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Numerical solution of some fractional dynamical systems in medicine involving non-singular kernel with vector order

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Abstract

In this paper, we propose systems of variable-order fractional equations for some problems in medicine. These problems include the dynamics of Zika virus fever and HIV infection of $CD4^+$ T-cells. Two types of non-local fractional derivatives are considered and compared in these dynamics: The Liouville-Caputo's definition and a definition involving non-singular Mittag-Leffler kernel. Predictor-corrector methods are described for simulating the corresponding dynamical systems.

Keywords: Dynamical systems System of fractional differential equations Zika virus fever HIV infection of $CD4^+$ T-cells Predictor-corrector methods.
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1. Introduction

Despite good advances in modeling systems for civil, mechanical and electrical engineering, various medical fields have not yet used mathematical tools well for modeling. In this paper, we introduce some well-studied modeling of medical problems. The dynamic behavior of these problems involves many unknown parameters and they are not as simple as a routine physical model. The battle of the immune system against individual germs like bacteria, viruses, and fungi and other toxins or chemicals is similar to the model of predator-prey. We are aware of a large number of models based on a method similar to predator-prey equation in the field of medicine, most of which rely on the local moment rate of change [1, 3, 11, 12, 14, 24, 25, 27, 34].

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But, we can not avoid the effect of memory and heredity in the population and density of cells or invaders and proteins which are produced by immune systems. Also, we can not experience well with simple dynamics in this field. One solution is to use operators involved both with the rate of change and non-locality. Fractional operators have been used successfully in many disciplines of science that have the properties expressed [2, 4, 5, 7, 9, 10, 15, 29, 32, 33]. Therefore, the non-local fractional derivatives are the best recommendations for modeling such complex dynamics [8, 22, 26, 28, 31].

Recently, fractional calculus is affected by definitions of new operators with a diversity of properties. Also, there is a warm discussion about "what is fractional derivatives?" [6, 18, 20]. The approach of this paper is to introduce the possibility of using such definitions in the modeling of some dynamical systems in medicine. Actually, in this paper, we consider the Liouville-Caputo's definition of a fractional derivative and a non-singular fractional derivative involving Mittag-Leffler kernel. We introduce a reliable numerical method for simulating the related dynamical systems and compare the results with different operators of fractional derivatives.

In this paper, we consider fractional derivatives in the convolution form:

$$\mathfrak{D}^{\alpha} y = \int_0^t k_{\alpha}(t-\tau) y'(\tau) d\tau, \quad 0 < \alpha < 1. \tag{1.1}$$

In our models, two types of prevalent kernels are considered:

1. Singular (Liouville-Caputo's definition (LC), see [13]):

$$k_{\alpha}(t-\tau) = \frac{1}{\Gamma(1-\alpha)(t-\tau)^{\alpha}}. \tag{1.2}$$

2. Nonsingular and nonlocal (Mittag-Leffler kernel (ML), see [5]):

$$k_{\alpha}(t-\tau) = \frac{B(\alpha)}{1-\alpha} E_{\alpha}\left(\frac{-\alpha}{1-\alpha}(t-\tau)^{\alpha}\right) \tag{1.3}$$

where $B(\alpha)$ is a normalization function obeying $B(0) = B(1) = 1$, and E_{α} is a one parameter Mittag-Leffler function [19].

The authors of [30] have realized that vector notations are more convenient for definitions of the index in algebraic fractional equations. Moreover, this type of notation not only is convenient for modeling systems with fractional order but also is convenient to use it with a high-level programming language like MATLAB. We note that software like MATLAB enjoys element-wise operations. Therefore, the author of this paper strongly recommends the writers in fractional dynamical systems use this type of notations for formulating their problems which contain more generality.

Definition 1. *Suppose* $\mathbf{y} = [y_1, \dots, y_{\nu}]^T$ *be a vector function and* $\overline{\alpha} = [\alpha_1, \dots, \alpha_{\nu}]^T$ *be a vector of dimension* $\nu \in \mathbb{N}$, *with* $\alpha_i \in \mathbb{R}$ *for* $i = 1, \dots, \nu$. *Then, the vector order fractional integral and derivative are defined by*

$$\mathfrak{J}^{\overline{\alpha}} \mathbf{y} = [\mathfrak{J}^{\alpha_1} y_1, \dots, \mathfrak{J}^{\alpha_{\nu}} y_{\nu}]^T,$$

and

$$\mathfrak{D}^{\overline{\alpha}} \mathbf{y} = [\mathfrak{D}^{\alpha_1} y_1, \dots, \mathfrak{D}^{\alpha_{\nu}} y_{\nu}]^T.$$

Regularly, many models in medicine obey nonlinear systems of fractional differential equations of the form

$$\begin{aligned} {}_0^C\mathfrak{D}_t^{\bar{\alpha}} \mathbf{y}(t) &= \mathbf{f}(t, \mathbf{y}(t)), \ t \in I := [0, T], \\ \mathbf{y}(0) &= \mathbf{y}_0, \end{aligned} \tag{1.4}$$

where $\bar{\alpha} = [\alpha_1, \ldots, \alpha_\nu]$ is a variable order, $T \in \mathbb{R}$, and $\mathbf{y} = [y_1, \ldots, y_\nu]^T$ is a vector function of dimension $\nu \in \mathbb{N}$. The vector $\mathbf{y}_0 \in \mathbb{R}^\nu$ is a constant initial value and $\mathbf{f} : [t_0, T] \times \mathbb{R}^\nu \mapsto \mathbb{R}^\nu$ can be a linear or nonlinear multivariate vector function.

This article is organized as follows: In Section 2, some preliminaries from fractional calculus reviewed. In Section 3, a system of fractional differential equations transformed into a system of weakly Volterra integral equations. In Section 4, a predictor-corrector method is introduced for solving nonlinear systems of fractional differential equations, numerically. Finally, in Section 5, numerical examples with simulations of some dynamical systems in medicine are considered.

2. Preliminaries

2.1. Fractional integral operator

For each definition of Caputo's fractional derivatives (1.2)-(1.3), there exists a corresponding integral operator $\mathfrak{I}^{\bar{\alpha}}$ such that

$$\mathfrak{I}^{\bar{\alpha}}\mathfrak{D}^{\bar{\alpha}}\mathbf{f}(t) = \mathbf{f}(t) - \mathbf{f}(0). \tag{2.1}$$

- Integral operator for LC's definition, see [21]:

$$\mathfrak{I}^{\bar{\alpha}}\mathbf{f}(t) = \frac{1}{\Gamma(\bar{\alpha})}\int_0^t \frac{\mathbf{f}(\tau)}{(t-\tau)^{1-\bar{\alpha}}}d\tau. \tag{2.2}$$

- Integral operator corresponding to ML kernel, see [7]:

$$\mathfrak{I}^{\bar{\alpha}}\mathbf{f}(t) = \frac{1-\bar{\alpha}}{B(\bar{\alpha})}\mathbf{f}(t) + \frac{\bar{\alpha}}{B(\bar{\alpha})\Gamma(\bar{\alpha})}\int_{t_0}^t \frac{\mathbf{f}(\tau)}{(t-\tau)^{1-\bar{\alpha}}}d\tau. \tag{2.3}$$

3. Reformulations of fractional differential equations into integral equations

The system (1.4), can be reformulated as integral equations:

- The system of integral equations corresponding to LC's definition:

$$\mathbf{y}(t) = \mathbf{y}_0 + \frac{1}{\Gamma(\bar{\alpha})}\int_0^t \frac{\mathbf{f}(\tau, \mathbf{y}(\tau))}{(t-\tau)^{1-\bar{\alpha}}}d\tau. \tag{3.1}$$

- The system of integral equations corresponding to ML kernel:

$$\mathbf{y}(t) = \mathbf{y}_0 + \frac{1-\bar{\alpha}}{B(\bar{\alpha})}\mathbf{f}(t, \mathbf{y}(t)) + \frac{\bar{\alpha}}{B(\bar{\alpha})\Gamma(\bar{\alpha})}\int_0^t \frac{\mathbf{f}(\tau, \mathbf{y}(\tau))}{(t-\tau)^{1-\bar{\alpha}}}d\tau. \tag{3.2}$$

Here, all operations corresponding to $\bar{\alpha}$ is element-wise.

4. Predictor Corrector method

Consider a uniform grid $I_h = \{t_j = jh : j = 0, 1, \ldots, N\}$, where $h = \frac{T}{N}$, and $N \in \mathbb{N}$. In finite difference methods, the object is finding $\mathbf{y}_{n+1} := \mathbf{y}(t_{n+1})$ $(n = 1, \ldots, N-1)$ based on previous values $\mathbf{y}_j$ $(j = 0, \ldots, n)$. Recursively, the solution on I_h can be obtained just by knowing $\mathbf{y}_j$. For a system of nonlinear fractional differential equations, approximate solution is obtained by solving a system of nonlinear equations. Fortunately, an iterative method can be used for solution of algebraic equations related to this system (1.4). But, every iterations need an initial value and therefore a predictor method is required. In construction of predictor we need to propose an explicit formula. In the following subsection we introduce a formula for predictor.

4.1. The formula for predictor

The quadrature method

$$\int_0^{t_{n+1}} \frac{\mathbf{f}(\tau, \mathbf{y}(\tau))}{(t-\tau)^{1-\bar{\alpha}}} d\tau \approx \sum_{j=0}^{n} b_{j,n+1}(\bar{\alpha}) \mathbf{f}(t_j, \mathbf{y}(t_j)). \tag{4.1}$$

base on the piecewise constant functions [16], is used to approximate weakly singular integrals. Here,

$$b_{j,n+1}(\bar{\alpha}) = \frac{(t_{n+1}-t_j)^{\bar{\alpha}} - (t_{n+1}-t_{j+1})^{\bar{\alpha}}}{\bar{\alpha}}.$$

Therefore, corresponding to each definitions of fractional derivatives, following generalized one-step Adams-Bashforth can be introduced:

- The explicit formula corresponding to LC's definition:

$$\mathbf{y}_{n+1}^0 = \mathbf{y}_0 + \frac{1}{\Gamma(\bar{\alpha})} \sum_{j=0}^{n} b_{j,n+1}(\bar{\alpha}) \mathbf{f}(t_j, \mathbf{y}_j). \tag{4.2}$$

- The explicit formula corresponding to ML kernel:

$$\mathbf{y}_{n+1}^0 = \mathbf{y}_0 + \frac{1-\bar{\alpha}}{B(\bar{\alpha})} \mathbf{f}(t_{n+1}, \mathbf{y}_n) + \frac{\bar{\alpha}}{B(\bar{\alpha})\Gamma(\bar{\alpha})} \sum_{j=0}^{n} b_{j,n+1}(\bar{\alpha}) \mathbf{f}(t_j, \mathbf{y}_j). \tag{4.3}$$

4.2. The formula for Corrector

Now, we should propose a high order formula for corrector. Both, the collocation methods based on piecewise polynomials or "hat shaped" functions can be used for constructing a corrector. Generally, in graded mesh it is better to chose piecewise polynomials as a basis of quadrature approximations since they have higher order with this meshes. For uniform mesh, quadrature approximations based on piecewise linear "hat shaped" functions are appropriate because they have order of convergence greater than 1. This approximation can be obtained by just interpolating on the basis with piecewise linear "hat shaped" functions [16]. For weakly singular equations, we then have

$$\int_0^{t_{n+1}} \frac{\mathbf{f}(\tau, \mathbf{y}(\tau))}{(t-\tau)^{1-\bar{\alpha}}} d\tau \approx \sum_{j=0}^{n+1} a_{j,n+1}(\bar{\alpha}) \mathbf{f}(t_j, \mathbf{y}_j). \tag{4.4}$$

The $a_{j,n+1}(\bar{\alpha})$ can be computed using following formula [16]:

$$a_{j,n+1}(\bar{\alpha}) = \frac{h^{\bar{\alpha}}}{\bar{\alpha}(\bar{\alpha}+1)} \begin{cases} n^{\bar{\alpha}+1} - (n-\bar{\alpha})(n+1)^{\bar{\alpha}}, & \text{if } j=0, \\ (n-j+2)^{\bar{\alpha}+1} + (n-j)^{\bar{\alpha}+1} & \text{if } j=1,\dots,n, \\ -2(n-j+1)^{\bar{\alpha}+1}, & \\ 1, & \text{if } j=n+1. \end{cases}$$

Therefore, corresponding to each definitions of fractional derivatives, following generalized one-step Adams-Moulton method, can be introduced:

- The implicit formula corresponding to LC's definition:

$$\mathbf{y}_{n+1} = \mathbf{y}_0 + \frac{1}{\Gamma(\bar{\alpha})} \sum_{j=0}^{n+1} a_{j,n+1}(\bar{\alpha}) \mathbf{f}(t_j, \mathbf{y}_j). \tag{4.5}$$

- The implicit formula corresponding to ML kernel:

$$\mathbf{y}_{n+1} = \mathbf{y}_0 + \frac{1-\bar{\alpha}}{B(\bar{\alpha})} \mathbf{f}(t_{n+1}, \mathbf{y}_{n+1}) + \frac{\bar{\alpha}}{B(\bar{\alpha})\Gamma(\bar{\alpha})} \sum_{j=0}^{n+1} a_{j,n+1}(\bar{\alpha}) \mathbf{f}(t_j, \mathbf{y}_j). \tag{4.6}$$

4.3. The predictor corrector method

The predictor use as an initial value for iterative process in corrector equations. If we use $m \in \mathbb{N}$ iteration, then predictor corrector method (PC^m) can be compacted as

- The PC^m corresponding to LC's definition:

$$\mathbf{y}_{n+1}^{i+1} = \mathbf{F}_n(\mathbf{y}) + \frac{1}{\Gamma(\bar{\alpha})} a_{n+1,n+1}(\bar{\alpha}) \mathbf{f}(t_{n+1}, \mathbf{y}_{n+1}^{i}), \tag{4.7}$$

for $i = 0, \dots, m-1$. Here,

$$\mathbf{F}_n(\mathbf{y}) := \mathbf{y}_0 + \frac{1}{\Gamma(\bar{\alpha})} \sum_{j=0}^{n} a_{j,n+1}(\bar{\alpha}) \mathbf{f}(t_j, \mathbf{y}_j).$$

- The PC^m corresponding to ML kernel:

$$\mathbf{y}_{n+1}^{i+1} = \mathbf{F}_n(\mathbf{y}) + \left(\frac{1-\bar{\alpha}}{B(\bar{\alpha})} + \frac{\bar{\alpha} a_{n+1,n+1}(\bar{\alpha})}{B(\bar{\alpha})\Gamma(\bar{\alpha})} \right) \mathbf{f}(t_{n+1}, \mathbf{y}_{n+1}^{i}), \tag{4.8}$$

for $i = 0, \dots, m-1$. Here,

$$\mathbf{F}_n(\mathbf{y}) := \mathbf{y}_0 + \frac{\bar{\alpha}}{B(\bar{\alpha})\Gamma(\bar{\alpha})} \sum_{j=0}^{n} a_{j,n+1}(\bar{\alpha}) \mathbf{f}(t_j, \mathbf{y}_j).$$

Finally, we accept $\mathbf{y}_{n+1} = \mathbf{y}_{n+1}^{m}$ as an approximate solutions and repeat the recursions until $n = N-1$.

5. Numerical examples and simulation

We note that the dot operation in MATLAB makes it very convenient to program these algorithms with vector order fractional derivatives or integrals. Therefore, all examples are simulated in MATLAB software. In the first example, we validate the method by a system that we have its exact solution and we discuss the parameters of the numerical methods. Next, we apply the method for some models in medicine.

5.1. Validation of the introduced method

Example 1. *Let us consider System (1.4), with $\bar{\alpha} = [0.8, 0.9]^T$,*

$$\mathbf{f}(t, \mathbf{y}) = \mathbf{A}\mathbf{y} + \mathbf{q}(t), \tag{5.1}$$

with

$$\mathbf{A} = \begin{bmatrix} 24 & -24 \\ 12 & 24 \end{bmatrix}$$

and the source function

$$\mathbf{q}(t) = \begin{bmatrix} 5tE_{\alpha_1,2}(-4t^{\alpha_1}) - 5t^3 E_{\alpha_1,4}(-4t^{\alpha_1}) + \frac{t^4}{12} + \frac{t^3}{6} - t^2 - t + 2 \\ -10t^2 E_{\alpha_2,3}(-9t^{\alpha_2}) + 10t^4 E_{\alpha_2,5}(-9t^{\alpha_2}) - \frac{t^4}{12} + \frac{t^3}{6} + t^2 - t - 2 \end{bmatrix}$$

corresponding to Liouville-Caputo's definition and

$$\mathbf{q}(t) = \begin{bmatrix} \frac{t^{1-\alpha_1}}{\Gamma(2-\alpha_1)} - \frac{t^{3-\alpha_1}}{\Gamma(4-\alpha_1)} + \frac{t^4}{12} + \frac{t^3}{6} - t^2 - t + 2 \\ -\frac{t^{2-\alpha_2}}{\Gamma(3-\alpha_2)} + \frac{t^{4-\alpha_2}}{\Gamma(5-\alpha_2)} - \frac{t^4}{12} + \frac{t^3}{6} + t^2 - t - 2 \end{bmatrix}$$

corresponding to Mittag-Leffler kernel. Choosing $\mathbf{y}_0 = [0,1]^T$*, the exact solution of the System* (1.4) *is*

$$\mathbf{y}(t) = [t - \frac{t^3}{6}, 1 - \frac{t^2}{2} + \frac{t^4}{24}]^T$$

for both proposed fractional derivatives with corresponding source functions. We approximate an index of error by

$$E_N(b) = \max_{i=0,\ldots,N} \{\|\mathbf{y}(t_i) - \mathbf{y}_i^m\|\}$$

where $\|.\|$ *is max norm for vectors. The results of simulations on* $[0,2]$ *are reported in Tables 1 and 2. In the first example, by increasing* N *the effect of the* m *on accuracy is reduced. However, in the second example the greater* m *is necessary and the method with* $m = 1$*, is divergent. Generally, one can also use a variable mode* PC^m *method by computing error estimate in each iteration controlled by desired tolerance.*

Table 1: The errors for various N and m in Example 1 with Liouville-Caputo's fractional derivative

$E_N(m)$	$m=1$	$m=2$	$m=3$	$m=4$
$N=50$	1.7806e-01	1.5695e-01	1.5607e-01	1.5609e-01
$N=100$	7.4463e-02	6.8696e-02	6.8561e-02	6.8563e-02
$N=200$	3.1658e-02	2.9998e-02	2.9974e-02	2.9975e-02
$N=400$	1.3570e-02	1.3080e-02	1.3076e-02	1.3076e-02
$N=800$	5.8449e-03	5.6991e-03	5.6984e-03	5.6984e-03

Table 2: The errors for various N and m in Example 1 with fractional derivative involving Mittag-Leffler kernel

$E_N(m)$	$m=1$	$m=2$	$m=3$	$m=4$
$N=50$	1.2091e+02	1.5484e-01	5.0857e-02	4.8617e-03
$N=100$	1.2574e+03	1.5123e-01	4.5273e-02	4.4312e-03
$N=200$	1.6342e+05	1.4871e-01	4.2180e-02	4.1892e-03
$N=400$	1.8555e+09	1.4707e-01	4.0445e-02	4.0584e-03
$N=800$	1.7548e+17	1.4605e-01	3.9462e-02	3.9881e-03

5.2. Simulating of some medical models

Example 2. *Zika virus fever is a viral disease caused by Zika Virus (ZIKV), a member of the family Flaviridae and the genus Flavivirus [23]. ZIKV is primarily transmitted to humans through the bite of infected Aedes species mosquitoes, including Aedes aegypti and Aedes albopictus, the most important vectors for transmitting DENV and CHIKV globally. A fractional model of this disease recently proposed [4]. In this example, we use the parameters of [23] for this model and after substitution this parameter, we obtain a simplified model of this disease described by linear fractional system* (1.4) *and* (5.1) *with*

$$\mathbf{A} = \begin{bmatrix} -0.0917 & 0 & 0 & 0 & 0 \\ 0.0750 & -0.0167 & 0 & 0 & 0 \\ 0 & 0 & -0.075 & 0 & 0.1 \\ 0 & 0 & 0.075 & -0.2 & 0 \\ 0 & 0 & 0 & 0.2 & -0.1 \end{bmatrix},$$

$$\mathbf{q} = [0.0095, 0.0005, 0.0001, 0, 0]^T,$$

and

$$\mathbf{y} = [S_a, I_a, S_h, I_h, R_h]^T$$

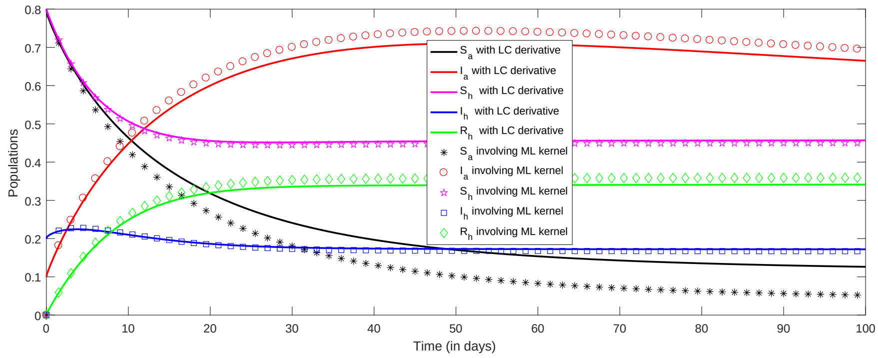

Figure 1: The simulated results for systems of fractional differential equations related to Zika virus fever with CL fractional derivative and ML kernel.

where S_a and I_a stands for the population of susceptible and infectious adults in Aedese mosquitoes, respectively. The notations S_h, I_h and R_a stand for population of susceptible, infectious and recovered humans. The dynamic of this system simulated in Figure 1 with $\bar{\alpha} = [0.90, 0.95, 0.98, 0.85, 0.95]^T$. The simulated results with CL fractional derivative and ML kernel are in agreement with the result of integer order depicted in [23].

Example 3. *In this example, we consider a system of nonlinear fractional differential equations. One of the popular model that has been studied in recent decades is the model of HIV infection of CD4$^+$ T-cells [24]. Let $\mathbf{y} = [T, I, V]^T$. Then, the system (1.4) with nonlinear function [17]*

$$\mathbf{f}(t, \mathbf{y}(t)) = \begin{bmatrix} 10 - 0.02y_1 + 0.3y_1(1 - \frac{y_1+y_2}{1500}) - 0.000024y_1y_3 \\ 0.00002y_1y_3 - 0.26y_2 \\ 192y_2 - 0.000024y_1y_3 - 2.4y_3 \end{bmatrix}$$

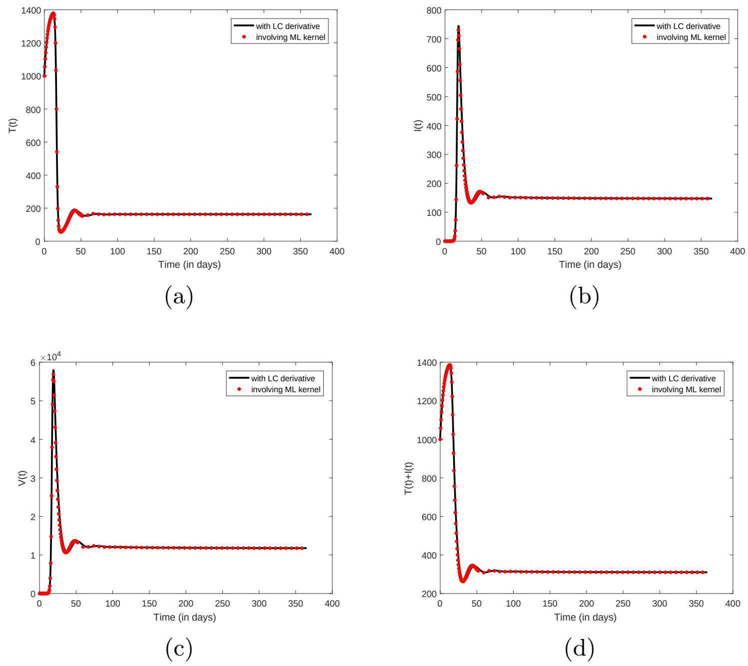

Figure 2: The simulated results for systems of fractional differential equations related to HIV infection of CD4$^+$ T-cells with CL fractional derivative and ML kernel: (A) Concentration of healthy CD4$^+$ T-cells; (B) Concentration of infected CD4$^+$ T-cells; (C) Free HIVs virus; (D) Concentration of all CD4$^+$ T-cells.

describes this model. Here, the dynamical variables $T(t)$, $I(t)$ *and* $V(t)$ *represent the concentration of healthy CD4*$^+$ *T-cells, infected CD4*$^+$ *T-cells and free HIVs virus in time* t*, respectively. This system is simulated with initial condition* $\mathbf{y} = [1000, 0, 0.001]^T$*, and vector order* $[0.9, 0.95, 0.98]^T$*. The Numerical method is tuned with* $N = 3000$, $m = 3$*. The results are depicted in Figures* (2) *(a)-(d). The results are in good agreement with the result of integer order reported in [17].*

Conclusion

Most of the dynamical systems are studied in the modeling of medical problems, use a local change of rate in their modeling. However, we expect memory and non-locality in the dynamics of medical problems. Therefore, in this paper, we considered variable-order fractional models for describing such dynamics. We considered two types of non-local fractional derivatives for modeling such systems. An efficient numerical method is proposed for solving corresponding variable-order fractional dynamical systems. The results show the behavior of both fractional derivatives is similar to the integer one. Considering the memory on these dynamics, these models are recommended to be considered instead of integer cases.

Disclosure statement

The authors declare no potential conflict of interest.

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