Positivity and boundedness preserving schemes for the fractional reaction-diffusion equation

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Abstract  In this paper, we design a semi-implicit scheme for the scalar time fractional reaction-diffusion equation. We theoretically prove that the numerical scheme is stable without the restriction on the ratio of the time and space stepsizes, and numerically show that the convergence orders are 1 in time and 2 in space. As a concrete model, the subdiffusive predator-prey system is discussed in detail. First, we prove that the analytical solution to the system is positive and bounded. Then, we use the provided numerical scheme to solve the subdiffusive predator-prey system, and theoretically prove and numerically verify that the numerical scheme preserves the positivity and boundedness.

Keywords  time fractional reaction-diffusion equation, subdiffusive predator-prey system, positivity, boundedness

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1 Introduction

Mathematically, the reaction-diffusion systems take the form of semi-linear parabolic partial differential equations. Usually, in real-world applications, the reaction term describes the birth-death or reaction occurring inside the habitat or reactor. The diffusion term models the movement of many individuals in an environment or media. The individuals can be very small particles in physics, bacteria, molecules, or cells, or very large objects such as animals, plants. The diffusion is often described by a power law, $\langle x^2(t) \rangle - \langle x(t) \rangle^2 \sim Dt^\alpha$, where $D$ is the diffusion coefficient and $t$ is the elapsed time (see [13]). In a normal diffusion, $\alpha = 1$. If $\alpha > 1$, the particle undergoes superdiffusion, and it results from active cellular transport processes. If $\alpha < 1$, the phenomenon is called subdiffusion, it can be protein diffusion within cells, or diffusion through porous media. This paper concerns the subdiffusive reaction-diffusion system, which corresponds to the classical reaction-diffusion equation with its first order time derivative replaced by the $\alpha$-th order fractional time derivative.

As an important concrete example, we discuss the subdiffusive predator-prey model in detail. All living things within an ecosystem are interdependent. A change in the size of one population or the environment they live affects all other organisms within the ecosystem. This is shown clearly by the relationship between predator and prey populations. Cavani and Farkas [4] introduced diffusion to the

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Michaelis-Menten-Holling predator-prey model. More general models are considered in [3,15,17]. Here, we further discuss the Michaelis-Menten-Holling predator-prey model with the subdiffusive mechanism [2,19]:

\[
\begin{align*}
\frac{\partial^\alpha N}{\partial t^\alpha} &= \frac{\partial^2 N}{\partial x^2} + N \left( 1 - N - \frac{aP}{P+N} \right), \quad x \in (l,r), \quad t > 0, \\
\frac{\partial^\alpha P}{\partial t^\alpha} &= \frac{\partial^2 P}{\partial x^2} + \sigma P \left( \frac{\gamma + \delta \beta P}{1 + \beta P} + \frac{N}{P+N} \right), \quad x \in (l,r), \quad t > 0,
\end{align*}
\]

(1.1)

with the positive initial conditions and the homogeneous Dirichlet boundary conditions

\[
N(l,t) = N(r,t) = P(l,t) = P(r,t) = 0,
\]

(1.2)

or the homogeneous Neumann boundary conditions

\[
(\partial N(x,t)/\partial x)|_{x=l} \text{ and } r, \text{ respectively } = (\partial P(x,t)/\partial x)|_{x=l} \text{ and } r, \text{ respectively } = 0,
\]

(1.2′)

where \(a, \sigma\) and \(\beta\) are positive real numbers, and \(0 < \gamma \leq \delta\). We prove that the analytical solution to (1.1) and (1.2) (or (1.2)′) is positive and bounded.

For the analytical solution to the subdiffusion equation, the reader can refer to [1,9,12,14,18] and the references therein. There are also some works for the numerical solutions to subdiffusion equations, see [5–8,10,11,20]. In particular, Zhang and Sun [21] developed the semi-implicit schemes for the subdiffusive equations. For the past few decades, the semi-implicit schemes are widely used in various complicated time dependent non-linear equations. Usually, the semi-implicit schemes use two time levels; in time level 1, the nonlinear terms are explicitly computed, and then to implicitly solve the high order linear terms. The expected advantage of the semi-implicit scheme is that as the nonlinear terms are computed efficiently but not losing good numerical stability. Here, we construct the semi-implicit scheme to numerically solve the subdiffusive reaction-diffusion equation. The stability of the numerical scheme is strictly proved, and it has no restriction on the ratio of the sizes of space steps and time ones. The convergent orders 1 in time and 2 in space are theoretically obtained and numerically verified. Moreover, we use the provided scheme to numerically solve the subdiffusive predator-prey model. We show both theoretically and numerically that it preserves the positivity and boundedness of the solutions to the subdiffusive predator-prey model.

The outline of the paper is as follows. In Section 2, we propose the time fractional semi-implicit scheme for the subdiffusive reaction-diffusion equation. We discuss the stability and convergence of the proposed scheme in Section 3, and prove that the temporal approximation order is 1 and the order in space is 2. In Section 4, we first prove the positivity and boundedness of the solution to the subdiffusive predator-prey model, then certify that the numerical scheme preserves its positivity and boundedness. In Section 5, we perform the numerical experiments to confirm the convergent orders and positivity and boundedness preserving. We conclude the paper with some remarks in the last section.

2 Scheme for the subdiffusive reaction-diffusion equation

We first consider the following scalar subdiffusive reaction-diffusion equation:

\[
\begin{align*}
\frac{\partial^\alpha u(x,t)}{\partial t^\alpha} &= \frac{\partial^2 u(x,t)}{\partial x^2} + f(u(x,t)),
\end{align*}
\]

(2.1)

with \(x \in \Omega = (0,1), 0 < t \leq T, 0 < \alpha < 1\), the initial condition

\[
u(x,0) = g(x), \quad x \in \Omega,
\]

(2.2)

and the boundary conditions

\[
u(0,t) = u(1,t) = 0, \quad 0 \leq t \leq T,
\]

(2.3)
or
\[
(\partial u(x,t)/\partial x)|_{x=0} = (\partial u(x,t)/\partial x)|_{x=1} = 0, \quad 0 \leq t \leq T,
\]  
(2.3)'

where \(\partial^\alpha u(x,t)/\partial t^\alpha\) is the time fractional Caputo derivative [16] defined as
\[
\frac{\partial^\alpha u(x,t)}{\partial t^\alpha} = \frac{1}{\Gamma(1-\alpha)} \int_0^t \frac{\partial u(x,s)}{\partial s} \left(\frac{t-s}{\tau}\right)^\alpha ds, \quad 0 < \alpha < 1.
\]  
(2.4)

For ease of presentation, we uniformly divide the spacial domain \(\Omega = (0,1)\) into \(M\) subintervals with stepsize \(h\) and the time domain \((0,T)\) into \(N\) subintervals with steplength \(\tau\). Let \(x_i = ih, i = 0, 1, \ldots, M; t_j = j\tau, j = 0, 1, \ldots, N\). Let the grid function be \(u_i^j = u(x_i,t_j), 0 \leq i \leq M, 0 \leq j \leq N\), denote
\[
\delta_x^2 u_i^j = \frac{u_{i+1}^j - 2u_i^j + u_{i-1}^j}{h^2},
\]  
(2.5)

and define
\[
D_t^\alpha u_i^0 = \frac{\tau^{-\alpha}}{\Gamma(2-\alpha)} \left[u_i^0 - \sum_{j=1}^{n-1} (b_n-j-1 - b_{n-j})u_i^j - b_{n-1}u_i^0\right]
\]  
(2.6)

as the discrete time fractional derivative by [16], where \(b_j = (j+1)^{1-\alpha} - j^{1-\alpha}\). It can be noted that \(b_j > 0\) and \(1 = b_0 > b_1 > \cdots > b_n > (1-\alpha)(n+1)^{-\alpha}\). There exists the following error estimate between \((\partial^\alpha u(x,t)/\partial t^\alpha)|_{t=t_n}\) and \(D_t^\alpha u_i^n\):

**Lemma 2.1** (See [21]). Suppose \(0 < \alpha < 1\), and let \(u(x_i,t) \in C^2[0,t_i]\), then
\[
\left|\frac{\partial^\alpha u(x_i,t)}{\partial t^\alpha}\right|_{t=t_n} - D_t^\alpha u_i^n \leq \frac{6}{\Gamma(2-\alpha)} \cdot \max_{0 \leq t \leq t_n} |\partial^2 u(x_i,t)/\partial t^2| \cdot \tau^{2-\alpha}.
\]

And it is well known that \(\delta_x^2 u_i^j\) is 2-order central difference approximation of \(\partial^2 u(x,t)/\partial x^2\) at \((x_i,t_j)\). Replacing \(n\) by \(n+1\), (2.6) can also be recast as
\[
D_t^\alpha u_{i+1}^{n+1} = \frac{\tau^{-\alpha}}{\Gamma(2-\alpha)} \sum_{j=0}^{n} b_j u_{i-j+1}^{n+1} - u_{i-j}^{n+1} + \frac{1}{\Gamma(1-\alpha)\tau^\alpha} \left[u_{i+1}^{n+1} - \sum_{j=0}^{n-1} (b_j - b_{j+1})u_{i-j}^{n+1} - b_n u_i^0\right].
\]  
(2.7)

Combining (2.5) and (2.7), we design the semi-implicit finite difference scheme of (2.1) as
\[
D_t^\alpha U_{i+1}^n = \delta_x^2 U_i^{n+1} + f(U_i^n),
\]  
(2.8)

where \(i = 1, 2, \ldots, M-1\) for the below mentioned boundary condition (2.11), and \(i = 0, 1, \ldots, M\) for (2.11)', \(n = 1, 2, \ldots, N-1\). Denoting \(\Gamma(2-\alpha)\tau^\alpha\) by \(C_\alpha\), we rewrite the above semi-implicit finite difference scheme as
\[
\sum_{j=0}^{n} b_j U_{i-j+1}^{n+1} - U_{i-j}^{n+1} = C_\alpha \delta_x^2 U_i^{n+1} + C_\alpha f(U_i^n).
\]  
(2.9)

From (2.2) the initial condition is specified as
\[
U_i^0 = g(x_i), \quad \text{for } i = 0, 1, \ldots, M;
\]  
(2.10)

and from (2.3) or (2.3)' the boundary conditions are given as
\[
U_0^n = U_M^n = 0, \quad \text{for } n = 0, 1, \ldots, N,
\]  
(2.11)

or
\[
U_{i-1}^n = U_i^n, \quad U_{M+1}^n = U_{M-1}^n, \quad \text{for } n = 0, 1, \ldots, N,
\]  
(2.11)'
i.e., the central difference discretization is used for the Neumann boundary.
3 Stability and convergence of the numerical scheme (2.9)–(2.11)

We discuss the stability and convergence of the numerical schemes. Throughout the paper, we assume that the function \( f \) satisfies the local Lipschitz condition with the Lipschitz constant \( L \), i.e.,
\[
|f(u(x,t)) - f(\tilde{u}(x,t))| \leq L|u(x,t) - \tilde{u}(x,t)|,
\]
when \( |u(x,t) - \tilde{u}(x,t)| < \varepsilon_0, x \in \Omega \) and \( t \in [0, T] \), where \( \varepsilon_0 \) is a given positive constant. We define the \( L_\infty \) norm of \( \{u^n_i\}_{i=1}^{M-1} \) as
\[
\|u^n\| = \max_{1 \leq i \leq M-1} |u^n_i|.
\]
The convergence result is as follows.

**Theorem 3.1.** Let \( \{u(x_i, t_n)\}_{i=1}^{M-1} \) and \( \{U^n_i\}_{i=1}^{M-1} \) be the exact solutions to the subdiffusive reaction-diffusion equation (2.1)–(2.3) and to the numerical scheme (2.9)–(2.11), respectively, define \( \varepsilon^n_i = u(x_i, t_n) - U^n_i \) and \( E^n = (\varepsilon^n_1, \varepsilon^n_2, \ldots, \varepsilon^n_{M-1})^T \). Then \( E^n \) satisfies the following error estimate:
\[
\|E^n\| \leq C(\tau + h^2),
\]  
when \( T < (1/(\Gamma(1 - \alpha)L))^1/\alpha \).

**Proof.** According to (2.8), we know
\[
D^2_{\tau}U^n_i \varepsilon^{n+1} = \delta^2_x \varepsilon^{n+1} + f(U^n_i).
\]  
By Lemma 2.1, there exists a positive constant \( C \), such that
\[
\left| \frac{\partial \alpha u(x_i, t)}{\partial t^\alpha} \bigg|_{t=t_{n+1}} - D^\alpha_{\tau} \varepsilon^{n+1} \right| \leq C\tau^{2-\alpha},
\]
and it is well known that
\[
\left| \frac{\partial^2 u(x_i, t_{n+1})}{\partial x^2} - \delta^2_x \varepsilon^{n+1} \right| \leq C h^2.
\]
Thanks to the Lipschitz continuity of \( f \) with respect to \( u \), we have
\[
|f(u^{n+1}_i) - f(u^n_i)| \leq L|u^{n+1}_i - u^n_i| \leq C\tau.
\]
Based on (3.3)–(3.5), there exists
\[
D^\alpha_{\tau} \varepsilon^{n+1} = \delta^2_x \varepsilon^{n+1} + f(u^n_i) + R^n_i,
\]
where \( R^n_i = O(\tau + h^2) \). For convenience, denoting \( C_\alpha R^n_i + r^n_i \) as \( r^{n+1}_i \), we can get
\[
\left(1 + \frac{2C_\alpha}{h^2}\right) \varepsilon^{n+1}_i = \sum_{j=0}^{n-1} (b_j - b_{j+1}) \varepsilon^{n-j}_i + b_n \varepsilon^{0}_i + \frac{C_\alpha}{h^2} (\varepsilon^{n+1}_i + \varepsilon^{n-1}_i) + C_\alpha (f(u(x_i, t_n)) - f(U^n_i)) + r^{n+1}_i.
\]
Taking \( n = 0 \) in (3.6), we have
\[
\left(1 + \frac{2C_\alpha}{h^2}\right) \varepsilon^0_i = b_0 \varepsilon^0_i + \frac{C_\alpha}{h^2} (\varepsilon^1_{i+1} + \varepsilon^1_{i-1}) + C_\alpha (f(u(x_i, t_0)) - f(U^0_i)) + r^1_i.
\]
Then there exists
\[
\|E^1\| \leq b_0 \|E^0\| + C_\alpha L \|E^0\| + \|r^1\|,
\]
where \( r^1 = (r^1_1, \ldots, r^1_{M-1}) \). Then
\[
\|E^1\| \leq (1 + C_\alpha L) \|E^0\| + \|r^1\|.
\]
Proof. Notice that Theorem 3.2. The numerical scheme

Now suppose that

which is the desired result, and the proof is completed.

Together with

So

According to (3.8), combining with \( b_j^{-1} < b_{j+1}^{-1} \), we have

Notice that

Together with \( b_n^{-1} \leq \frac{(n+1)^n}{1-\alpha} \) and \( (n+1)\tau \leq T \), we obtain

which is the desired result, and the proof is completed.

According to the above convergence theorem, we know that the numerical solution is in the neighborhood of the exact solution. We consider the numerical stability under the small perturbation. Let \( \tilde{U}_i^n \) be the approximate solution to the numerical scheme (2.9)-(2.11), and denote \( \epsilon_i^n = U_i^n - \tilde{U}_i^n \), \( e^n = (\epsilon_1^n, \epsilon_2^n, \ldots, \epsilon_M^n)^T \). Then there exists the following numerical stability result.

**Theorem 3.2.** The numerical scheme (2.9)-(2.11) is stable and there exists

\[
\|\epsilon^n\| \leq \frac{1}{(1-\alpha) - T^\alpha \Gamma(2-\alpha)L} \|\epsilon^0\|,
\]

when \( T < (1/(\Gamma(1-\alpha)L))^{1/\alpha} \).

**Proof.** We prove this theorem by mathematical induction. From (2.9), we immediately obtain

\[
(1 + \frac{2C_0}{h^2}) \epsilon_i^{n+1} = \sum_{j=0}^{n-1} (b_j - b_{j+1})\epsilon_i^{n-j} + b_n\epsilon_i^0 + \frac{C_0}{h^2} (\epsilon_i^{n+1} + \epsilon_i^{n-1}) + C_0(f(U_i^n) - f(\tilde{U}_i^n)),
\]
and the perturbation errors of boundary conditions are

\[ c^n_0 = e^n_M = 0, \quad 1 \leq n \leq N. \tag{3.11} \]

Taking \( n = 0 \) in (3.10), we have

\[ (1 + \frac{2C_\alpha}{h^2}) e^1_i = e^0_i + \frac{C_\alpha}{h^2} (e^1_{i+1} + e^1_{i-1}) + C_\alpha (f(U^0_i) - f(U^0_i)). \tag{3.12} \]

Then there exists

\[ (1 + \frac{2C_\alpha}{h^2}) |e^1_i| \leq |e^0_i| + \frac{C_\alpha}{h^2} (|e^1_{i+1}| + |e^1_{i-1}|) + C_\alpha |f(U^0_i) - f(U^0_i)| \leq \|e^0\| + \frac{C_\alpha}{h^2} (\|e^1\| + \|e^1\|) + C_\alpha L \|e^0\|, \quad 1 \leq i \leq M - 1. \]

So we obtain

\[ \|e^1\| \leq (1 + C_\alpha L) \|e^0\|, \]

it can be easily checked that this means (3.9) holds for \( e^1 \). Now supposing (3.9) holds for \( e^1, e^2, \ldots, e^n \), we prove

\[ \|e^{n+1}\| \leq \frac{1}{(1 - \alpha) - T^\alpha \Gamma(2 - \alpha)L} \|e^0\|. \]

Just as the above process, from (3.10), we get

\[ (1 + \frac{2C_\alpha}{h^2}) |e^{n+1}_i| \leq \sum_{j=0}^{n-1} (b_j - b_{j+1}) \|e^{n-j}\| + b_n \|e^0\| + \frac{2C_\alpha}{h^2} \|e^{n+1}\| + C_\alpha L \|e^n\|. \]

So

\[ \|e^{n+1}\| \leq \sum_{j=0}^{n-1} (b_j - b_{j+1}) \|e^{n-j}\| + b_n \|e^0\| + C_\alpha L \|e^n\|. \]

Then, owing to \( b_{n-1}^{-1} < b^{-1}_n, C_\alpha = \Gamma(2 - \alpha)T^\alpha \) and \( T^\alpha < 1/\Gamma(1 - \alpha)L \), there exists

\[ \|e^{n+1}\| \leq \left( \frac{1 - b_n + C_\alpha L}{(1 - \alpha) - T^\alpha \Gamma(2 - \alpha)L} + b_n \right) \|e^0\| \leq \frac{1}{(1 - \alpha) - T^\alpha \Gamma(2 - \alpha)L} \|e^0\|. \]

**Remark 3.3.** The above analysis focuses on scalar equation, but it can be easily extended to the vector one. Take (1.1) as an example, and denote the nonlinear term of the first equation as \( f(N, P) \) and the nonlinear term of the second equation as \( g(N, P) \). Denoting \( \rho^n = N(x_i, t_n) - N^n_i \) and \( \eta^n = P(x_i, t_n) - P^n_i \), and using the following simple trick:

\[ |f(N^{n+1}_i, P^{n+1}_i) - f(N^n_i, P^n_i)| = |f(N^{n+1}_i, P^{n+1}_i) - f(N^{n+1}_i, P^n_i) + f(N^{n+1}_i, P^n_i) - f(N^n_i, P^n_i)| \leq |f(N^{n+1}_i, P^{n+1}_i) - f(N^{n+1}_i, P^n_i)| + |f(N^{n+1}_i, P^n_i) - f(N^n_i, P^n_i)| \leq L(|P^{n+1}_i - P^n_i| + |N^{n+1}_i - N^n_i|), \]

we have

\[ \|\rho^m\| \leq \frac{b^{-1}_{m-1}}{(1 - \alpha) - T^\alpha \Gamma(2 - \alpha)L} \left( \|\rho^0\| + \|\eta^0\| + \max_{1 \leq j \leq m} \|r^j\| \right), \]

and

\[ \|\eta^m\| \leq \frac{b^{-1}_{m-1}}{(1 - \alpha) - T^\alpha \Gamma(2 - \alpha)L} \left( \|\rho^0\| + \|\eta^0\| + \max_{1 \leq j \leq m} \|r^j\| \right), \]

for \( m = 1, 2, \ldots, n \), by the analysis similar to Theorem 3.1.
4 Positivity and boundedness of the analytical and numerical solutions to the subdiffusive predator-prey model

In this section, we first prove that the analytical solutions to (1.1)–(1.2) are positive and bounded, then demonstrate that both the numerical schemes (2.9)–(2.10) with (2.11) and with (2.11)′ preserve their positivity and boundedness when utilized to numerically solve (1.1)–(1.2) and (1.1) and (1.2)′, respectively.

4.1 Maximum principle for analytical solutions

For analyzing the properties of the analytical solutions, we introduce the following maximum principle. The considered equation is

\[ Lu = \frac{\partial^\alpha u}{\partial t^\alpha} - \frac{\partial^2 u}{\partial x^2} + c(x, t)u = f(x, t), \quad (x, t) \in \Omega_T = \Omega \times (0, T], \]

where \( \Omega_T \) is a bounded domain with Lipschitz continuous boundary.

**Theorem 4.1.** Assuming that the coefficient \( c(x, t) \geq 0 \) and \( f(x, t) \leq 0 \) (resp. \( f(x, t) \geq 0 \)) in \( \Omega_T \) and \( u \in C^{2,1}(\Omega_T) \cap C(\Omega_T) \) is the solution to (4.1), then the non-negative maximum (resp. non-positive minimum) value of \( u(x, t) \) in \( \Omega_T \) (if exists) must reach at the parabolic boundary \( \Gamma_T \), i.e.,

\[ \max_{\Omega_T} u(x, t) \leq \max_{\Gamma_T} \{ u(x, t), 0 \}, \quad \text{resp.} \quad \min_{\Omega_T} u(x, t) \geq \min_{\Gamma_T} \{ u(x, t), 0 \}. \]

In fact, if the non-negative maximum value of \( u(x, t) \) is not at the boundary \( \Gamma_T \) and \( f(x, t) \leq 0 \), then there exists a point \((x^*, t^*) \in \Omega_T\) such that

\[ u(x^*, t^*) = \max_{\Gamma_T} \{ u(x, t), 0 \} \quad \text{and} \quad u(x^*, t^*) = \max_{\Omega_T} u(x, t). \]

Let \( b > 0 \), for any \( \varepsilon > 0 \), we introduce the auxiliary function

\[ v(x, t) = u(x, t) - \varepsilon e^{bt}. \]

On the one hand, we know that, for any sufficient small \((x, t) \in \Omega_T\), \( v(x, t) \) satisfies

\[ \frac{\partial^\alpha v}{\partial t^\alpha} - \frac{\partial^2 v}{\partial x^2} + c(x, t)v = \frac{\partial^\alpha u}{\partial t^\alpha} - \frac{\partial^2 u}{\partial x^2} + c(x, t)u - \varepsilon e^{bt}c(x, t) \]

\[ = f(x, t) - \varepsilon (bt^{1-\alpha}E_{1,2-\alpha}(bt) + e^{bt}c(x, t)) < 0, \]

where \( E_{\alpha,\beta}(z) \) is the Mittag-Leffler function. On the other hand, at the maximum point \((x^*, t^*)\), according to the definition of Caputo derivative, we have

\[ \left. \frac{\partial^\alpha u(x^*, t)}{\partial t^\alpha} \right|_{t=t^*} = \frac{1}{\Gamma(1-\alpha)} \int_0^{t^*} \frac{\partial u(x^*, s)}{\partial s} \frac{1}{(t^*-s)^\alpha} ds \]

\[ = \lim_{\tau \to 0} \frac{\tau^{1-\alpha}}{\Gamma(2-\alpha)} \sum_{j=0}^{n-1} b_j \frac{1}{\tau} (u(x^*, t^*-j\tau) - u(x^*, t^*-(j+1)\tau)) \]

\[ = \lim_{\tau \to 0} \frac{\tau^{-\alpha}}{\Gamma(2-\alpha)} (u(x^*, t^*) - (1-b_1)u(x^*, t^*-\tau) - \cdots - b_n u(x_0^*, 0)) \]

\[ = \lim_{\tau \to 0} \frac{\tau^{-\alpha}}{\Gamma(2-\alpha)} ((1-b_1)(u(x^*, t^*) - u(x^*, t^*-\tau)) + \cdots \]

\[ + b_n (u(x^*, t^*) - u(x^*, 0))) \]

\[ \geq \lim_{\tau \to 0} \frac{\tau^{-\alpha}}{\Gamma(2-\alpha)} b_n (u(x^*, t^*) - u(x^*, 0)) \]
where \( \tau = t^*/n \), \( b_j \) is defined in (2.6), and \( 1 = b_0 > b_1 > \cdots > b_n > (1 - \alpha) (n + 1) - \alpha \) is used. Since \( u(x^*, t^*) > u(x^*, 0) \), denoting \( m^* = u(x^*, t^*) - u(x^*, 0) \), there exists
\[
\frac{\partial^\alpha v(x^*, t^*)}{\partial t^\alpha} \bigg|_{t = t^*} = \frac{\partial^\alpha u(x^*, t^*)}{\partial t^\alpha} - \varepsilon b(t^*)^{1 - \alpha} E_{1,2 - \alpha} (bt^*) \geq 0,
\]
when \( \varepsilon \leq \frac{(1 - \alpha) T^{1 - \alpha} m^*}{\Gamma(2 - \alpha)b(t^*)^{1 - \alpha} E_{1,2 - \alpha} (bt^*)} \). Together with \( \frac{\partial^2 u}{\partial x^2} = \frac{\partial^2 u}{\partial x^2} \leq 0 \) at \((x^*, t^*)\), we know
\[
\frac{\partial^\alpha v}{\partial t^\alpha} - \frac{\partial^2 v}{\partial x^2} + c(x, t)v \geq 0 \quad \text{at} \quad (x^*, t^*),
\]
which is contradictory with (4.3). Similar analysis can be done for the case \( f(x, t) \geq 0 \). So, from the above analysis, we arrive at Theorem 4.1.

Remark 4.2. If we take the initial condition of (4.1) as \( u(x, 0) = 0 \), and its boundary conditions are Dirichlet’s and homogeneous, then from Theorem 4.1 we have \( u(x, t) \leq 0 \) when \( f(x, t) \leq 0 \) and \( u(x, t) \geq 0 \) when \( f(x, t) \geq 0 \). The same results still hold if the homogeneous Neumann boundary conditions are used, since the maximum (minimum) value of \( u(x, t) \) at the boundary is non-positive (nonnegative) under the homogeneous Neumann boundary conditions. In fact, if the maximum value of \( u(x, t) \) at the boundary is positive, suppose it is located at the left boundary (similar analysis can be done if at the right boundary) and denote the one closest to the line \( t = 0 \) by \( u(x_i, t^*) \), then for any given sufficiently small \( \varepsilon \), there exists \( \xi_\varepsilon \in (x_i, x_i + \varepsilon) \) such that \( u(x_i + \varepsilon, t^*) - u(x_i, t^*) = \frac{\partial^\alpha u(x_i, t^*)}{\partial x^\alpha} |_{x = x_i} \varepsilon^2 < 0 \) since \( \frac{\partial^\alpha u(x_i, t^*)}{\partial x^\alpha} |_{x = x_i} < 0 \). So there exists sufficiently big \( M > 2 \) and small \( \delta t > 0 \) such that \( \frac{\partial^\alpha u(x, t)}{\partial x^\alpha} < 0 \) for any \( (x, t) \in \Omega^* = \{(x, t) \mid x_i < \xi_\varepsilon - \frac{\delta t}{M} < x < \xi_\varepsilon + \frac{\delta t}{M} < x_i + \varepsilon; t^* - \delta t < t < t^* \} \). Now consider (4.1) in the domain \( \Omega^* = \{(x, t) \mid \xi_\varepsilon < x < x_i + \varepsilon; 0 < t < t^* \} \), obviously the maximum value of \( u(x, t) \) still is obtained at the parabolic boundary \( \Gamma^* \) of \( \Omega^* \). Furthermore, if taking \( \varepsilon \) small enough, then the maximum value is located in the domain \( \Gamma_{\varepsilon} \cap \Omega_{\varepsilon} \). Now at the maximum point, \( \frac{\partial^\alpha u}{\partial t^\alpha} - \frac{\partial^2 u}{\partial x^2} + cu > 0 \), a contradiction is reached.

4.2 Positivity and boundedness of the analytical solutions

Using upper and lower solutions method, we prove the positivity and boundedness of the analytical solutions to (1.1)–(1.2) and (1.1) and (1.2)'. First, we introduce the definition of upper and lower solutions.

Definition 4.3. For the system of equations \((i = 1, 2)\)
\[
\frac{\partial^\alpha u_i}{\partial t^\alpha} - \frac{\partial^2 u_i}{\partial x^2} = f_i(u_1, u_2), \quad x \in \Omega, \quad t \in (0, T],
\]
\[
Bu_i (u_i \text{ or } \partial u_i / \partial x) = g_i(x, t), \quad x \in \partial \Omega, \quad t \in (0, T],
\]
\[
u_i(x, 0) = \varphi_i(x), \quad x \in \Omega,
\]
and suppose that \( \bar{u}_i(x, t) \) and \( \underline{u}_i(x, t) \) satisfy
\[
B \bar{u}_i - g_i(x, t) \geq 0 \geq B \underline{u}_i - g_i(x, t), \quad x \in \partial \Omega, \quad t \in (0, T],
\]
\[
\bar{u}_i(x, 0) - \varphi_i(x) \geq 0 \geq \underline{u}_i(x, 0) - \varphi_i(x), \quad x \in \Omega,
\]
and \( f_1(\cdot, \cdot) \) is quasi-monotone decreasing, \( f_2(\cdot, \cdot) \) is quasi-monotone increasing, and
\[
\frac{\partial^\alpha \bar{u}_1}{\partial t^\alpha} - \frac{\partial^2 \bar{u}_1}{\partial x^2} - f_1(\bar{u}_1, u_2) \geq \frac{\partial^\alpha \bar{u}_1}{\partial t^\alpha} - f_1(\bar{u}_1, \bar{u}_2),
\]
\[
\frac{\partial^\alpha \underline{u}_2}{\partial t^\alpha} - \frac{\partial^2 \underline{u}_2}{\partial x^2} - f_2(\underline{u}_1, \underline{u}_2) \geq \frac{\partial^\alpha \underline{u}_2}{\partial t^\alpha} - f_2(\bar{u}_1, \bar{u}_2),
\]
and \( \frac{\partial^\alpha \underline{u}_1}{\partial t^\alpha} - \frac{\partial^2 \underline{u}_1}{\partial x^2} - f_1(\underline{u}_1, u_2) \geq \frac{\partial^\alpha \underline{u}_1}{\partial t^\alpha} - f_1(\underline{u}_1, \underline{u}_2), \)
\[
\frac{\partial^\alpha \bar{u}_2}{\partial t^\alpha} - \frac{\partial^2 \bar{u}_2}{\partial x^2} - f_2(\bar{u}_1, \bar{u}_2) \geq \frac{\partial^\alpha \bar{u}_2}{\partial t^\alpha} - f_2(\bar{u}_1, \bar{u}_2).
\]
Then \( U(x,t) = (\tilde{u}_1(x,t), \tilde{u}_2(x,t)) \) and \( V(x,t) = (u_1(x,t), u_2(x,t)) \) are respectively called upper solution and lower solution to the system (4.4).

The theoretical result obtained using upper and lower solutions is given as follows.

**Theorem 4.4.** Suppose \( \{f_1, f_2\} \) is mixed quasi-monotone and local Lipschitz continuous

\[
|f_1(u_1, u_2) - f_1(v_1, v_2)| \leq L(|u_1 - v_1| + |u_2 - v_2|),
\]

where \( L \) is constant, \( |u_1 - v_1| < \varepsilon_0 \) and \( |u_2 - v_2| < \varepsilon_0 \) is a given constant. If upper and lower solutions, \( U(x,t) \) and \( V(x,t) \), satisfy \( V(x,t) \leq U(x,t) \), then (4.4) has a unique solution in \([V(x,t), U(x,t)]\).

**Proof.** See Appendix A.

Let us denote \( f(N, P) = N(1 - \frac{\sigma P}{P + N}) \) and \( g(N, P) = \sigma P(-\frac{\gamma + \delta \beta P}{1 + \beta P} + \frac{N}{P + N}) \). We certify that both (1.1)–(1.2) and (1.1) and (1.2)' have lower and upper solutions, \((0,0)\) and \((1, L_1)\), where \( L_1 > 1/\gamma \).

First, it is needed to check that \( f \) is a quasi-monotone decreasing function and \( g \) is a quasi-monotone increasing function. Since the derivatives of the nonlinear terms are

\[
\frac{\partial f(N, P)}{\partial P} = -\frac{aN^2}{(P + N)^2}
\]
and

\[
\frac{\partial g(N, P)}{\partial N} = \frac{\sigma P^2}{(P + N)^2},
\]

it is obvious that \( f \) is decreasing w.r.t \( P \) and \( g \) is increasing w.r.t \( N \). At the same time, it can be noted that both (1.2) and (1.2)' satisfy the conditions (4.5) directly. And it can be easily checked that the upper solution \( U(x,t) = (\tilde{N}(x,t), \tilde{P}(x,t)) = (1, L_1) \) and the lower solution \( V(x,t) = (N(x,t), P(x,t)) = (0,0) \) satisfy

\[
\begin{align*}
\frac{\partial^\alpha \tilde{N}}{\partial t^\alpha} - \frac{\partial^2 \tilde{N}}{\partial x^2} - f(\tilde{N}, \tilde{P}) &\geq 0 \geq \frac{\partial^\alpha \tilde{N}}{\partial t^\alpha} - \frac{\partial^2 \tilde{N}}{\partial x^2} - f(N, P), \\
\frac{\partial^\alpha \tilde{P}}{\partial t^\alpha} - \frac{\partial^2 \tilde{P}}{\partial x^2} - g(\tilde{N}, \tilde{P}) &\geq 0 \geq \frac{\partial^\alpha \tilde{P}}{\partial t^\alpha} - \frac{\partial^2 \tilde{P}}{\partial x^2} - g(N, P).
\end{align*}
\]

(4.8)

If we specify the initial condition of (1.1) such that \( N(x,0) \in [0,1] \) and \( P(x,0) \in [0,L_1] \) for any \( x \in (l,r) \), the initial condition satisfy (4.6). From Theorem 4.4 the exact solution to (1.1)–(1.2) (or (1.1) and (1.2)') is bounded and positive.

### 4.3 Positivity and boundedness of the numerical solutions

We show that the numerical schemes (2.9)–(2.11)' preserve the positivity and boundedness of the corresponding analytical solutions to (1.1)–(1.2)'.

First, for (1.1) with the initial conditions \( N(x,0) \in [0,1] \) and \( P(x,0) \in [0,L_1] \), \( L_1 < \frac{1}{\gamma} \), for any \( x \in (l,r) \), we have its discretization scheme

\[
\begin{align*}
N_i^{n+1} - C_\alpha \delta_x^2 N_i^{n+1} &= \sum_{j=0}^{n-1} (b_j - b_{j+1}) N_i^{n-j} + b_n N_i^0 + C_\alpha N_i^n \left( 1 - N_i^n - \frac{a P_i^n}{P_i^n + N_i^n} \right), \\
P_i^{n+1} - C_\alpha \delta_x^2 P_i^{n+1} &= \sum_{j=0}^{n-1} (b_j - b_{j+1}) P_i^{n-j} + b_n P_i^0 + C_\alpha \sigma P_i^n \left( -\frac{\gamma + \delta \beta P_i^n}{1 + \beta P_i^n} + \frac{N_i^n}{P_i^n + N_i^n} \right).
\end{align*}
\]

Then we use the induction method to prove \( 0 < N_i^n \leq 1 \) and \( 0 < P_i^n \leq L_1 \) for any \( i \) and \( n \). It can be noted that, \( 0 < N_i^0 \leq 1 \) and \( 0 < P_i^0 \leq L_1 \) hold obviously. Now suppose \( 0 < N_i^k \leq 1 \) and \( 0 < P_i^k \leq L_1 \) for any \( k \leq n \), we prove that it still holds when \( k = n + 1 \).
Denote $w := C_\alpha N_i^n(1 - N_i^n - \frac{\alpha b_i}{P_i^n + N_i^n})$ and $v := C_\alpha \sigma P_i^n\left(-\frac{\gamma + \delta N_i^n}{1 + \beta P_i^n} + \frac{1}{P_i^n + N_i^n}\right)$. When $C_\alpha \leq 1$, it is easy to obtain

$$w \leq C_\alpha N_i^n(1 - N_i^n) \leq C_\alpha (1 - N_i^n),$$

(4.9)

$$w \geq C_\alpha N_i^n(1 - N_i^n - a) \geq -C_\alpha a N_i^n,$$

(4.10)

and

$$v \leq C_\alpha \sigma P_i^n\left(-\frac{\gamma + \delta N_i^n}{1 + \beta P_i^n} + \frac{1}{P_i^n + N_i^n}\right) \leq C_\alpha \sigma (1 - P_i^n \gamma),$$

(4.11)

$$v \geq C_\alpha \sigma P_i^n\left(-\delta + \frac{N_i^n}{P_i^n + N_i^n}\right) \geq -C_\alpha \sigma P_i^n \delta.$$ 

(4.12)

Because of $b_j > b_{j+1}$, $0 < N_i^n \leq 1$ and $0 < P_i^n \leq L_1$, we know

$$(1 - b_1)N_i^n \leq \sum_{j=0}^{n-1} (b_j - b_{j+1})N_i^{n-j} + b_n N_i^n \leq \frac{1 - b_1}{2} N_i^n + \frac{1 + b_1}{2},$$

(4.13)

and

$$(1 - b_1)P_i^n \leq \sum_{j=0}^{n-1} (b_j - b_{j+1})P_i^{n-j} + b_n P_i^n \leq \frac{1 - b_1}{2} P_i^n + \frac{1 + b_1}{2} L_1.$$ 

(4.14)

Owing to (4.9), (4.10) and (4.13), when $C_\alpha < \min\{\frac{1-b_1}{2}, \frac{1-b_1}{\sigma \beta}\}$, we get

$$0 < N_i^{n+1} - C_\alpha a^2 N_i^{n+1} \leq 1.$$ 

(4.15)

In the similar way, owing to (4.11), (4.12) and (4.14), when $C_\alpha < \frac{(1-b_1)}{\sigma \beta}$, we get

$$0 < P_i^{n+1} - C_\alpha a^2 P_i^{n+1} \leq L_1.$$ 

(4.16)

From (4.15) and (4.16), we can get $0 < N_i^{n+1} \leq 1$ and $0 < P_i^{n+1} \leq L_1$. In fact, if $0 < N_i^{n+1} \leq 1$ does not hold, then there exists $i$ such that

$$N_i^{n+1} \leq 0 \quad \text{or} \quad N_i^{n+1} > 1.$$ 

If $N_i^{n+1} \leq 0$, then we choose the minimum in $i = 0, \ldots, M$, and denote it by $N_k^{n+1}$, which is non-positive. Thanks to (4.15), we know that

$$N_k^{n+1} - \frac{C_\alpha}{h^2} (N_k^{n+1} - 2N_i^{n+1} + N_{k+1}^{n+1}) > 0.$$ 

So $N_k^{n+1} \leq 0$ implies

$$N_i^{n+1} > \frac{N_k^{n+1} + N_{k+1}^{n+1}}{2}.$$ 

We get $N_i^{n+1} < N_k^{n+1}$ or $N_i^{n+1} < N_{k+1}^{n+1}$, which still hold even at the boundary, including the Dirichlet and Neumann boundaries. This is contradictory with the assumption that $N_k^{n+1}$ is the minimum. If $N_i^{n+1} > 1$, then choose the maximum in $i = 0, \ldots, M$, and denote it by $N_l^{n+1}$, and $N_l^{n+1} > 1$ holds. Since $N_l^{n+1} - \frac{C_\alpha}{h^2} (N_{l-1}^{n+1} - 2N_l^{n+1} + N_{l+1}^{n+1}) \leq 1$, we have

$$\frac{C_\alpha}{h^2} (N_{l-1}^{n+1} - 2N_l^{n+1} + N_{l+1}^{n+1}) \geq N_l^{n+1} - 1 > 0.$$ 

So

$$N_l^{n+1} < \frac{N_{l-1}^{n+1} + N_{l+1}^{n+1}}{2}.$$ 

We get $N_i^{n+1} < N_l^{n+1}$ or $N_i^{n+1} < N_{l+1}^{n+1}$, which still hold even at the boundary, including the Dirichlet and Neumann boundaries. This is contradictory with the assumption.

Similarly, we can verify that $0 < P_i^{n+1} \leq L_1$. 

5 Numerical experiments

We present the simulation results of the schemes (2.9)–(2.11) for Dirichlet boundary and (2.9)–(2.10) and (2.11)' for Neumann boundary to verify all the above theoretical results. In particular, the subdiffusive predator-prey model (1.1) with homogeneous Neumann boundary conditions (1.2)' is simulated, and the pictures are displayed. Examples 5.1 and 5.2 numerically confirm the unconditional stability of the numerical schemes and first order convergence in time for any $\alpha \in (0, 1)$. Example 5.3 is for the subdiffusive predator-prey model with specified initial and boundary conditions.

In the computations of Examples 5.1 and 5.2, we take the spatial steplength $h = 0.0005$, which is small enough so that the spatial error can be neglected for obtaining convergent rate in time direction. The errors are measured at time $T = 1$ and by $L_\infty$ norm. And $\alpha$ is, respectively, taken as 0.3, 0.6 and 0.9.

Example 5.1. For (2.1)–(2.3), we take its exact analytical solution as

$$u(x, t) = t^2 \sin(2\pi x),$$

and the non-linear term as

$$f(u) = \frac{1}{u + 4}.$$

Then, on the right-hand side, we need to add the forcing term

$$g(x, t) = \frac{2}{\Gamma(3 - \alpha)(2 - \alpha)} \sin(2\pi x) + 4\pi^2 t^2 \sin(2\pi x) - \frac{1}{t^2 \sin(2\pi x) + 4},$$

and the corresponding initial and boundary conditions are respectively

$$u(x, 0) = 0,$$

$$u(0, t) = u(1, t) = 0.$$

Tables 1–3 show the errors for the numerical solutions, and the first-order convergence in time $T$ for different $\alpha$.

| Table 1 | The error and convergent rate of the proposed scheme for Example 5.1, when $\alpha = 0.3$ and $h = 0.0005$ |
|---------|--------------------------------------------------|
| $\tau$  | $e(h, \tau)$ | Rate |
| $\frac{1}{8}$ | 1.628403729893591e−003 |  |
| $\frac{1}{16}$ | 8.461705972403477e−004 | 0.94444 |
| $\frac{1}{32}$ | 4.303180907271331e−004 | 0.97555 |
| $\frac{1}{64}$ | 2.166950795682299e−004 | 0.98974 |
| $\frac{1}{128}$ | 1.08815076031326e−004 | 0.99379 |
| $\frac{1}{256}$ | 5.474834928109740e−005 | 0.99099 |

| Table 2 | The error and convergent rate of the proposed scheme for Example 5.1, when $\alpha = 0.6$ and $h = 0.0005$ |
|---------|--------------------------------------------------|
| $\tau$  | $e(h, \tau)$ | Rate |
| $\frac{1}{8}$ | 2.021632915774174e−003 |  |
| $\frac{1}{16}$ | 9.783209560871864e−004 | 1.0471 |
| $\frac{1}{32}$ | 4.709883249863767e−004 | 1.0546 |
| $\frac{1}{64}$ | 2.270387164748922e−004 | 1.0528 |
| $\frac{1}{128}$ | 1.100565972464995e−004 | 1.0447 |
| $\frac{1}{256}$ | 5.382548524024222e−005 | 1.0319 |
Table 3 The error and convergent rate of the proposed scheme for Example 5.1, when $\alpha = 0.9$ and $h = 0.0005$

| $\tau$    | $e(h, \tau)$  | Rate   |
|-----------|---------------|--------|
| $\frac{1}{8}$ | 3.392154303510031e-003 |        |
| $\frac{1}{16}$ | 1.657079757972468e-003 | 1.0336 |
| $\frac{1}{32}$ | 8.0353858083563e-004   | 1.0442 |
| $\frac{1}{64}$ | 3.88384156070585e-004   | 1.0489 |
| $\frac{1}{128}$ | 1.876360100631080e-004   | 1.0495 |
| $\frac{1}{256}$ | 9.083194250991689e-005   | 1.0467 |

Example 5.2. For (2.1), (2.2) and (2.3)', the exact solution and the boundary condition are, respectively, taken as $t^2 \cos(2\pi x)$ and

$$
\frac{\partial u(x,t)}{\partial x} \bigg|_{x=0} = \frac{\partial u(x,t)}{\partial x} \bigg|_{x=1} = 0.
$$

We still use (5.2) and (5.4) as the non-linear term and initial condition, respectively. And the following forcing term is needed to add to the right-hand side of the equation,

$$
g(x,t) = 2 \frac{\Gamma(3-\alpha)}{\Gamma(2-\alpha)} t^{(2-\alpha)} \cos(2\pi x) + 4 \pi^2 t^2 \cos(2\pi x) - \frac{1}{t^2 \cos(2\pi x) + 4},
$$

(5.6)

The simulation errors and first-order convergence for different $\alpha$ are demonstrated in Tables 4–6.

Example 5.3. Consider the reaction diffusion equation

$$
D_\alpha^t u = d_1 \frac{\partial^2 u}{\partial x^2} + u \left(1 - u - \frac{aP}{P + u} \right),
$$

$$
D_\alpha^t P = d_2 \frac{\partial^2 P}{\partial x^2} + \sigma P \left(- \frac{\gamma + \delta \beta P}{1 + \beta P} + \frac{N}{P + N} \right),
$$

(5.7)

with the homogeneous Neumann boundary conditions on the domain $\Omega = [0, 1]$.

Table 4 The error and convergent rate of the proposed scheme for Example 5.2, when $\alpha = 0.3$ and $h = 0.0005$

| $\tau$    | $e(h, \tau)$  | Rate   |
|-----------|---------------|--------|
| $\frac{1}{8}$ | 2.88757570653641e-003 |        |
| $\frac{1}{16}$ | 1.52719887164893e-003 | 0.91897 |
| $\frac{1}{32}$ | 7.855525404816266e-004   | 0.95911 |
| $\frac{1}{64}$ | 3.983144175851994e-004   | 0.97980 |
| $\frac{1}{128}$ | 2.006793113920047e-004   | 0.98902 |
| $\frac{1}{256}$ | 1.0095370785771210e-004   | 0.99120 |

Table 5 The error and convergent rate of the proposed scheme for Example 5.2, when $\alpha = 0.6$ and $h = 0.0005$

| $\tau$    | $e(h, \tau)$  | Rate   |
|-----------|---------------|--------|
| $\frac{1}{8}$ | 2.713892842113319e-003 |        |
| $\frac{1}{16}$ | 1.337146145350632e-003 | 1.0212 |
| $\frac{1}{32}$ | 6.55017868808295e-004   | 1.0296 |
| $\frac{1}{64}$ | 3.205477251759792e-004   | 1.0310 |
| $\frac{1}{128}$ | 1.572572233041474e-004   | 1.0274 |
| $\frac{1}{256}$ | 7.755217692539951e-005   | 1.0199 |
Table 6  The error and convergent rate of the proposed scheme for Example 5.2, when \( \alpha = 0.9 \) and \( h = 0.0005 \)

| \( \tau \) | \( e(h, \tau) \) | Rate  |
|--------|---------------|-------|
| \( \frac{1}{4} \) | 3.769255105664726e−003 |     |
| \( \frac{1}{8} \) | 1.832929458344568e−003 | 1.0401 |
| \( \frac{1}{16} \) | 8.885772877893494e−004 | 1.0446 |
| \( \frac{1}{32} \) | 4.30289430325280e−004 | 1.0462 |
| \( \frac{1}{64} \) | 2.084713949954686e−004 | 1.0455 |
| \( \frac{1}{128} \) | 1.012302249301378e−004 | 1.0422 |

For more details of the equation, one can see [2]. Let us denote \( f(N, P) = N(1 - N - \frac{P}{\sqrt{1 + N}}) \), \( g(N, P) = \sigma P(-\frac{\gamma + \delta \beta}{1 + \beta} + \frac{N}{1 + N}) \), and define \((\bar{N}, \bar{P})\) as the equilibrium point of (5.7). In the case, \( \sigma = 1, a = 1.1, \gamma = 0.05, \beta = 1 \) and \( \delta = 0.5 \), then as \( f(\bar{N}, \bar{P}) = 0 \) and \( g(\bar{N}, \bar{P}) = 0 \), we can obtain the equilibrium point \((\bar{N}, \bar{P}) = (0.113585, 0.471397)\). The simulations were performed for the system on a fixed grid with spatial stepsize \( h = 0.005 \) and time stepsize \( \tau = 0.1 \). As the initial condition, we use \( N(x, 0) = \bar{N} + 0.0214 \cos(\pi x), P(x, 0) = \bar{P} + 0.0066 \cos(\pi x) \).  

We focus predominantly on displaying the properties of the numerical solutions to different time fractional order \( \alpha \), see Figures 1–3.
6 Conclusions

We introduce the unconditional stable semi-implicit numerical schemes for subdiffusive reaction diffusion equation with Dirichlet boundary condition and Neumann boundary condition, respectively. And the subdiffusive predator-prey model is detailedly discussed. We prove that its analytical solution is positive and bounded. Then we show that the proposed numerical schemes preserve the positivity and boundedness of the analytical solutions. The extensive numerical experiments are performed to confirm the theoretical results and show the dissipative properties of subdiffusive predator-prey model.

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A Appendix

Proof of Theorem 4.4. Taking the initial iteration function as

\[ (\bar{u}_1^{(0)}, \bar{u}_2^{(0)}) = (\bar{u}_1, \bar{u}_2), \]  
(A.1)
with $u_1 \leq \tilde{u}_1$ and $u_2 \leq \tilde{u}_2$, define the following iteration:

\[
\begin{cases}
\frac{\partial^\alpha \tilde{u}_1^{(k)}}{\partial t^\alpha} - \frac{\partial^2 \tilde{u}_1^{(k)}}{\partial x^2} + L \cdot \tilde{u}_1^{(k)} = L \cdot \tilde{u}_1^{(k-1)} + f_1(\tilde{u}_1^{(k-1)}, \tilde{u}_2^{(k-1)}), \\
\frac{\partial^\alpha \tilde{u}_2^{(k)}}{\partial t^\alpha} - \frac{\partial^2 \tilde{u}_2^{(k)}}{\partial x^2} + L \cdot \tilde{u}_2^{(k)} = L \cdot \tilde{u}_2^{(k-1)} + f_2(\tilde{u}_1^{(k-1)}, \tilde{u}_2^{(k-1)}), \\
\frac{\partial^\alpha \tilde{u}_1^{(k)}}{\partial t^\alpha} - \frac{\partial^2 \tilde{u}_1^{(k)}}{\partial x^2} + L \cdot \tilde{u}_1^{(k)} = L \cdot \tilde{u}_1^{(k-1)} + f_1(\tilde{u}_1^{(k-1)}, \tilde{u}_2^{(k-1)}), \\
\frac{\partial^\alpha \tilde{u}_2^{(k)}}{\partial t^\alpha} - \frac{\partial^2 \tilde{u}_2^{(k)}}{\partial x^2} + L \cdot \tilde{u}_2^{(k)} = L \cdot \tilde{u}_2^{(k-1)} + f_2(\tilde{u}_1^{(k-1)}, \tilde{u}_2^{(k-1)}), \\
\end{cases}
\]

where $L$ is the maximum of Lipschitz constants of $f_1$ and $f_2$. Subtracting (4.7) from (A.3) leads to

\[
\begin{cases}
\frac{\partial^\alpha (\tilde{u}_1^{(1)} - \tilde{u}_1^{(0)})}{\partial t^\alpha} - \frac{\partial^2 (\tilde{u}_1^{(1)} - \tilde{u}_1^{(0)})}{\partial x^2} + L \cdot (\tilde{u}_1^{(1)} - \tilde{u}_1^{(0)}) \leq 0, \\
\frac{\partial^\alpha (\tilde{u}_2^{(1)} - \tilde{u}_2^{(0)})}{\partial t^\alpha} - \frac{\partial^2 (\tilde{u}_2^{(1)} - \tilde{u}_2^{(0)})}{\partial x^2} + L \cdot (\tilde{u}_2^{(1)} - \tilde{u}_2^{(0)}) \leq 0, \\
\frac{\partial^\alpha (\tilde{u}_1^{(0)} - \tilde{u}_1^{(1)})}{\partial t^\alpha} - \frac{\partial^2 (\tilde{u}_1^{(0)} - \tilde{u}_1^{(1)})}{\partial x^2} + L \cdot (\tilde{u}_1^{(0)} - \tilde{u}_1^{(1)}) \leq 0, \\
\frac{\partial^\alpha (\tilde{u}_2^{(0)} - \tilde{u}_2^{(1)})}{\partial t^\alpha} - \frac{\partial^2 (\tilde{u}_2^{(0)} - \tilde{u}_2^{(1)})}{\partial x^2} + L \cdot (\tilde{u}_2^{(0)} - \tilde{u}_2^{(1)}) \leq 0, \\
B(\tilde{u}_1^{(1)} - \tilde{u}_1^{(0)}),B(\tilde{u}_2^{(1)} - \tilde{u}_2^{(0)}),|_{\partial \Omega \times (0,T)} = B(\tilde{u}_1^{(0)} - \tilde{u}_1^{(1)}),B(\tilde{u}_2^{(0)} - \tilde{u}_2^{(1)}),|_{\partial \Omega \times (0,T)} = 0, \\
\tilde{u}_1^{(1)}(x,0) - \tilde{u}_1^{(0)}(x,0) = \tilde{u}_1^{(0)}(x,0) - \tilde{u}_1^{(1)}(x,0) = 0, \\x \in \Omega, \\
i = 1,2.
\end{cases}
\]

According to the maximum principle Theorem 4.1 and Remark 4.2, we know that

\[
\tilde{u}_1^{(1)} \leq \tilde{u}_1^{(0)}, \quad \tilde{u}_2^{(1)} \leq \tilde{u}_2^{(0)}, \quad k = 0,1,\ldots
\]

Supposing $\tilde{u}_i^{(k)} \leq \tilde{u}_i^{(k-1)}$, $\tilde{u}_i^{(k-1)} \leq \tilde{u}_i^{(k)}$, and then that the nonlinear term $f_1$ is quasi-monotone decreasing results in

\[
\begin{align*}
&f_1(\tilde{u}_1^{(k)}, \tilde{u}_2^{(k)}) - f_1(\tilde{u}_1^{(k-1)}, \tilde{u}_2^{(k-1)}) \\
&= f_1(\tilde{u}_1^{(k)}, \tilde{u}_2^{(k)}) - f_1(\tilde{u}_1^{(k-1)}, \tilde{u}_2^{(k-1)}) + f_1(\tilde{u}_1^{(k)}, \tilde{u}_2^{(k-1)}) - f_1(\tilde{u}_1^{(k-1)}, \tilde{u}_2^{(k-1)}) \\
&\leq 0 + L \cdot |\tilde{u}_1^{(k)} - \tilde{u}_1^{(k-1)}| \\
&\leq L \cdot (\tilde{u}_1^{(k-1)} - \tilde{u}_1^{(k)}).
\end{align*}
\]

In a similar way, we also get

\[
\begin{align*}
f_2(\tilde{u}_1^{(k)}, \tilde{u}_2^{(k)}) - f_2(\tilde{u}_1^{(k-1)}, \tilde{u}_2^{(k-1)}) &\leq L \cdot (\tilde{u}_2^{(k-1)} - \tilde{u}_2^{(k)}), \\
f_1(\tilde{u}_1^{(k)}, \tilde{u}_2^{(k)}) - f_1(\tilde{u}_1^{(k-1)}, \tilde{u}_2^{(k-1)}) &\leq L \cdot (\tilde{u}_1^{(k)} - \tilde{u}_1^{(k-1)}), \\
f_2(\tilde{u}_1^{(k)}, \tilde{u}_2^{(k)}) - f_2(\tilde{u}_1^{(k-1)}, \tilde{u}_2^{(k-1)}) &\leq L \cdot (\tilde{u}_2^{(k)} - \tilde{u}_2^{(k-1)}).
\end{align*}
\]
So, together with (A.4)–(A.7), the iteration (A.3) implies
\[
\begin{aligned}
\frac{\partial^\alpha (\tilde{u}_1^{(k+1)} - \tilde{u}_1^{(k)})}{\partial t^\alpha} - \frac{\partial^2 (\tilde{u}_1^{(k+1)} - \tilde{u}_1^{(k)})}{\partial x^2} + L \cdot (\tilde{u}_1^{(k+1)} - \tilde{u}_1^{(k)}) \\
\leq L \cdot (\tilde{u}_1^{(k+1)} - \tilde{u}_1^{(k)}) + f_1(\tilde{u}_1^{(k+1)}, \tilde{u}_2^{(k)}) - f_1(\tilde{u}_1^{(k)}, \tilde{u}_2^{(k)}) \\
\frac{\partial^\alpha (\tilde{u}_2^{(k+1)} - \tilde{u}_2^{(k)})}{\partial t^\alpha} - \frac{\partial^2 (\tilde{u}_2^{(k+1)} - \tilde{u}_2^{(k)})}{\partial x^2} + L \cdot (\tilde{u}_2^{(k+1)} - \tilde{u}_2^{(k)}) \\
\leq L \cdot (\tilde{u}_2^{(k+1)} - \tilde{u}_2^{(k)}) + f_2(\tilde{u}_1^{(k+1)}, \tilde{u}_2^{(k)}) - f_2(\tilde{u}_1^{(k)}, \tilde{u}_2^{(k)}) \\
\frac{\partial^\alpha (\tilde{u}_3^{(k)} - \tilde{u}_3^{(k)})}{\partial t^\alpha} - \frac{\partial^2 (\tilde{u}_3^{(k)} - \tilde{u}_3^{(k)})}{\partial x^2} + L \cdot (\tilde{u}_3^{(k)} - \tilde{u}_3^{(k)}) \\
\leq L \cdot (\tilde{u}_3^{(k)} - \tilde{u}_3^{(k)}) + f_3(\tilde{u}_1^{(k)}, \tilde{u}_2^{(k)}) - f_3(\tilde{u}_1^{(k)}, \tilde{u}_2^{(k)}) \\
B (\tilde{u}_1^{(k+1)} - \tilde{u}_1^{(k)})|_{\partial \Omega \times (0,T)} = B (\tilde{u}_1^{(k)} - \tilde{u}_1^{(k)})|_{\partial \Omega \times (0,T)} = 0, \quad i = 1, 2,
\end{aligned}
\]
\[
\tilde{u}_1^{(k+1)}(x,0) - \tilde{u}_1^{(k)}(x,0) = \tilde{u}_1^{(k)}(x,0) - \tilde{u}_1^{(k)}(x,0) = 0, \quad x \in \bar{\Omega}, \quad i = 1, 2.
\]

Then there exist
\[
\tilde{u}_1^{(k+1)} \leq \tilde{u}_1^{(k)}, \quad \tilde{u}_3^{(k)} \leq \tilde{u}_3^{(k)}, \quad k = 0, 1, \ldots
\]

Recalling the iteration (A.3) again, we deduce
\[
\begin{aligned}
\frac{\partial^\alpha (\tilde{u}_1^{(k)} - \tilde{u}_1^{(k)})}{\partial t^\alpha} - \frac{\partial^2 (\tilde{u}_1^{(k)} - \tilde{u}_1^{(k)})}{\partial x^2} + L \cdot (\tilde{u}_1^{(k)} - \tilde{u}_1^{(k)}) \\
\leq L \cdot (\tilde{u}_1^{(k)} - \tilde{u}_1^{(k)}) + f_1(\tilde{u}_1^{(k)}, \tilde{u}_2^{(k)}) - f_1(\tilde{u}_1^{(k)}, \tilde{u}_2^{(k)}) \leq 0,
\end{aligned}
\]
\[
\begin{aligned}
\frac{\partial^\alpha (\tilde{u}_2^{(k)} - \tilde{u}_2^{(k)})}{\partial t^\alpha} - \frac{\partial^2 (\tilde{u}_2^{(k)} - \tilde{u}_2^{(k)})}{\partial x^2} + L \cdot (\tilde{u}_2^{(k)} - \tilde{u}_2^{(k)}) \\
\leq L \cdot (\tilde{u}_2^{(k)} - \tilde{u}_2^{(k)}) + f_2(\tilde{u}_1^{(k)}, \tilde{u}_2^{(k)}) - f_2(\tilde{u}_1^{(k)}, \tilde{u}_2^{(k)}) \leq 0,
\end{aligned}
\]
\[
\begin{aligned}
\frac{\partial^\alpha (\tilde{u}_3^{(k)} - \tilde{u}_3^{(k)})}{\partial t^\alpha} - \frac{\partial^2 (\tilde{u}_3^{(k)} - \tilde{u}_3^{(k)})}{\partial x^2} + L \cdot (\tilde{u}_3^{(k)} - \tilde{u}_3^{(k)}) \\
\leq L \cdot (\tilde{u}_3^{(k)} - \tilde{u}_3^{(k)}) + f_3(\tilde{u}_1^{(k)}, \tilde{u}_2^{(k)}) - f_3(\tilde{u}_1^{(k)}, \tilde{u}_2^{(k)}) \leq 0,
\end{aligned}
\]
\[
B (\tilde{u}_i^{(k)} - \tilde{u}_i^{(k)})|_{\partial \Omega \times (0,T)} = 0, \quad i = 1, 2,
\]
\[
\tilde{u}_i^{(k)}(x,0) - \tilde{u}_i^{(k)}(x,0) = 0, \quad x \in \bar{\Omega}, \quad i = 1, 2,
\]

then \(\tilde{u}_i^{(k)} \leq \tilde{u}_i^{(k)} \). So
\[
\tilde{u}_i^{(k)} \leq \tilde{u}_i^{(1)} \leq \cdots \leq \tilde{u}_i^{(k)} \leq \cdots \leq \tilde{u}_i^{(1)} \leq \tilde{u}_i^{(1)}, \quad i = 1, 2.
\]

Note that \(f_1\) is quasi-monotone decreasing and \(f_2\) is quasi-monotone increasing. Then there are
\[
\lim_{k \to +\infty} \tilde{u}_i^{(k)} = \tilde{u}_i(x,t),
\]
\[
\lim_{k \to +\infty} \tilde{u}_i^{(k)} = \tilde{u}_i(x,t), \quad i = 1, 2,
\]

which satisfy \(\tilde{u}_i \geq \tilde{u}_i\) and
\[
\begin{aligned}
\frac{\partial^\alpha \tilde{u}_1}{\partial t^\alpha} - \frac{\partial^2 \tilde{u}_1}{\partial x^2} - f_1(\tilde{u}_1, \tilde{u}_2) = 0,
\frac{\partial^\alpha \tilde{u}_2}{\partial t^\alpha} - \frac{\partial^2 \tilde{u}_2}{\partial x^2} - f_2(\tilde{u}_1, \tilde{u}_2) = 0,
\frac{\partial^\alpha \tilde{u}_1}{\partial t^\alpha} - \frac{\partial^2 \tilde{u}_1}{\partial x^2} - f_1(\tilde{u}_1, \tilde{u}_2) = 0,
\frac{\partial^\alpha \tilde{u}_2}{\partial t^\alpha} - \frac{\partial^2 \tilde{u}_2}{\partial x^2} - f_2(\tilde{u}_1, \tilde{u}_2) = 0,
\end{aligned}
\]
\[
B \tilde{u}_i|_{\partial \Omega \times (0,T)} = B \tilde{u}_i|_{\partial \Omega \times (0,T)} = g_i(x,t),
\]
\[
\tilde{u}_i(x,0) = \tilde{u}_i(x,0) = \varphi_i(x), \quad x \in \bar{\Omega}, \quad i = 1, 2.
\]
Next, we will certify 
\[ \bar{u}_i = \frac{u_i}{u_i}, \quad i = 1, 2. \]

Defining \( w_1 = \bar{u}_1 - \frac{u}{w}, \ w_2 = \bar{u}_2 - \frac{u}{w}, \) we have known \( w_1 \geq 0 \) and \( w_2 \geq 0 \) from above discussions. According to the iteration, we can obtain

\[
\frac{\partial^\alpha w_1}{\partial t^\alpha} - \frac{\partial^2 w_1}{\partial x^2} = f_1(\bar{u}_1, \frac{u}{w}) - f_1(\frac{u}{w}, \bar{u}_2) \\
= f_1(\bar{u}_1, \frac{u}{w}) - f_1(\bar{u}_1, \frac{u}{w}) + f_1(\frac{u}{w}, \bar{u}_2) - f_1(\frac{u}{w}, \bar{u}_2) \\
\leq L \cdot (\bar{u}_1 - \frac{u}{w}) + L \cdot (\bar{u}_2 - \frac{u}{w}) \\
= L \cdot (w_1 + w_2),
\]

\[
\frac{\partial^\alpha w_2}{\partial t^\alpha} - \frac{\partial^2 w_2}{\partial x^2} = f_2(\bar{u}_1, \frac{u}{w}) - f_2(\frac{u}{w}, \bar{u}_2) \\
= f_2(\bar{u}_1, \frac{u}{w}) - f_2(\bar{u}_1, \frac{u}{w}) + f_2(\frac{u}{w}, \bar{u}_2) - f_2(\frac{u}{w}, \bar{u}_2) \\
\leq L \cdot (\bar{u}_2 - \frac{u}{w}) + L \cdot (\bar{u}_1 - \frac{u}{w}) \\
= L \cdot (w_1 + w_2).
\]

So

\[
\begin{aligned}
&\frac{\partial^\alpha w_1}{\partial t^\alpha} - \frac{\partial^2 w_1}{\partial x^2} - L \cdot (w_1 + w_2) \leq 0, \\
&\frac{\partial^\alpha w_2}{\partial t^\alpha} - \frac{\partial^2 w_2}{\partial x^2} - L \cdot (w_1 + w_2) \leq 0, \\
&\quad Bw_1 = 0, \quad Bw_2 = 0, \\
&w_1(x, 0) = 0, \quad w_2(x, 0) = 0.
\end{aligned}
\]

Denoting \( w = w_1 + w_2 \geq 0 \), it is obvious that

\[
\begin{aligned}
&\frac{\partial^\alpha w}{\partial t^\alpha} - \frac{\partial^2 w}{\partial x^2} - L \cdot w \leq 0, \\
&Bw = 0, \\
&w(x, 0) = 0.
\end{aligned}
\] (A.10)

Based on (A.10), next, we try to prove that \( w \equiv 0 \) in \( \Omega_T \). Suppose that \( w \) obtains its maximum value at \( (\hat{x}, \hat{t}) \), if \( (\hat{x}, \hat{t}) \in \Gamma_T \) and the boundary conditions are Dirichlet’s, \( w \equiv 0 \) holds obviously; if \( (\hat{x}, \hat{t}) \in \Gamma_T \) and \( u(\hat{x}, \hat{t}) \) is strictly bigger than \( u(x, t) \) for any \( (x, t) \in \Omega_T \), and the boundary conditions are Neumann’s, it can be shown that \( w \equiv 0 \) holds by the ideas in Remark 4.2 and the following proof.

Now assume \( (\hat{x}, \hat{t}) \in \Omega_T \) and \( w(\hat{x}, \hat{t}) > 0 \), then there exists \( t^* (< \hat{t}) \) such that \( w(x, t) < \frac{1}{2} w(\hat{x}, \hat{t}) \) for any \( t \in (0, t^*) \) and \( x \in \Omega \). Introduce the function \( u \) of \( t \) such that it satisfies

\[
\begin{aligned}
&\frac{\partial u(t)}{\partial t} = -\frac{1}{2} \frac{w(\hat{x}, \hat{t})}{t^*} \quad \text{in} \quad (0, t^*), \\
&u(0) = \frac{1}{2} w(\hat{x}, \hat{t}),
\end{aligned}
\]

and \( u(t) = 0, \ t \in [t^*, T] \), denote

\[
\bar{w}(x, t) = w(x, t) + u(t) \quad \text{in} \quad \Omega \times [0, T].
\]

Then the maximum of \( \bar{w} \) is still at \( (\hat{x}, \hat{t}) \), and \( \bar{w} \) satisfies the following inequality:

\[
\frac{\partial^\alpha \bar{w}}{\partial t^\alpha} - \frac{\partial^2 \bar{w}}{\partial x^2} \leq Lw + \frac{\partial^\alpha u(t)}{\partial t^\alpha}.
\]

At \( (\hat{x}, \hat{t}) \), it follows that \( \frac{\partial^\alpha \bar{w}(\hat{x}, t)}{\partial t^\alpha} \big|_{t=\hat{t}} \geq 0 \) and \( -\frac{\partial^\alpha \bar{w}(x, t)}{\partial x^2} \big|_{x=\hat{x}} \geq 0 \). While

\[
\left. \frac{\partial^\alpha u(t)}{\partial t^\alpha} \right|_{t=\hat{t}} = \frac{1}{\Gamma(1-\alpha)} \int_0^{\hat{t}} (\hat{t} - \tau)^{-\alpha} \frac{du(\tau)}{d\tau} d\tau
\]
\[= -\frac{1}{2\Gamma(1-\alpha)} \int_{0}^{\hat{t}^*} (\hat{t} - \tau)^{-\alpha} \frac{w(\hat{x}, \hat{t})}{t^*} d\tau\]
\[= -\frac{w(\hat{x}, \hat{t})}{2\Gamma(1-\alpha)t^*} \int_{0}^{\hat{t}^*} (\hat{t} - \tau)^{-\alpha} d\tau\]
\[< -\frac{w(\hat{x}, \hat{t})}{2\Gamma(1-\alpha)t^*} \int_{0}^{\hat{t}^*} \hat{t}^{-\alpha} d\tau\]
\[= \frac{w(\hat{x}, \hat{t})}{2\Gamma(1-\alpha)} \hat{t}^{-\alpha}\]

Since \(\hat{t} \leq T\), if \(T \leq (\frac{1}{2\Gamma(1-\alpha)})^{\frac{1}{\alpha}}\), then \(T^\alpha \leq \frac{1}{2\Gamma(1-\alpha)}\) and
\[Lw(\hat{x}, \hat{t}) + \frac{\partial^\alpha u(\hat{t})}{\partial t^\alpha} < 0.\]

We arrive at a contradiction, so that \(w \equiv 0\) holds.

If \((\frac{1}{2\Gamma(1-\alpha)})^{\frac{1}{\alpha}} < T \leq 2(\frac{1}{2\Gamma(1-\alpha)})^{\frac{1}{\alpha}}\), we take \(\hat{T} = (\frac{1}{2\Gamma(1-\alpha)})^{\frac{1}{\alpha}}\). In the domain \(\Omega \times [0, \hat{T}]\), we can get \(w \equiv 0\). For \(\hat{T} \leq t \leq T\), set \(\hat{t} = t - \hat{T}\) and \(\hat{w}(\hat{t}) = w(t + \hat{T})\). So when \(0 \leq \hat{t} \leq T - \hat{T}\), \(\hat{w}\) satisfies
\[
\begin{cases}
\frac{\partial\hat{w}}{\partial t^\alpha} - \frac{\partial^2 \hat{w}}{\partial x^2} - L \cdot \hat{w} \leq 0, \\
B\hat{w} = 0, \\
\hat{w}(x, 0) = 0.
\end{cases}
\]

Since \(T - \hat{T} \leq (\frac{1}{2\Gamma(1-\alpha)})^{\frac{1}{\alpha}}\), we have \(\hat{w} = 0\) in \(\Omega \times [0, T - \hat{T}]\). Then \(w = 0\) in \(\Omega \times [\hat{T}, T]\). Consequently, \(w = 0\) in \(\Omega \times [0, T]\). This process can be continued for any finite times, so we obtain \(w \equiv 0\) in \(\overline{\Omega_T}\) for any \(T\).

Combining with the known \(w_1 \geq 0\) and \(w_2 \geq 0\), \(w \equiv 0\) implies \(w_1 \equiv 0\) and \(w_2 \equiv 0\). Then we get \(\bar{u}_1 = u_1\) and \(\bar{u}_2 = u_2\). Set
\[u_i(x, t) = \bar{u}_i = \bar{u}_i, \quad i = (1, 2),\]
then \(u(x, t) = (u_1, u_2)\) solves (4.4).

Next, we prove the uniqueness of the solution.

Suppose that there exists another solution \(u^*(x, t) = (u_1', u_2')\) which satisfies \(V(x, t) \leq u^*(x, t) \leq U(x, t)\). Obviously, \(\bar{u}_i^{(0)} \leq u_i' \leq \bar{u}_i^{(0)} (i = 1, 2)\). On the one hand, since \(u^*(x, t)\) can be considered as an upper solution, according to \(V(x, t) \leq u^*(x, t)\), we know \(\bar{u}_i^{(k)} \leq u_i'\). Therefore, \(\lim_{k \to \infty} \bar{u}_i^{(k)}(x, t) = u_i \leq u_i'\). On the other hand, \(u^*(x, t)\) can also be considered as a lower solution, according to \(u^*(x, t) \leq U(x, t)\), we know \(\lim_{k \to \infty} \bar{u}_i^{(k)}(x, t) = u_i \geq u_i'\). Consequently \(u_i' = u_i\). \(\square\)