Finite difference schemes for variable-order time fractional diffusion equation

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Outline

• Introduction

• Three finite difference methods

• Stability and convergence

• Numerical example

• Conclusive remarks and future works
Definition of variable order operator

Definition of integral

\[ I_{0+}^{\alpha(t)} f(t) = \frac{1}{\Gamma(\alpha(t))} \int_0^t (t-\tau)^{\alpha(t)-1} f(\tau) \, d\tau, \]

\[ \text{Re} \left( \alpha(t) \right) > 0. \]

Definition of Caputo type derivative

\[ \mathcal{C} D_{0+}^{\alpha(t)} f(t) = \frac{1}{\Gamma(1-\alpha(t))} \int_0^t \frac{f'(\tau) \, d\tau}{(t-\tau)^{\alpha(t)}}, \quad 0 < \alpha(t) < 1. \]
Background

• The concept of variable-order operator is introduced by Samko et al. in 1993. The variable-order operator has been found as a powerful tool to deal with the problems in the fields of viscoelasticity, viscoelastic deformation, viscous fluid, anomalous diffusion, etc.

• These current applications of variable-order (VO) fractional differential equations, and many others that may well be proposed in the near future, make it necessary to search for methods of exact or numerical solution.

• The numerical methods for ODE and space fractional diffusion equation have been studied. Until now, the finite difference methods for VO time fractional diffusion equation are still unreported.
The considered equation and some symbols

\[
D_t^{\alpha(x,t)} c(x, t) = K \frac{\partial^2 c(x, t)}{\partial x^2} + q(x, t), \quad x \in (0, L), \ t \in (0, T]
\]
\[
c(x, 0) = f(x),
\]
\[
c(0, t) = g(t); \ c(L, t) = h(t),
\]

\(\alpha(x, t)\) is the Caputo type variable-order

\(K > 0\) is a generalized diffusion coefficient

\(q(x, t)\) is a source term

\(c(x,t)\) is concentration, mass or other quantities of interest
Discretization of Caputo type definition

VO time fractional derivative

\[
\frac{\partial^{\alpha_{i}^{k+1}} c(x_l, t_{k+1})}{\partial t^{\alpha_{i}^{k+1}}} = \frac{\tau^{-\alpha_{i}^{k+1}}}{\Gamma(2 - \alpha_{i}^{k+1})} \left\{ c(x_l, t_{k+1}) - c(x_l, t_k) \right\} + \sum_{j=1}^{k} \left[ c(x_l, t_{k+1-j}) - c(x_l, t_{k-j}) \right] \left[ (j+1)^{1-\alpha_{i}^{k+1}} - j^{1-\alpha_{i}^{k+1}} \right] + O(\tau).
\]

Second order space derivative

\[
\frac{\partial^2 c(x_l, t_k)}{\partial x^2} = \frac{c(x_{l+1}, t_k) - 2c(x_l, t_k) + c(x_{l-1}, t_k)}{h^2} + O(h^2)
\]
Explicit method

\[
\begin{align*}
    c_l^1 &= r_l^1 c_{l+1}^0 + (1 - 2r_l^1) c_l^0 + r_l^1 c_{l-1}^0 + \tau^{\alpha_l^{k+1}} \Gamma(2 - \alpha_l^{k+1}) q_{l+1}^0, \quad k = 0, \\
    c_l^{k+1} &= r_l^{k+1} c_{l+1}^k + (1 - b_1^{l,k+1} - 2r_l^{k+1}) c_l^k + r_l^{k+1} c_{l-1}^k \\
    &\quad + \sum_{j=1}^{k-1} c_l^{k-j} d_{j+1}^{l,k+1} + b_k^{l,k+1} c_l^0 + \tau^{\alpha_l^{k+1}} \Gamma(2 - \alpha_l^{k+1}) q_{l+1}^k, \quad k \geq 1.
\end{align*}
\]

where

\[
\begin{align*}
    r_l^{k+1} &= \frac{K \tau^{\alpha_l^{k+1}} \Gamma(2 - \alpha_l^{k+1})}{h^2},
    b_j^{l,k+1} &= (j + 1)^{1 - \alpha_l^{k+1}} - j^{1 - \alpha_l^{k+1}} \\
    d_j^{l,k+1} &= b_j^{l,k+1} - b_j^{l,k+1}
\end{align*}
\]
Implicit method

\[
\begin{align*}
(1 + 2r_i^1)c_i^1 - r_i^1 c_{i+1}^1 - r_i^1 c_{i-1}^1 &= c_i^0 + \tau \alpha_i^1 \Gamma(2 - \alpha_i^1)q_i^1, \quad k = 0 \\
(1 + 2r_i^{k+1})c_i^{k+1} - r_i^{k+1} c_{i+1}^{k+1} - r_i^{k+1} c_{i-1}^{k+1} &= \\
\sum_{j=0}^{k-1} c_i^{k-j} d_{j+1}^{l,k+1} + b_i^{l,k+1} c_i^0 + \tau \alpha_i^{k+1} \Gamma(2 - \alpha_i^{k+1})q_i^{k+1}, \quad k > 0.
\end{align*}
\]
Matrix form of implicit method

\[
\begin{aligned}
\left\{ \begin{array}{c}
A(1)C^1 &= IC^0 + Q(1), \\
A(k + 1)C^{k+1} &= \bar{d}_1^{k+1}C^k + \ldots + \bar{d}_k^{k+1}C^1 + \bar{b}_k^{k+1}C^0 + Q(k + 1), \ k \geq 1.
\end{array} \right.
\end{aligned}
\]

\[A(k) = \begin{bmatrix}
1 + 2r_1^k & -r_1^k & 0 & \ldots & 0 & 0 \\
-r_2^k & 1 + 2r_2^k & -r_2^k & \ldots & 0 & 0 \\
0 & -r_3^k & 1 + 2r_3^k & \ldots & 0 & 0 \\
\vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\
0 & 0 & 0 & \ldots & 1 + 2r_{M-2}^k & -r_{M-2}^k \\
0 & 0 & 0 & \ldots & -r_{M-1}^k & 1 + 2r_{M-1}^k
\end{bmatrix},
\]

\[C^k = \begin{bmatrix}
c_1^k \\
c_2^k \\
\vdots \\
c_{M-2}^k \\
c_{M-1}^k
\end{bmatrix}, \quad \bar{d}_j^{k+1} = \begin{bmatrix}
d_j^{1,k+1} \\
d_j^{2,k+1} \\
\vdots \\
d_j^{M-2,k+1} \\
d_j^{M-1,k+1}
\end{bmatrix}, \quad \bar{b}_j^{k+1} = \begin{bmatrix}
b_j^{1,k+1} \\
b_j^{2,k+1} \\
\vdots \\
b_j^{M-2,k+1} \\
b_j^{M-1,k+1}
\end{bmatrix}, \quad Q(k + 1) = \begin{bmatrix}
r_1^{k+1}g(t_{k+1}) + \tau^{\alpha_1^{k+1}}(2 - \alpha_1^{k+1})q_1^{k+1} \\
\tau^{\alpha_2^{k+1}}(2 - \alpha_2^{k+1})q_2^{k+1} \\
\tau^{\alpha_3^{k+1}}(2 - \alpha_3^{k+1})q_3^{k+1} \\
\vdots \\
\tau^{\alpha_{M-2}^{k+1}}(2 - \alpha_{M-2}^{k+1})q_{M-2}^{k+1} \\
\tau^{\alpha_{M-1}^{k+1}}(2 - \alpha_{M-1}^{k+1})q_{M-1}^{k+1}
\end{bmatrix}.
\]
Crank-Nicholson method

\[
\begin{aligned}
-r_l^1 c_{l+1}^{1} + (1 + 2r_l^1) c_l^{1} - r_l^1 c_{l-1}^{1} &= \\
r_l^1 c_{l+1}^{0} + (1 - 2r_l^1) c_l^{0} + r_l^1 c_{l-1}^{0} + \tau^{\alpha_l^1} \Gamma(2 - \alpha_l^1) q_l^{1/2}, & k = 0; \\
-r_l^{k+1} c_{l+1}^{k+1} + (1 + 2r_l^{k+1}) c_l^{k+1} - r_l^{k+1} c_{l-1}^{k+1} &= \\
r_l^{k+1} c_{l+1}^{k} - 2r_l^{k+1} c_l^{k} + r_l^{k+1} c_{l-1}^{k} + \sum_{j=0}^{k-1} d_j^{l,k+1} c_l^{k-j} + b_k^{l,k+1} c_l^{0} \\
+ \tau^{\alpha_l^{k+1}} \Gamma(2 - \alpha_l^{k+1}) q_l^{k+1/2}, & k \geq 1.
\end{aligned}
\]

\[
\frac{\partial^2 c(x_l, t)}{\partial x^2} = \frac{1}{2} \left( \frac{c(x_{l+1}, t_{k+1}) - 2c(x_l, t_{k+1}) + c(x_{l-1}, t_{k+1})}{h^2} \right) + O(h^2).
\]
Matrix form of Crank-Nicholson method

\[
\begin{aligned}
A(1)C^1 &= B(1)C^0 + Q(0), \\
A(k + 1)C^{k+1} &= B(k + 1)C^k + d_1^{k+1}C^k + d_2^{k+1}C^{k-1} + \ldots \\
& \quad + d_k^{k+1}C^1 + b_k^{k+1}C^0 + Q(k), \quad k \geq 1.
\end{aligned}
\]

\[
A(k) = \begin{bmatrix}
1 + 2r_1^k & -r_1^k & 0 & \ldots & 0 & 0 \\
-r_2^k & 1 + 2r_2^k & r_2^k & \ldots & 0 & 0 \\
0 & -r_3^k & 1 + 2r_3^k & \ldots & 0 & 0 \\
\vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\
0 & 0 & 0 & \ldots & 1 + 2r_{M-2}^k & -r_{M-2}^k \\
0 & 0 & 0 & \ldots & -r_{M-1}^k & 1 + 2r_{M-1}^k
\end{bmatrix}
\]

\[
B(k) = \begin{bmatrix}
-2r_1^k & +r_1^k & 0 & \ldots & 0 & 0 \\
0 & -2r_2^k & r_2^k & \ldots & 0 & 0 \\
0 & -r_3^k & -2r_3^k & \ldots & \ldots & \ldots \\
\vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\
0 & 0 & 0 & \ldots & -2r_{M-2}^k & -r_{M-2}^k \\
0 & 0 & 0 & \ldots & -r_{M-1}^k & -2r_{M-1}^k
\end{bmatrix}
\]

\[
Q(k) = \begin{bmatrix}
r_1^k(g(t_k) + g(t_{k-1})) + \tau^{\alpha_1^{k+1}}\Gamma(2 - \alpha_1^{k+1})q_1^{k+1/2} \\
\tau^{\alpha_2^{k+1}}\Gamma(2 - \alpha_2^{k+1})q_2^{k+1/2} \\
\vdots \\
\tau^{\alpha_{M-2}^{k+1}}\Gamma(2 - \alpha_{M-2}^{k+1})q_{M-2}^{k+1/2} \\
r_{M-1}^k(h(t_k) + h(t_{k-1})) + \tau^{\alpha_{M-1}^{k+1}}\Gamma(2 - \alpha_{M-1}^{k+1})q_{M-1}^{k+1/2}
\end{bmatrix}.
\]
Stability of three finite difference methods

Here we use the Fourier method to prove the stability of three methods

**Proposition 1.** The coefficients $r_{l}^{k}$ and $d_{j}^{l,k}$ have the following properties

1. $r_{l}^{k} > 0$, $0 < b_{j}^{l,k} < b_{j-1}^{l,k} < 1$, $\forall l = 1, 2, \ldots, M$; $\forall j, k = 1, 2, \ldots, N$,

2. $0 < d_{j}^{l,k} < 1$, $\sum_{j=0}^{k-1} d_{j+1}^{l,k+1} = 1 - b_{k}^{l,k+1}$. 
Stability of explicit method

Theorem 1. The explicit difference scheme (5) is stable with the condition that
\[ \forall (l, k), r^k_l \leq \frac{1}{4} (1 - b_{1,l,k}), \quad (l = 1, 2, ..., M; \; k = 1, 2, ..., N). \]

Remark. From Theorem 1, we can know that the stable condition of explicit method is dependent with the evolution trajectory of \( \alpha(x, t) \). Hereby, the stable condition will changes with time evolution and space location.
Stability of implicit and Crank-Nicholson methods

Theorem 2. The implicit difference scheme is unconditionally stable.

Theorem 3. The Crank-Nicholson difference scheme is unconditionally stable.
An interesting result

Let $\rho^k_l = u^k_l - U^k_l$, where $U^k_l$ represents the approximate solution at $(x_l, t_k)$

$$\rho^k_l = \delta_k e^{i\sigma l k},$$

For Crank-Nicholson method, we can get the following result

$$\frac{\delta_{k+1}}{\delta_k} = \frac{1 - 4r^k_l \sin^2\left(\frac{qh}{2}\right) - b^l,k+1_1 + \sum_{j=1}^{k-1} (b^l,k+1_j - b^l,k+1_{j+1}) \frac{\delta_{k-j}}{\delta_k} + b^l,k+1_k \frac{\delta_0}{\delta_k}}{1 + 4r^k_l \sin^2\left(\frac{qh}{2}\right)}$$
Figure 1: Comparison of the ratios $\delta_{k+1}/\delta_k$ for $k=0,1,2,3$ and $4$ with $h = 0.1$, $\tau = 0.1$, $K = 1.0$. 
Convergence of three methods

**Theorem 5.** The explicit method is convergent when $\forall (l, k), r^k_l \leq \frac{1}{4}(1-b^{l,k}_1), \ (l = 1, 2, ..., M; \ k = 1, 2, ..., N)$, and there is a positive constant $C$, such that

$$|c^k_l - c(x_l, t_k)| \leq C(\tau + h^2), \ l = 1, 2, ..., M - 1; \ k = 1, 2, ..., N. \quad (53)$$

**Theorem 4.** The implicit method is convergent, and there is a positive constant $C$, such that

$$|c^k_l - c(x_l, t_k)| \leq C(\tau + h^2), \ l = 1, 2, ..., M - 1; \ k = 1, 2, ..., N. \quad (52)$$

**Theorem 6.** The Crank-Nicholson method is convergent, and there is a positive constant $C$, such that

$$|c^k_l - c(x_l, t_k)| \leq C(\tau + h^2), \ l = 1, 2, ..., M - 1; \ k = 1, 2, ..., N. \quad (54)$$
Numerical example

\[
\begin{aligned}
\frac{\partial^{\alpha(x,t)} c(x, t)}{\partial x^{\alpha(x,t)}} &= K \frac{\partial^2 c(x, t)}{\partial x^2} + q(x, t), \quad x \in (0, L), \ t \in (0, L], \\
&\quad c(x, 0) = 0, \\
&\quad c(0, t) = c(L, t) = 0,
\end{aligned}
\]

where

\[
q(x, t) = \frac{2}{\Gamma(3 - \alpha(x,t))} t^{2-\alpha(x,t)} \sin\left(\frac{x\pi}{L}\right) + \frac{K \pi^2 t^2}{L^2} \sin\left(\frac{x\pi}{L}\right),
\]

\(0 < \alpha(x, t) \leq 1, \text{ for } \forall(x, t).\)

The exact analytical solution for the above equation can be stated as

\[
c(x, t) = t^2 \sin(x\pi/L).
\]
Figure 2: The numerical result of variable-order time fractional diffusion equation by Crank-Nicholson method. The time step is $\tau = 0.01$, space step is $h = 0.1$. The variable-order function of time fractional derivative is $\alpha(x, t) = 0.8 + 0.2xt/(TL)$, where $L = 10.0$, $T = 0.5$. 
Table 1: Absolute errors ($|U(x_t, t_k) - u^k_t|$, $U$ is exact solution and $u$ is numerical solution) of explicit method, implicit method and Crank-Nicholson method for constant-order fractional diffusion equation at $x = 5.0$. The time step is $\tau = 0.01$, the space step is $h = 0.1$ and the time fractional order is $\alpha = 0.8$.

<table>
<thead>
<tr>
<th>Time</th>
<th>Explicit method</th>
<th>Implicit method</th>
<th>Crank-Nicholson method</th>
</tr>
</thead>
<tbody>
<tr>
<td>t=0.1</td>
<td>0.007E-2</td>
<td>0.526E-3</td>
<td>0.465E-3</td>
</tr>
<tr>
<td>t=0.2</td>
<td>0.314E-2</td>
<td>1.080E-3</td>
<td>0.919E-3</td>
</tr>
<tr>
<td>t=0.3</td>
<td>1.114E-2</td>
<td>1.836E-3</td>
<td>1.167E-3</td>
</tr>
<tr>
<td>t=0.4</td>
<td>2.556E-2</td>
<td>2.932E-3</td>
<td>1.109E-3</td>
</tr>
<tr>
<td>t=0.5</td>
<td>4.766E-2</td>
<td>4.434E-3</td>
<td>0.620E-3</td>
</tr>
</tbody>
</table>
Table 2: Absolute errors of explicit method, implicit method and Crank-Nicholson method for constant-order fractional diffusion equation at $x = 5.0$. The time step is $\tau = 0.01$, the space step is $h = 0.1$ and the variable-order function of time fractional derivative is $\alpha(x, t) = 0.8 + 0.2t/T$.

<table>
<thead>
<tr>
<th>Time</th>
<th>Explicit method</th>
<th>Implicit method</th>
<th>Crank-Nicholson method</th>
</tr>
</thead>
<tbody>
<tr>
<td>$t=0.1$</td>
<td>0.012E-2</td>
<td>0.574E-3</td>
<td>0.418E-3</td>
</tr>
<tr>
<td>$t=0.2$</td>
<td>0.356E-2</td>
<td>1.304E-3</td>
<td>0.698E-3</td>
</tr>
<tr>
<td>$t=0.3$</td>
<td>1.257E-2</td>
<td>2.453E-3</td>
<td>0.568E-3</td>
</tr>
<tr>
<td>$t=0.4$</td>
<td>2.898E-2</td>
<td>4.282E-3</td>
<td>0.233E-3</td>
</tr>
<tr>
<td>$t=0.5$</td>
<td>5.425E-2</td>
<td>7.118E-3</td>
<td>2.027E-3</td>
</tr>
</tbody>
</table>
Table 3: Absolute errors of explicit method, implicit method and Crank-Nicholson method for constant-order fractional diffusion equation at $x = 5.0$. The time step is $\tau = 0.01$, the space step is $h = 0.1$ and the variable-order function of time fractional derivative is $\alpha(x, t) = 0.8 + 0.2xt/(LT)$.

<table>
<thead>
<tr>
<th>Time</th>
<th>Explicit method</th>
<th>Implicit method</th>
<th>Crank-Nicholson method</th>
</tr>
</thead>
<tbody>
<tr>
<td>$t=0.1$</td>
<td>0.009E-2</td>
<td>0.550E-3</td>
<td>0.442E-3</td>
</tr>
<tr>
<td>$t=0.2$</td>
<td>0.335E-2</td>
<td>1.188E-3</td>
<td>0.813E-3</td>
</tr>
<tr>
<td>$t=0.3$</td>
<td>1.184E-2</td>
<td>2.132E-3</td>
<td>0.885E-3</td>
</tr>
<tr>
<td>$t=0.4$</td>
<td>2.722E-2</td>
<td>3.556E-3</td>
<td>0.484E-3</td>
</tr>
<tr>
<td>$t=0.5$</td>
<td>5.085E-2</td>
<td>5.650E-3</td>
<td>0.578E-3</td>
</tr>
</tbody>
</table>
Figure 3: The error $(U(x = 5.0, t_k) - u_{20k}^{h})$, $U$ is exact solution and $u$ is numerical solution) evolution curve with time at $x = 5.0$. The time step is $\tau = 0.01$, space step is $h = 0.1$. The variable-order function of time fractional derivative is $\alpha(x, t) = 0.8 + 0.2xt/(TL)$, where $L = 10.0$, $T = 1.0$. 
Some remarks

• The numerical method for variable-order diffusion equation is harder to perform than constant-order one.

• The stability and accuracy of the finite difference methods for variable-order time fractional diffusion equation have close relationship with the function of variable-order.

• The accuracy of the finite difference methods is case sensitive.
Further works

• Make further study about dynamic-order fractional dynamic system, based on the experiment of temperature-dependent variable-order fractal.

• Investigation about the relationship between CTRW and variable-order diffusion equation.

• Numerical method of variable-order space fractional advection-diffusion equation, and make a comparison between numerical method and experimental result.
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