

2. Mutation operation for generating a candidate

   $$\overrightarrow{v_l}^t = \overrightarrow{x}_{r0}^t + \alpha(\overrightarrow{x}_{r1}^t - \overrightarrow{x}_{r2}^t)$$

   where α is a perturbation factor, here arbitrarily defined as 0.7, and the vectors $\overrightarrow{x}_{r0}^t$, $\overrightarrow{x}_{r1}^t$ and $\overrightarrow{x}_{r2}^t$ are randomly chosen from within the population and must be distinct from each other.

3. The next step is the crossover operation where the generated vector can be accepted or not depending on the criterion

   $$\overrightarrow{x}_l^{t+1} = \begin{cases} \overrightarrow{v_l}^t, \text{if } p_c \leqslant rand_{k,l} \\ \overrightarrow{x}_l^t, \text{otherwise} \end{cases}$$

   where p_c is the crossover probability defined for the present study as 0.7.

4. Finally, if the new vector $\overrightarrow{v_l}^t$ provides a better value for the objective function than vector $\overrightarrow{x}_l^t$, the latter is replaced by the former in the next generation, otherwise $\overrightarrow{x}_l^t$ remains in the population for one more generation

5. Repeat steps 2-4 until a predefined maximum number generations is achieved.

5. RESULTS

5.1 Direct Problem and Case of Study

In this study, the direct problem was solved with $K_2 = 0.1$ and $K_4 = 10^{-5}$, the initial condition is given by

$$p(x, t = 0) = 0.5(1 + \cos(\pi(x - 1))) \qquad 0 \leq x \leq 2 \tag{20}$$

and the boundary condition defined as

$$p(0, t) = p(2, t) \quad = \quad 0 \tag{21}$$

$$\left.\frac{\partial p(x,t)}{\partial x}\right|_{x=0} = \left.\frac{\partial p(x,t)}{\partial x}\right|_{x=2} \quad = \quad 0 \tag{22}$$

Figure 2a shows the $\beta_{exact}(x)$ function and Fig. 2b its derivative.

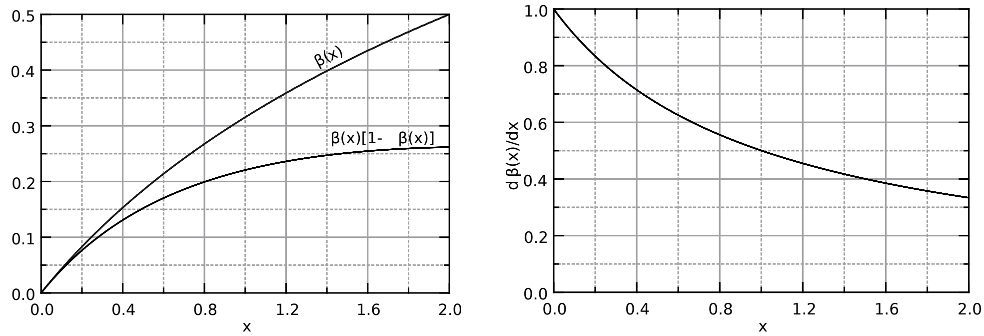

Figure 2. (a) Function $\beta(x) = \beta_{exact}s(x) = log(x+1)$, and the product $\beta(x)[1-\beta(x)]$. (b) The derivative of $\beta(x)$ with respect to x.

In this particular case, the solution of the biflux anomalous diffusion model without noise is presented in Fig. 3a.

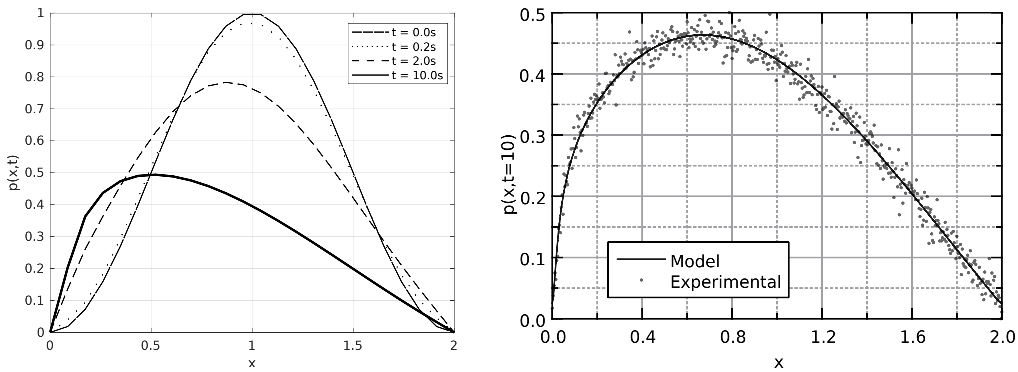

Figure 3. (a) The solution of the BG Model with constant parameters. $\beta(x) = \log(x+1)$, $K_2 = 0.1$ and $K_4 = 10^{-5}$ without noise. (b) The solution of the BG Model at t=10 with $\beta = \log(x+1)$, $K_2 = 0.1$, $K_4 = 10^{-5}$ and with noise from a gaussian distribution $\mathcal{N}(\mu = 0, \sigma = 0.01)$.

With the output of the direct problem the synthetic data was generated by adding random noise from a gaussian distribution to it, the noisy data is shown in Fig. 3b and it'll be the data considered as our case of study.

5.2 Parameters Estimation

In the process of estimating the coefficients it is important to define a search interval for each element, in the current study we defined the lower limit as -1.0 and upper limit to 1.0 except for coefficient A_N that is contained in the interval 0.0 to 1.0. The maximum degree of the polynomial was set as 7.

After 30 runs of the Differential Evolution algorithm with 30 particles each, the 10 best solutions in terms of the cost function value are ranked in Table 1.

Figure 4 shows Solutions 1, 2, 5, 7 and 8 in comparison with the exact values of $\beta(x)$ along x.

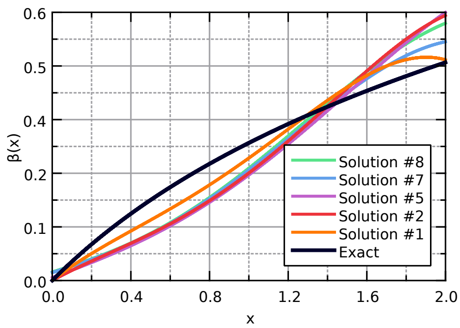

Figure 4. A few selected solutions from Table 1 of the estimated polynomial $\beta(x)$

The results in Table 1 shows that the two best solutions in terms of the value of the cost function was a 4th degree polynomial, and the approach used did not have any 7 degree polynomial after several runs of the algorithm.

In Figure 5 the # 1 and # 10 solutions were used to solve the BG Model and plotted along side the synthetic experimental data used for a visual comparison reason.

Table 1. The 10 Best solutions obtained with the Differential Evolution algorithm after 30 runs of the algorithm with 30 as the maximum generation number and population size of 30 each.

Solution	**Z**							
	A_0	A_0	A_0	A_1	A_2	A_3	A_4	A_5
#1	0.000000	0.000000	0.000000	-0.087332	0.283434	-0.265461	0.337245	0.000000
#2	0.000000	0.000000	0.000000	-0.064951	0.222200	-0.157164	0.235142	0.000000
#3	0.000000	0.000000	0.023557	-0.079058	0.187456	-0.192952	0.267132	0.000884
#4	0.000000	0.000000	0.058743	-0.205408	0.285988	-0.146824	0.223975	0.000000
#5	0.000000	0.000000	0.000156	-0.031347	0.094223	0.000000	0.161489	0.006469
#6	0.000000	0.000000	0.029741	-0.080288	0.165702	-0.202598	0.278812	0.013596
#7	0.000000	0.000000	0.009255	-0.086152	0.164124	-0.000173	0.137480	0.017369
#8	0.000000	0.000000	0.010510	-0.087223	0.165826	0.000436	0.137618	0.018525
#9	0.000000	0.000000	0.046135	-0.144138	0.172362	-0.052807	0.182588	0.018140
#10	0.000000	0.000000	0.055398	-0.095613	0.077877	-0.117823	0.253057	0.021231
Std. Dev.	0.000000	0.000000	0.023171	0.047393	0.068503	0.095899	0.065965	0.008984

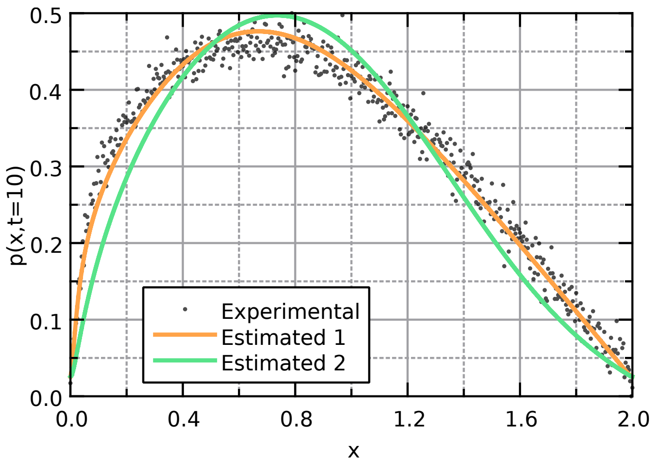

Figure 5. (a) The solution of the BG Model with two candidates solutions for **Z**, with Result #1 and Result #10.

6. CONCLUSIONS

Our approach of an inverse problem of coefficients estimation with the aid of the Differential Evolution algorithm has proved itself successful as the final result was a really close prediction with error of magnitude of order 10^{-2} with respect to that predicted by the model with the exact parameters which indicates that this approach can be a solution for those who wants to try out the BG Model but has no available knowledge about $\beta(x)$.

For future works, firstly $\beta(x)$ can be treated as a multivariate polynomial as a function not only of spatial position but also of time and the concentration itself. This would allow for the analysis of the hidden flux of particles from the primary flux to the secondary flux. Secondly, a two and three dimensional cases should be explored with this polynomial approach.

7. ACKNOWLEDGEMENTS

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