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Parameter estimation for the fractional fractal diffusion model based on its numerical solution

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ABSTRACT

In this paper, we mainly consider a problem of parameter estimation for the fractional fractal diffusion model used to describe the anomalous diffusion in porous media. The Bayesian method is proposed to estimate parameters for the fractional fractal diffusion model based on its numerical solution. Firstly, the center Box difference method is employed to solve the fractional fractal diffusion equation subject to the initial–boundary conditions. Then we apply the Bayesian method to estimate three parameters for the model simultaneously, that is the fractional order α, the fractal dimension d_f and the structure parameter θ. To testify the validity of the results for the model's parameter estimation, experimental data from the fast desorption process of methane in coal are used. It is shown that the numerical results modeled with parameters given by the Bayesian method coincide well with the desorption experimental data, indicating that the Bayesian method is efficient and valid in identifying multi-parameter for the fractional fractal diffusion model. Besides, the fractional fractal diffusion model is demonstrated to be more capable than the classical Fick's model to describe the anomalous diffusion behavior of gas in coal. To clarify the parameters' effect on the relative diffusion amount of methane for the fractional fractal diffusion model, parameter sensitivity analysis is also carried out. This paper provides a specific and efficient parameter estimation method for the fractional fractal diffusion model.

1. Introduction

In recent years, many cases referred to as anomalous diffusion, in which the Fick's classical model fails to capture the diffusion behavior of substance, have caused increasing interests of researchers. It turns out that the fractional diffusion model provides more accurate description of memory and hereditary properties of anomalous transport process. Fractional constitutive equations instead of the classic counterparts have been widely used to well capture the more complex features of objects [1–5].

In the heterogeneous porous media, the fractal structure is proved to have great effects on particle diffusion processes [6]. Therefore, the fractal dimension has been introduced into the constitutive equation and demonstrated to be more efficient than the integer dimension in representing the diversity and complexity of objective things. O'Shaugnessy and Procaccia [7] proposed the widely used OP model for diffusive transport in a porous media by introducing the fractal dimension d_f.

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Yuste. et al. [8] considered the long-time behavior of the survival probability for anomalous d-dimensional diffusion problems with radial symmetry. Wang et al. [9] used the classical fractal diffusion model to describe the diffusion of gases in a porous material within the limited volume of a stiff container(LVSC).

Though many analytical methods have been expanded to solve fractional differential equations, for example, Gepreel et al. [10] found the exact solutions for some nonlinear partial fractional differential equations used the fractional sub-equation method, Baleanu et al. [11] established the long-time asymptotic formula of solutions to a $(1+\alpha)$-order fractional differential equation, extensive research has been carried out on developing efficient numerical methods, including finite difference methods [12–14], the finite element method [15,16], the finite volume method [17,18], and the spectral method [19,20]. Currently, numerical methods have held dominant position in the aspect of solving fractional partial differential equations. For example, Weihua Deng and his coworkers [21] discussed the semi-implicit schemes for the nonlinear predator–prey reaction–diffusion model with the space–time fractional derivatives, and analyzed the stability and convergence of the schemes. Yu et al. [22] considered a two-dimensional non-linear fractional reaction–subdiffusion equation, and derived a novel compact numerical method with second-order temporal accuracy and fourth-order spatial accuracy. Zeng et al. [23] first proposed two fully discrete schemes for the time-fractional subdiffusion equation with space discretized by finite element method and time discretized by the fractional linear multistep methods, both the two numerical algorithms were demonstrated to be unconditionally stable with maximum global convergence order. Yang et al. [24] provided three numerical methods, namely, the L1/L2-approximation method, the standard/shifted Grünwald method, and the matrix transform method to deal with the fractional partial differential equation with Riesz space fractional derivatives on a finite domain.

As an important problem connected with the fractional constitutive models, to develop special parameter estimation methods to identify model parameter from experimental data has induced much research. Many methods have been applied to estimate parameter for classic problems [25,26], while that developed for fractional differential equations are quite few. Liu et al. [27] applied a modified hybrid simplex search and a particle swarm optimization method to estimate parameters for fractional dynamical models arising from biological systems. Yu et al. [28] proposed numerical algorithms to estimate relaxation parameters and Caputo fractional derivative for a fractional thermal wave model in spherical composite medium. Cheng et al. [29] studied the determination of the order of the Caputo fractional derivative and the diffusion coefficient in a fractional diffusion equation and gave a uniqueness result. Yu et al. [30] proposed the Levenberg–Marquardt algorithm based on a fractional derivative to estimate the unknown order of a Riemann–Liouville fractional derivative for a fractional Stokes first problem for a heated generalized second grade fluid. Zheng et al. [31] studied a new regularization method for solving a time-fractional inverse diffusion problem in a one-dimensional semi-infinite domain. As an statistical technique, the Bayesian method connected with Monte Carlo sampling [32] has been shown to be efficient in inverse problem for kinds of models. Angelov et al. [33] applied a Bayesian approach to estimate the basic reproduction number for the model of the spread of an infectious disease in a population. Wang et al. [34] used a Bayesian method to reconstruct an unknown transient heat source in a three-dimensional participating medium from temperature measurements. Ma et al. [35] introduced a method for accelerating Bayesian inference based on the use of an adaptive sparse grid collocation technique to construct a stochastic surrogate model. Fan et al. [36] successfully proposed the Bayesian method to estimate parameters for fractional equation based on the analytical solutions.

In this paper, we mainly consider the parameter estimation for the fractional fractal diffusion model used to describe the anomalous diffusion in porous media. The problem is carried out by means of the Bayesian method based on the model's numerical solution. More specifically, we first construct the numerical scheme for the fractional fractal diffusion model. And then, based on the model's numerical solution, we use the Bayesian method to conduct multi-parameter estimation for the model.

The rest of this paper is organized as follows: In Section 2, a brief derivation of the fractional fractal diffusion model is shown. In Section 3, we give the center Box difference scheme for the fractional fractal diffusion model subject to the initial–boundary conditions. Parameter estimation of the three unknowns, that is the fractional order α, the fractal dimension d_f and the structure parameter θ, by the Bayesian method are shown in Section 4. Results and discussions are analyzed in Section 5. In the end, some conclusions are made.

2. The fractional diffusion model based on the fractal theory

For diffusive transport in porous media, the diffusivity D was proposed to take the form [7] of

$$D = D_0 r^{-\theta}, \tag{1}$$

where D is the diffusion coefficient, D_0 is the pre-exponential factor, r is the radius of particles, and θ is a structure parameter describing the transport path of the diffusing molecule that is walking in the fractal porous material.

The Fick's model used for the Euclidean geometry with radial symmetry in dimension [37] is

$$\frac{\partial c(r,t)}{\partial t} = \frac{D}{r^{d-1}} \frac{\partial}{\partial r}\left(r^{d-1}\frac{\partial c(r,t)}{\partial r}\right). \tag{2}$$