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Laplace-fPINNs: Laplace-Based Fractional Physics-Informed Neural Networks for Solving Forward and Inverse Problems of a Time Fractional Equation

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Abstract. Physics-informed neural networks (PINNs) are an efficient tool for solving forward and inverse problems for fractional diffusion equations. However, since the automatic differentiation is not applicable to fractional derivatives, solving fractional diffusion equations by PINNs meets a number of challenges. To deal with the arising problems, we propose an extension of PINNs called the Laplace-based fractional physics-informed neural networks (Laplace-fPINNs). It can effectively solve forward and inverse problems for fractional diffusion equations. Note that this approach avoids introducing a mass of auxiliary points and simplifies the loss function. We validate the effectiveness of using the Laplace-fPINNs by several examples. The numerical results demonstrate that the Laplace-fPINNs method can effectively solve the forward and inverse problems for fractional diffusion equations.

AMS subject classifications: 35R11

Key words: Physics-informed neural networks, Laplace transform, numerical inverse Laplace transform, time fractional equations.

1. Introduction

Fractional diffusion equations have been extensively studied in engineering, physics, and mathematics due to their superior capability for modeling anomalous diffusion phenomena. The model differs from the standard diffusion models since it follows a basic assumption that the diffusion obeys the standard Brownian motion and has been applied to animal coat patterns and nerve cell signals. A distinctive feature of standard Brownian motions is that the mean squared displacement $\langle x^2(t)\rangle$ of diffusing species linearly increases with time — i.e. $\langle x^2(t)\rangle \sim K_1 t$. However, in an anomalous diffusion, the mean squared

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displacement shows a non-linear power law growth with time — i.e. $\langle x^2(t)\rangle \sim K_\alpha t^\alpha$, where $0<\alpha<1$ represents a subdiffusion and $\alpha>1$ a superdiffusion. At the microscopic level, such anomalous diffusion processes can be accurately described by a continuous-time random walk where the waiting time between successive particle leaps follows a heavy-tailed distribution with a diverging mean. At the macroscopic level, anomalous diffusion describes the evolution of the probability density function of a particle that appears at a given spatial location x and time t. A list of successful applications of fractional diffusion equations are extensive and continually expanding. These applications include, but are not limited to, solute transport in heterogeneous media [4,9], thermal diffusion on fractal domains [31], protein transport within membranes [17,36], and flow in highly heterogeneous aquifers [5]. Comprehensive review of the physics modeling and a diverse range of applications can be found in [6,30].

In this paper, we consider the following general time-fractional diffusion equation on a bounded domain $\Omega\subset\mathbb{R}^d$ with homogeneous Dirichlet boundary condition:

$$\begin{aligned}
&\left(D_k^c u\right)(x,t)=\nabla\cdot\big(a(x)\nabla u(x,t)\big)+c(x)u(x,t)+f(x,t), \quad x\in\Omega, \quad t>0,\\
&u(x,0)=u_0(x), \quad x\in\Omega,\\
&u(x,t)=0, \qquad x\in\partial\Omega, \quad t>0,
\end{aligned} \tag{1.1}$$

where $(D_k^c u)(x,t)$ denotes the Caputo type fractional derivative defined by

$$\left(D_k^c u\right)(x,t)=\int_0^t k(t-\tau)\frac{d}{d\tau}u(x,\tau)d\tau, \tag{1.2}$$

and k is a nonnegative locally integrable function. Setting

$$k(\tau)=\frac{\tau^{-\alpha}}{\Gamma(1-\alpha)}, \quad 0<\alpha<1 \tag{1.3}$$

in the Eq. (1.2), we have the conventional Caputo fractional derivative [33]. Another important particular case of (1.2) is given by

$$k(\tau)=\sum_{k=1}^n \gamma_k \frac{\tau^{-\alpha_k}}{\Gamma(1-\alpha_k)}, \quad 0<\alpha_1<\cdots<\alpha_n<1. \tag{1.4}$$

It corresponds to the multi-term time fractional derivatives. $\Gamma(\cdot)$ denotes the gamma function, $a(x)$, $c(x)$, $f(x,t)$, and $u_0(x)$ are the diffusion coefficient, reaction coefficient, source, and initial value, respectively.

Solving partial differential equations numerically is a well-known challenge, and it becomes even more difficult when dealing with fractional diffusion equations that involve nonlocal operators. Recently, there has been a growing trend to apply machine learning techniques for solving forward and inverse problems of partial differential equations. Several examples include the use of Gaussian process regression [13,19,34] and deep learning-based methods [2,10,18,28,35,44] to solve these types of problems.