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Do We Need Decay-Preserving Error Estimate for Solving Parabolic Equations with Initial Singularity?

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Abstract. Solutions exhibiting weak initial singularities arise in various equations, including diffusion and subdiffusion equations. When employing the well-known L1 scheme to solve subdiffusion equations with weak singularities, numerical simulations reveal that this scheme exhibits varying convergence rates for different choices of model parameters (i.e., domain size, final time T, and reaction coefficient κ). This elusive phenomenon is not unique to the L1 scheme but is also observed in other numerical methods for reaction-diffusion equations such as the backward Euler (IE) scheme, Crank-Nicolson (C-N) scheme, and two-step backward differentiation formula (BDF2) scheme. The existing literature lacks an explanation for the existence of two different convergence regimes, which has puzzled us for a long while and motivated us to study this inconsistency between the standard convergence theory and numerical experiences. In this paper, we provide a general methodology to systematically obtain error estimates that incorporate the exponential decaying feature of the solution. We term this novel error estimate the 'decay-preserving error estimate' and apply it to the aforementioned IE, C-N, and BDF2 schemes. Our decay-preserving error estimate consists of a low-order term with an exponential coefficient and a high-order term with an algebraic coefficient, both of which depend on the model parameters. Our estimates reveal that the varying convergence rates are caused by a trade-off between these two components in different model parameter regimes. By considering the model parameters, we capture different states of the convergence rate that traditional error estimates fail to explain. This approach retains more properties of the continuous solution. We validate our analysis with numerical results.

AMS subject classifications: 65M06, 65M12, 65M25

Key words: Diffusion equation, subdiffusion equation, weak initial singularity, decay-preserving error estimate, convergence rate.

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1 Introduction

Many studies have been carried out on numerical analysis of the following linear reaction subdiffusion equations

$$\begin{aligned} \partial_t^\alpha u-\Delta u&=\kappa u+f, \quad x\in\Omega,\ t\in(0,T],\\ u(x,t)&=0, \quad x\in\partial\Omega,\ t\in(0,T],\\ u(x,0)&=u_0(x), \quad x\in\bar{\Omega}, \end{aligned} \tag{1.1}$$

where the reaction coefficient κ is a given constant, and ∂_t^α denotes the fractional Caputo derivative of order α with respect to t, namely

$$\partial_t^\alpha u(x,t)=\frac{1}{\Gamma(1-\alpha)}\int_0^t \frac{\partial_s u(x,s)}{(t-s)^\alpha}ds, \quad 0<\alpha<1.$$

Diffusion is one of the most prominent transport mechanisms in nature. The classical diffusion models generally describe the Brownian motion of particles. However, over the last few decades, numerous experimental findings suggest that the Brownian motion assumption may not be adequate for accurately describing some physical processes, such as anomalous diffusion or non-Gaussian process. Instead, these processes are better described by the model (1.1). For a comprehensive exploration of various applications and physical modeling, one can refer to the surveys in [18,19] and the monograph [6].

In any numerical methods for solving problem (1.1), a key consideration is that the solution exhibits a weak singularity near the initial time $t=0$ even though the initial value is smooth. Specifically, if $u_0(x)\in H_0^1(\Omega)\cap H^2(\Omega)$, the solution of problem (1.1) with $f=0$ satisfies [5]

$$\|\partial_t u(t)\|_{L^2(\Omega)}\le Ct^{\alpha-1}. \tag{1.2}$$

Under the regularity condition (1.2), the convergence rate with the maximum norm in time is proven to be $\mathcal{O}(\tau^\alpha)$ for various numerical schemes, such as the L1 and L2-type [7, 10, 12, 20] and convolution quadrature schemes [5, 15]. Furthermore, the point-wise error estimate of the L1 scheme at time $t=t_n$ is established as $\mathcal{O}(\tau t_n^{\alpha-1})$ in [2,9], implying that the L1 scheme with a smooth initial value is first-order convergent at the final time level. Further discussions can be found in [3, 4, 17, 23]. An example is widely used to numerically verify the theory by taking $\Omega=(0,L)$, and the exact solution of problem (1.1) is constructed as

$$u=t^\alpha\sin(\pi x/L). \tag{1.3}$$

In the simulation, we use the L1 scheme to discretize the Caputo derivative with N uniformly distributed grid points, and use the finite difference method in space with M grid points. Table 1 displays temporal convergence rates of the L1 scheme for a fixed time level $t_N=T$, $\alpha=0.5$ and $M=20000$. An interesting and puzzling phenomenon is observed in Table 1 that the convergence rates are influenced by the choices of model parameters, i.e., the interval length L, the final time T and the reaction coefficient κ. Specifically, the