Role of fractional derivatives in the mathematical modeling of the transmission of Chlamydia in the United States from 1989 to 2019

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Abstract Nowadays, the mathematical modeling of infectious diseases is a big trend worldwide. The mathematical models help us to forecast future outbreaks of diseases in the presence of present data. In this article, we represent a model of the transmission of Chlamydia in the United States by using data from 1989 to 2019. In the formulation of the model, we used integer and fractional derivatives. Several graphs are plotted for the various possible cases of the given parameters. The aim of this paper is to justify how the mathematical models in terms of fractional derivatives have more degree of freedom to explore disease dynamics for a particular data set and capture memory effects. The separate parameter estimation for each value of the fractional order increases the novelty of this work. The use of a real-data set of Chlamydia in the United States makes this study more visible and important to the literature.

Keywords Chlamydia · Data-fitting · Mathematical model · Caputo fractional derivative · Numerical method

Mathematics Subject Classification 26A33 · 34C60 · 92C60 · 92D30

1 Introduction

Chlamydia, known as ‘the silent epidemic’ is one of the most generic sexually transmitted epidemics in the United States and European nations [1]. It was recorded that nearly 92 million in Chlamydia cases were found worldwide in 1999, with 42 million for men and 50 million for women [2]. It is noticed that people in the age group of 20 – 24 years are at big hazard of being infected on average because, in 2010, this age group contained 36% of all infected cases which is the maximum ratio among all age clusters [3]. This disease has a unique and complex biphasic growth cycle including eukaryotic cells. Genital Chlamydia infection is treatable with antibiotics [4]. Chlamydia persists in a reversible condition called chlamydial persistence, which leads to a protracted interaction between Chlamydia and the infected host cell [5].

To date, several modeling has been introduced to explore the transmission of Chlamydia. The authors in Ref. [6] were defined as an optimal control derivation for the Chlamydia modeling. In [7], an optimal control modeling of the chronic Chlamydia trachomatis dis-
ease considering a combination treatment with tranpyridine and antibiotic was derived. In [8], mathematical modeling of Chlamydia trachomatis in a human carrier was introduced. Some novel analyses on a chlamydia epidemic model have been given in Ref. [9]. In [10], the researchers have described a model to test intervention strategies for Chlamydia. In [11], the authors introduced a study of the in-host structure of Chlamydia trachomatis. Akinlotan et al. in [12] have modeled the play of mucosal vaccine on the within-host structure of Chlamydia disease. In [13], some analyses of Chlamydia transmission in a closed population were proposed. The study is given in Ref. [14] analyzed a Chlamydia model with a pulse vaccination factor. In [15], a study on optimizing coverage for a chlamydia trachomatis screening program was proposed.

Nowadays, different types of fractional derivatives have been defined and are highly used because of their advanced features which help us to analyze a real-world problem more deeply [16–18]. To date, several real-world problems have been successfully modeled using various types of fractional derivatives. Here we look at some recent works in this area: In [19], the authors analyzed the transmission of the COVID-19 epidemic by using integer and fractional derivatives. In [20], the authors performed the analyses of the existence and uniqueness of a fractional-order blood glucose-insulin minimal model. In [21], the cholera epidemic has been studied using a novel fractional-order model with real data. In [22], the authors derived an optimal control system for the mosaic epidemic in terms of Caputo fractional derivatives. Erturk et al. in Ref. [23] performed some novel analysis of the modeling of corneal shape using Caputo fractional derivatives. In [24], some novel analyses of stability and bifurcation of an HIV-1 model with a discrete-time delay have been proposed. In [25], the mechanism of the alkali-silica chemical reaction has been explored using a nonlinear model in the Caputo sense. In Ref. [26], the authors firstly introduced a nonlinear mathematical model for the transmission of tooth cavity in humans by using the novel results based on integer- and fractional-order derivatives. In [27], a fractional-order model of blood ethanol concentration with a real data has been proposed. In [28], the authors implemented the Atangana–Baleanu operators on a 3D Hopfield neural network model. In [29], an analytic solution of a nonlinear multi-order fractional boundary value problem existing in chemical reactor theory has been derived.

Odibat et al. in [30] derived a novel form of Predictor–Corrector scheme to simulate generalized Caputo-type delay differential equations. In [31], the mathematical models with fractional derivatives for the dye removal adsorption process have been proposed. In [32], some novel analyses with applications of a regularized Ψ–Hilfer fractional derivative have been given.

Getting the idea of the mathematical modeling and the features of fractional derivatives, we introduce a nonlinear model for the Chlamydia epidemic in terms of integer and fractional order derivatives. The aim of this article is to explore the future outbreaks of Chlamydia in the United States by using the data from 1989 to 2019. The application of the Caputo fractional derivatives includes the memory effects in the model which provides more degree of freedom in the experimental simulations. The article is framed as follows: In Sect. 2, the preliminaries are given. Section 3 introduces the dynamics of integer- and fractional-order mathematical models along with the novel parameter estimation and data fitting. For estimating the parameter values, we use some computational techniques. In the first one, we used an ODE solver (e.g. ode15s) in MATLAB to estimate the parameters of the classical model from a Least square perspective and then solved it numerically for a set of values for the Caputo fractional derivative. Another technique uses the Adams-type predictor–corrector method to investigate parameter estimation for the fractional-order model. In Sect. 4, several experimental observations are given to check the effects of fractional-order values and find the best-fit value of the order of Caputo fractional derivatives. Section 5 gives the conclusion of the study.

2 Preliminaries

Firstly, we write the following basics of fractional calculus useful for our investigations:

Definition 1 [16,17] The real-function $F(t)$, $t > 0$ belongs to the space

- a) $C_{\zeta^+}$, $\zeta \in \mathbb{R}$ if there exists a real number $q > \zeta$, such that $F(t) = t^{\gamma}F_1(t)$, $F_1 \in C[0, \infty)$. Clearly, $C_{\zeta^+} \subset C_{\gamma}$ if $\gamma \leq \zeta$.
- b) $C_{\zeta^m}$, $m \in \mathbb{N} \cup \{0\}$ if $F^m \in C_{\zeta}$.
Definition 2 [16, 17] The left- and right-hand Caputo fractional derivatives of $F \in C^n_{-1}$ of order $\alpha \in (\nu - 1, \nu]$, $\nu \in \mathbb{N}$ are given by

$$C^D_{t_0} F(t) = \frac{1}{\Gamma(\nu - \alpha)} \int_{t_0}^{t} (t - \tau)^{\nu - \alpha - 1} F^{(\nu)}(\tau) d\tau,$$

and

$$C^D_{t_0} F(t) = \frac{(-1)^{\nu}}{\Gamma(\nu - \alpha)} \int_{t_0}^{t} (\tau - t)^{\nu - \alpha - 1} F^{(\nu)}(\tau) d\tau,$$

provided they exist almost everywhere on $[t_0, t_1]$.

3 The mathematical models

In this section, we introduce our mathematical models to define the dynamics of the chlamydia epidemic in terms of integer- and fractional-order derivatives.

3.1 Integer-order model

Here we define the structure of sexually transmitted disease chlamydia in United states using the mathematical model derived by Odionyemna et al. [6]. The population size of the humans is considered into six compartments; unvaccinated susceptible individuals $S(t)$, vaccinated susceptible individuals $V(t)$, exposed peoples $E(t)$, infectious peoples $I(t)$, treated humans $T(t)$, and humans with recovery $R(t)$. Total population size is $N(t) = S(t) + V(t) + E(t) + I(t) + T(t) + R(t)$. Therefore, the model dynamics is expressed as follows:

$$\begin{align*}
\frac{dS}{dt} &= (1 - \phi)\Lambda - \frac{\beta S(I + \xi T)}{N} + wV - \mu S, \\
\frac{dV}{dt} &= \phi\Lambda - V(w + \mu) - \frac{\beta(1 - \pi)V(\xi T + I)}{N}, \\
\frac{dE}{dt} &= \beta \frac{(1 - \pi)V(\xi T + I)}{N} + \frac{\beta S(I + \xi T)}{N} - (\sigma + \mu)E + (1 - \rho)\theta T + \frac{\epsilon\beta(I + \xi T)R}{N}, \\
\frac{dI}{dt} &= \sigma E - (\gamma + \eta + \mu + \delta_1)I + \rho\theta T, \\
\frac{dT}{dt} &= \eta I - (\mu + \theta + \delta_2 + \tau)T, \\
\frac{dR}{dt} &= \gamma I - \frac{\epsilon\beta R(\xi T + I)}{N} + T\tau - \mu R,
\end{align*}$$

(1)

where the corresponding model parameters $\Lambda$ is the birth rate, $\beta$ is the transmission rate from $S$ to $I$ class, $\epsilon$ is the reinfection rate, $p$ is the fraction of humans that failed treatment, $\theta$ is the failure rate of treatment, $\mu$ is the natural mortality rate of the human populations, $\pi$ is the effectiveness of vaccine, $\phi$ is the fraction of recruited humans, $\delta_1$ is the disease-induced mortality rate for infectious peoples, $\delta_2$ is the disease-induced death rate of treated humans, $\sigma$ is the transmission rate from $E$ to $I$ class, $\xi$ is the modification parameter, $w$ is the waning of vaccine rate, $\eta$ is the treatment rate for infectious individuals, $\gamma$ is the recovery rate of infectious class, and $\tau$ is the recovery rate of treated class.

3.1.1 Data fitting and parameter estimation

For parameter estimation, we use an ODE solver (e.g. ode15s) in MATLAB to estimate the parameters of the classical model (1) from a Least square perspective. We investigate the parameter estimation and data fitting of the model 1 with yearly infected cases of United States from the year 1989 to 2019. The real data used in the estimation is available at CDC website [33]. We utilize the Levenberg–Marquardt algorithm with lsqcurvefit function in MATLAB to estimate the parameter values. From the recent data, the United States total population in 1989 was 235825000. The initial populations are taken as $S(0) = 233824096$, $V(0) = 1000000$, $E(0) = 500000$, $I(0) = 200904$, $T(0) = 250000$ and $R(0) = 50000$.

In Fig. 1, we can observe that the integer order Chlamydia mathematical model (1) is fitted really well with yearly infectious cases in the United States from the year 1989 to 2019. The corresponding real-data based parameter values of the integer-order case ($\alpha = 1$) are given in Table 1.
The integer-order derivatives are local in nature, so they do not contain the memory in the system. To capture memory effects in the proposed model, we go for further analysis by using Caputo fractional derivatives. In the fractional-order model, the present behaviour of the disease will depend on the outbreaks of the previous stage of time. So, the system will contain a history where the current time stage results will be reflected by the previous outcomes, which looks like the more realistic nature of a disease.

3.2 Fractional-order model

Here we generalize the previously given integer-order model (1) by using Caputo fractional derivatives. As we know the general rule of fractional-order generalization is that simply replacing the integer-order derivatives with fractional-order derivatives does not look correct because such-type of generalization can give an unphysical model. In that case, a perfect equal dimensionality is required for an accurate generalization. For this, we place the fractional-order powers \( \alpha \) on each time-dimensional parameter for making the equal time-dimension of time \( e^{-\alpha t} \) on both hands of the model. Therefore, the fractional-order model to define the chlamydia epidemic is given as follows:

\[
\begin{align*}
C^D_0 S(t) &= (1 - \phi)A^\alpha - \frac{\beta^\alpha S(I + \xi T)}{N} - \mu^\alpha S + \omega^\alpha V, \\
C^D_0 V(t) &= \phi A^\alpha - V(\mu^\alpha + \omega^\alpha) - (1 - \pi)\beta^\alpha V(I + \xi T), \\
C^D_0 E(t) &= \frac{(1 - \pi)\beta^\alpha V(I + \xi T)}{N} + \frac{\beta^\alpha S(I + \xi T)}{N} \\
&\quad - (\mu^\alpha + \sigma^\alpha)E + (1 - p)\theta^\alpha T + \frac{\epsilon^\alpha}{N} \beta^\alpha(I + \xi T)R + T\tau^\alpha, \\
C^D_0 I(t) &= \sigma^\alpha E - I(\mu^\alpha + \eta^\alpha + \gamma^\alpha + \delta^\alpha_1 + p\theta^\alpha T), \\
C^D_0 R(t) &= \eta^\alpha I - T(\mu^\alpha + \theta^\alpha + \delta^\alpha_2 + \tau^\alpha), \\
C^D_0 R(t) &= \gamma^\alpha I - \mu^\alpha R - \frac{\epsilon^\alpha}{N} \beta^\alpha(I + \xi T)R + T\tau^\alpha, \\
\end{align*}
\]

where 0 < \( \alpha \leq 1 \) is the order of the given fractional derivative \( C^D_0 \).

The disease-free equilibrium \( E^* \) of the proposed fractional-order model is

\[
E_1(S^*, V^*, E^*, I^*, T^*, R^*) = \left( \frac{(\mu^\alpha + \omega^\alpha)(1 - \phi)\Lambda^\alpha + \phi\Lambda^\alpha \omega^\alpha}{(w^\alpha + \mu^\alpha)\mu^\alpha}, \right.
\]

\[
\left. \frac{\Lambda^\alpha \phi}{\omega^\alpha + \mu^\alpha}, 0, 0, 0, 0 \right). 
\]

The estimated basic reproductive number \( R_0 \) is defined by

\[
R_0 = \frac{\sigma^\alpha(\xi \beta^\alpha \eta^\alpha A + \Lambda^\alpha A_2)}{N^*\left[ A_4 + A_2(\gamma^\alpha + \mu^\alpha + \delta^\alpha_1) + (\delta^\alpha_2 + \mu^\alpha + \tau^\alpha)(\eta^\alpha \alpha^\alpha + \eta^\alpha \mu^\alpha) + \eta^\alpha \mu^\alpha \theta^\alpha (1 - p) \right]},
\]

by the previous outcomes, which looks like the more realistic nature of a disease.

Before proceeding towards the data fitting for the proposed fractional-order model, here we check the stability condition of the disease-free equilibrium \( E^* \). In this regard, the following theorem is established.

**Theorem 1** The disease-free equilibrium \( E^* \) of the proposed fractional-order model (2) is locally asymptotically stable when \( R_0 \leq 1 \) and unstable when \( R_0 > 1 \).

**Proof** To investigate the stability of \( E^* \), firstly we write the linearization of the model (2) at any equilibrium \( E(S^*, V^*, E^*, I^*, T^*, R^*) \) as follows:

\[
\begin{align*}
C^D_0 S(t) &= -\frac{1}{N} \left( \beta^\alpha (I^* + \xi T^*) - \mu^\alpha \right) S + \omega^\alpha V, \\
&\quad - \frac{\beta^\alpha S^*}{N} I - \frac{\beta^\alpha S^* \xi}{N} T, \\
C^D_0 V(t) &= -\frac{(\mu^\alpha + \omega^\alpha) V - (1 - \pi)\beta^\alpha (I^* + \xi T^*)}{N} \\
&\quad - \frac{(1 - \pi)\beta^\alpha V^*}{N} I - \frac{(1 - \pi)\beta^\alpha V^* \xi}{N} T, \\
C^D_0 E(t) &= \frac{\beta^\alpha (I^* + \xi T^*)}{N} S + \frac{(1 - \pi)\beta^\alpha (I^* + \xi T^*)}{N} V \\
&\quad - \frac{(\mu^\alpha + \sigma^\alpha) E - (1 - p)\theta^\alpha T}{N} + \frac{\epsilon^\alpha}{N} \beta^\alpha(I + \xi T^*)R + T\tau^\alpha, \\
C^D_0 I(t) &= \sigma^\alpha E - I(\mu^\alpha + \eta^\alpha + \gamma^\alpha + \delta^\alpha_1 + p\theta^\alpha T). \\
\end{align*}
\]
The second column represents the parameter values of the integer order model (1). The third, and fourth columns represent the parameter values of the fractional-order model (2). The fifth column corresponds to the parameters estimated with an optimal value of \( \alpha \).

| Parameter | \( \alpha = 1 \) | \( \alpha = 0.9 \) | \( \alpha = 0.8 \) | \( \alpha = 0.9839 \) (estimated value) |
|-----------|----------------|----------------|----------------|----------------|
| \( \phi \) | 3.9491 | 0.5288 | 1.7013 | 1.4284 |
| \( \beta \) | 0.8755 | 1.1089 | 0.7433 | 1.0410 |
| \( \xi \) | 0.7845 | 0.7624 | 0.7451 | 0.9960 |
| \( \sigma \) | 0.4984 | 0.9999 | 0.9835 | 0.000006 |
| \( \rho \) | 0.6008 | 0.7269 | 0.6969 | 0.000006 |
| \( \epsilon \) | 0.2062 | 0.6884 | 0.5521 | 0.7074 |
| \( \eta \) | 0.4629 | 0.2187 | 0.1248 | 0.2489 |
| \( \gamma \) | 0.5702 | 0.6504 | 0.5293 | 0.6599 |
| \( \delta_1 \) | 0.0928 | 0.2086 | 0.000001 | 0.1526 |
| \( \delta_2 \) | 0.0580 | 0.0128 | 0.000034 | 0.1524 |
| \( \tau \) | 0.5851 | 0.4456 | 0.4729 | 0.7227 |
| \( \theta \) | 0.0020 | 0.1333 | 0.3143 | 0.0297 |

Implementing the Laplace transformation on the both sides of the proposed system (12), we get the following system:

\[
\begin{align*}
\mathcal{C}D_{t_0^+}^\alpha S(t) &= \eta^\alpha I - (\mu^\alpha + \theta^\alpha + \delta_2^\alpha + \tau^\alpha)T, \\
\mathcal{C}D_{t_0^+}^\alpha R(t) &= \gamma^\alpha I - \frac{e^\alpha \beta^\alpha R^*}{N} I - \frac{e^\alpha \beta^\alpha \xi R^*}{N} T \\
&+ e^\alpha T - \mu^\alpha R - \frac{e^\alpha \beta^\alpha (I^* + \xi T^*)}{N} R. \\
\end{align*}
\]

Implementing the Laplace transformation on the both sides of the proposed system (12), we get the following system:

\[
\begin{align*}
s^\alpha \mathcal{L}[S(s)] - s^{\alpha-1} S(0) &= \left[ \frac{1}{N} (\beta^\alpha (I^* + \xi T^*)) - \mu^\alpha \right] \\
&\quad - \frac{\beta^\alpha S^*}{N} \mathcal{L}[I(s)] - \frac{\beta^\alpha S* \xi}{N} \mathcal{L}[T(s)]. \\
s^\alpha \mathcal{L}[V(s)] - s^{\alpha-1} V(0) &= -(\mu^\alpha + \omega^\alpha) \mathcal{L}[V(s)] \\
&\quad - \frac{(1 - \pi) \beta^\alpha (I^* + \xi T^*)}{N} \mathcal{L}[V(s)] \\
&\quad - \frac{(1 - \pi) \beta^\alpha V^*}{N} \mathcal{L}[I(s)] \\
&\quad - \frac{(1 - \pi) \beta^\alpha V^* \xi}{N} \mathcal{L}[T(s)], \\
s^\alpha \mathcal{L}[E(s)] - s^{\alpha-1} E(0) &= \frac{\beta^\alpha (I^* + \xi T^*)}{N} \mathcal{L}[S(s)] \\
&\quad + \frac{(1 - \pi) \beta^\alpha (I^* + \xi T^*)}{N} \mathcal{L}[V(s)] \\
&\quad - (\mu^\alpha + \sigma^\alpha) \mathcal{L}[E(s)] \\
&\quad + \frac{\beta^\alpha S^*}{N} \mathcal{L}[I(s)] \\
&\quad + \frac{\beta^\alpha S^* \xi}{N} \mathcal{L}[T(s)] \\
&\quad + \frac{\beta^\alpha V^*}{N} \mathcal{L}[I(s)] \\
&\quad + \frac{\beta^\alpha V^* \xi}{N} \mathcal{L}[T(s)] \\
&\quad + \frac{\beta^\alpha \xi R^*}{N} \mathcal{L}[R(s)] \\
&\quad - \frac{e^\alpha \beta^\alpha V^*}{N} \mathcal{L}[I(s)] \\
&\quad - \frac{e^\alpha \beta^\alpha V^* \xi}{N} \mathcal{L}[I(s)] \\
&\quad + \frac{e^\alpha \beta^\alpha \xi R^*}{N} \mathcal{L}[R(s)] \\
&\quad - \frac{e^\alpha \beta^\alpha (I^* + \xi T^*)}{N} \mathcal{L}[R(s)]. \\
\end{align*}
\]

where \( \mathcal{L}[S(s)] \), \( \mathcal{L}[V(s)] \), \( \mathcal{L}[E(s)] \), \( \mathcal{L}[I(s)] \), \( \mathcal{L}[T(s)] \) and \( \mathcal{L}[R(s)] \) are the Laplace transforms of the given classes \( S(t) \), \( V(t) \), \( E(t) \), \( I(t) \), \( T(t) \) and \( R(t) \) respectively.
The above system (13) can be represented by
\[
\Delta(s) = \begin{cases} 
A_1(s) = s^{a-1} S(0) \\
A_2(s) = s^{a-1} V(0) \\
A_3(s) = s^{a-1} E(0) \\
A_4(s) = s^{a-1} I(0) \\
A_5(s) = s^{a-1} T(0) \\
A_6(s) = s^{a-1} R(0)
\end{cases}
\]
where
\[
\Delta(s) = \begin{bmatrix}
s^a + \frac{1}{T}(\beta^a(I^* + \xi T^*)) + \mu^a & -w^a & 0 & \frac{\beta^a S^*}{N^*} & \frac{\beta^a S^* \xi}{N^*} & 0 \\
0 & s^a + (\mu^a + w^a) & 0 & \frac{(1-\pi)\beta^a V^*}{N^*} & \frac{(1-\pi)\beta^a V^* \xi}{N^*} & 0 \\
0 & 0 & -(s^a + (\mu^a + w^a)) & \frac{(1-\pi)\beta^a V^*}{N^*} & \frac{(1-\pi)\beta^a V^* \xi}{N^*} & 0 \\
0 & 0 & 0 & \frac{\beta^a S^*}{N^*} + \frac{e^a \beta^a R^*}{N^*} & \frac{e^a \beta^a R^* \xi}{N^*} & 0 \\
0 & 0 & 0 & 0 & \frac{\beta^a S^*}{N^*} + \frac{e^a \beta^a R^*}{N^*} & 0 \\
0 & 0 & 0 & 0 & 0 & 0
\end{bmatrix}
\]

The above given expression is a characteristic matrix of model (12). At disease-free equilibrium \(E^*\), the matrix is defined by
\[
\Delta(s) = \begin{bmatrix}
s^a + \mu^a & -w^a & 0 & \frac{\beta^a S^*}{N^*} & \frac{\beta^a S^* \xi}{N^*} & 0 \\
0 & s^a + \mu^a & 0 & \frac{(1-\pi)\beta^a V^*}{N^*} & \frac{(1-\pi)\beta^a V^* \xi}{N^*} & 0 \\
0 & 0 & s^a + \mu^a & \frac{(1-\pi)\beta^a V^*}{N^*} & \frac{(1-\pi)\beta^a V^* \xi}{N^*} & 0 \\
0 & 0 & 0 & \frac{\beta^a S^*}{N^*} + \frac{e^a \beta^a R^*}{N^*} & \frac{e^a \beta^a R^* \xi}{N^*} & 0 \\
0 & 0 & 0 & 0 & \frac{\beta^a S^*}{N^*} + \frac{e^a \beta^a R^*}{N^*} & 0 \\
0 & 0 & 0 & 0 & 0 & 0
\end{bmatrix}
\]

Now, the characteristic equation of the given Jacobian matrix is
\[
(s^a + \mu^a)(s^a + Z_1)[s^{3a} + s^{2a}(Z_4 + Z_5 + Z_2)]
\]
For simplicity, we choose
\[
CD_{0+}^\alpha S(t) = K_1(t, S, V, E, I, T, R), \\
CD_{0+}^\alpha V(t) = K_2(t, S, V, E, I, T, R), \\
CD_{0+}^\alpha E(t) = K_3(t, S, V, E, I, T, R), \\
CD_{0+}^\alpha I(t) = K_4(t, S, V, E, I, T, R), \\
CD_{0+}^\alpha R(t) = K_6(t, S, V, E, I, T, R),
\]
with initial conditions \(S(0) = S_0, \ V(0) = V_0, \ E(0) = E_0, \ I(0) = I_0, \ T(0) = T_0, \ R(0) = R_0\). Here \(K_1, \ K_2, \ K_3, \ K_4, \ K_5\) and \(K_6\) are the singular-type kernels.

Now consider the following initial value problem (IVP) for representing the model (7)
\[
CD_{0+}^\alpha X(t) = K(X(t), t), \\
X(0) = X_0,
\]
where
\[
X(t) = [S(t), V(t), E(t), I(t), T(t), R(t)], \\
X_0 = [S(0), V(0), E(0), I(0), T(0), R(0)],
\]
and
\[
K(X(t), t) = \begin{cases} 
K_1(t, S, V, E, I, T, R), \\
K_2(t, S, V, E, I, T, R), \\
K_3(t, S, V, E, I, T, R), \\
K_4(t, S, V, E, I, T, R), \\
K_5(t, S, V, E, I, T, R), \\
K_6(t, S, V, E, I, T, R),
\end{cases}
\]

Here we define the following Volterra integral equation associated to the IVP (8)
\[
X(t) = X_0 + \frac{1}{\Gamma(\alpha)} \int_0^t (t-w)^{\alpha-1} K(X(w), w) dw.
\]
We see that \(K\) is a nonlinear kernel, so let us apply the iterative scheme to establish the results. Regarding it, we define the following equation
\[
X_n(t) = X_0 + \frac{1}{\Gamma(\alpha)} \int_0^t (t-w)^{\alpha-1} K(X_{n-1}(w), w) dw.
\]
We choose \(X_0(t) = X_0\). Then two successive terms’ difference is given by
\[
X_n(t) - X_{n-1}(t) = \frac{1}{\Gamma(\alpha)} \int_0^t (t-w)^{\alpha-1} \left[ K(X_{n-1}(w), w) - K(X_{n-2}(w), w) \right] dw.
\]
For simplicity, we choose \(\zeta_n = X_n(t) - X_{n-1}(t)\). Then
\[
\zeta_n(t) = \sum_{j=0}^n \zeta_j(t).
\]
We find
\[
\|\zeta_n(t)\| = \|X_n(t) - X_{n-1}(t)\| \\
\|\zeta_n(t)\| = \left\| \frac{1}{\Gamma(\alpha)} \int_0^t (t-w)^{\alpha-1} \left[ K(X_{n-1}(w), w) - K(X_{n-2}(w), w) \right] dw \right\|.
\]
Then
\[
\|\zeta_n(t)\| \leq \frac{1}{\Gamma(\alpha)} \int_0^t (t-w)^{\alpha-1} \|K(X_{n-1}(w), w) - K(X_{n-2}(w), w)\| dw.
\]
It is required to fix \(K\) as a Lipschitzian respect to \(X\), thus
\[
\|\zeta_n(t)\| \leq \frac{L}{\Gamma(\alpha)} \int_0^t (t-w)^{\alpha-1} \|\zeta_{n-1}(w)\| dw.
\]
Therefore, the following inequality achieved
\[
\|\zeta_n(t)\| \leq \frac{L}{\Gamma(\alpha)} \int_0^t (t-w)^{\alpha-1} \|\zeta_{n-1}(w)\| dw. \tag{12}
\]

**Theorem 2** The proposed IVP (8) exists a unique solution under the contraction for \(K\).

**Proof** The following result obtained from eqn. (12)
\[
\|\zeta_n(t)\| \leq \left( \frac{L t^\alpha}{\Gamma(\alpha+1)} \right)^n \|\zeta_0(t)\|. \\
\|\zeta_n(t)\| \leq \left( \frac{L t^\alpha}{\Gamma(\alpha+1)} \right)^3 \|\zeta_0(t)\|. \\
\|\zeta_n(t)\| \leq \left( \frac{L t^\alpha}{\Gamma(\alpha+1)} \right)^n \|\zeta_0(t)\|.
\]
Then successive iterations gives
\[
\|\zeta_n(t)\| \leq \left( \frac{L t^\alpha}{\Gamma(\alpha+1)} \right)^n \|\zeta_0(t)\|.
\]
Say \(X(t) = \sum_{j=0}^n \zeta_j(t)\), then \(X(t)\) exists and continuous.

Define \(X(t) = X_n(t) + \Lambda_n(t)\), where \(\Lambda_n(t)\) is the amount of error between exact and approximate solutions with \(\Lambda_n(t) \to 0\) when \(n \to \infty\). Therefore
\[
X(t) - X_n(t) = \frac{1}{\Gamma(\alpha)} \int_0^t [K(X(t) - \Lambda_n(w), w)] dw.
\]
Now
\[
\mathcal{X}(t) - \mathcal{X}_0 - \frac{1}{\Gamma(\alpha)} \int_0^t (t - w)^{\alpha - 1} K(\mathcal{X}(w), w) dw \\
= \Lambda_n(t) + \frac{1}{\Gamma(\alpha)} \int_0^t (t - w)^{\alpha - 1} \\
[ K(\mathcal{X}(w) - \Lambda_n(w), w) - K(\mathcal{X}(w), w) ] dw.
\]

Using the norm, we get
\[
\| \mathcal{X}(t) - \mathcal{X}_0 - \frac{1}{\Gamma(\alpha)} \int_0^t (t - w)^{\alpha - 1} K(\mathcal{X}(w), w) dw \| \\
\leq \| \Lambda_n(t) \| + \frac{1}{\Gamma(\alpha)} \int_0^t (t - w)^{\alpha - 1} \\
\times \| K(\mathcal{X}(w) - \Lambda_n(w), w) - K(\mathcal{X}(w), w) \| dw \\
\leq \| \Lambda_n(t) \| + \frac{L t^\alpha}{\Gamma(\alpha + 1)} \| \Lambda_n(t) \|. 
\tag{13}
\]

If \(n\) tends to \(\infty\), the right-hand side of equation (13) converges to zero.

Then
\[
\mathcal{X}(t) = \mathcal{X}_0 + \frac{1}{\Gamma(\alpha)} \int_0^t (t - w)^{\alpha - 1} K(\mathcal{X}(w), w) dw.
\]

Therefore, it is concluded that the solution \(\mathcal{X}(t)\) exists. For the uniqueness, let us consider the two different solutions \(\mathcal{X}(t)\) and \(\mathcal{X}_1(t)\), then
\[
\| \mathcal{X}(t) - \mathcal{X}_1(t) \| \leq \frac{L t^\alpha}{\Gamma(\alpha + 1)} \| \mathcal{X}(t) - \mathcal{X}_1(t) \| \\
\leq \left( \frac{L t^\alpha}{\Gamma(\alpha + 1)} \right)^2 \| \mathcal{X}(t) - \mathcal{X}_1(t) \| \\
\vdots \\
\leq \left( \frac{L t^\alpha}{\Gamma(\alpha + 1)} \right)^n \| \mathcal{X}(t) - \mathcal{X}_1(t) \|
\]
when \(n\) tends to \(\infty\), \(L^\infty\) tends to 0, which concludes \(\mathcal{X}(t) = \mathcal{X}_1(t)\).

Hence, there exists a unique solution of the proposed IVP (8). This gives the proof of the existence of a unique solution for the fractional order model (2). \(\square\)

### 3.2.2 Parameter estimation and data fitting

As given in Sect. 3.1.1 for integer-order case, here we do the same for fractional-order model. For estimating the parameter values, we use the Adams-type Predictor–Corrector method. The data is of the yearly infectious cases of United States from the year 1989 to 2019. Again, we use the Levenberg–Marquardt algorithm with lsqcurvefit function in MATLAB. Initial population is taken as \(S(0) = 233824096, V(0) = 1000000, E(0) = 500000, I(0) = 200904, T(0) = 250000\) and \(R(0) = 50000\).

The fitting performance of the fractional-order model at \(\alpha = 0.9\) and \(\alpha = 0.8\) is given in Figs. 2 and 3, respectively. The corresponding real-data based parameter values of the fractional-order cases \(\alpha = 0.9\) and \(\alpha = 0.8\) are presented in Table 1.
4 Numerical simulations and discussions

Now, to derive the numerical solution of the given Caputo-type model (2), we use the Adams–Bashforth–Moulton method. Using the related Volterra integral equations of the proposed model classes, $\alpha \in [0, 1]$, $0 \leq t \leq T$, step size $h = T/N$, and $t_n = nh$, for $n = 0, 1, 2, \ldots, N \in \mathbb{Z}^+$, the solution of the model (2) is written as follows:

$$S_{n+1} = S_0 + \frac{h^\alpha}{\Gamma(\alpha + 2)} \left( (1 - \phi) \Lambda^\alpha - \frac{\beta^\alpha S_{n+1}^P (I^P_{n+1} + \xi T^P_{n+1})}{S^P_{n+1} + V^P_{n+1} + E^P_{n+1} + I^P_{n+1} + T^P_{n+1} + R^P_{n+1}} \right) + \frac{h^\alpha}{\Gamma(\alpha + 2)} \sum_{j=0}^{n} a_{j,n+1} \left( \frac{(1 - \phi) \Lambda^\alpha - \beta^\alpha S_j (I_j + \xi T_j)}{S_j + V_j + E_j + I_j + T_j + R_j} \right) - \mu^\alpha S_j + w^\alpha V_j), \right.$$  

$$V_{n+1} = V_0 + \frac{h^\alpha}{\Gamma(\alpha + 2)} \left( \phi \Lambda^\alpha - V^P_{n+1} (\mu^\alpha + w^\alpha) - \frac{(1 - \pi) \beta^\alpha V_j (I_j + \xi T_j)}{S_j + V_j + E_j + I_j + T_j + R_j} \right) - \mu^\alpha V_j + w^\alpha V_j), \right.$$  

$$E_{n+1} = E_0 + \frac{h^\alpha}{\Gamma(\alpha + 2)} \left( (1 - \pi) \beta^\alpha V^P_{n+1} (I^P_{n+1} + \xi T^P_{n+1}) \right) + \frac{h^\alpha}{\Gamma(\alpha + 2)} \sum_{j=0}^{n} a_{j,n+1} \left( (1 - \pi) \beta^\alpha V_j (I_j + \xi T_j) \right) - (\mu^\alpha + \sigma^\alpha) E^P_{n+1} + (1 - p) \theta^\alpha T^P_{n+1}.$$  

where

$$S^P_{n+1} = S_0 + \frac{1}{\Gamma(\alpha)} \sum_{j=0}^{n} b_{j,n+1} \left( (1 - \phi) \Lambda^\alpha - \frac{\beta^\alpha S_j (I_j + \xi T_j)}{S_j + V_j + E_j + I_j + T_j + R_j} \right) - \frac{(1 - \pi) \beta^\alpha V_j (I_j + \xi T_j)}{S_j + V_j + E_j + I_j + T_j + R_j}.$$

$$V^P_{n+1} = V_0 + \frac{1}{\Gamma(\alpha)} \sum_{j=0}^{n} b_{j,n+1} \left( \phi \Lambda^\alpha - V_j (\mu^\alpha + w^\alpha) \right).$$

$$E^P_{n+1} = E_0 + \frac{1}{\Gamma(\alpha)} \sum_{j=0}^{n} b_{j,n+1} \left( (1 - \pi) \beta^\alpha V_j (I_j + \xi T_j) \right).$$
Fig. 4 Model outputs for $\alpha = 1, 0.95, 0.9$ and $0.85$ by using the parameter values given in Column 2, Table 1.
Role of fractional derivatives in the mathematical modeling

In the above derivation, we treat our fractional order parameters, we fit the fractional-order parameter values to perform the fractional-order simulations for checking how the model behaves at various fractional orders with the inclusion of memory effects (that is what we have just done in the previous section). Here to produce more degrees of freedom in the graphical simulations and the estimation of parameters, we treat our fractional order parameter to be estimated. In this case, by using the aforementioned parameter estimation algorithms, we get the optimal value of the fractional order \( \alpha = 0.9839 \) (Column 5, Table 1). The fitting performance of the given model (2) for \( \alpha = 0.9839 \) is clearly visible in Fig. 5.

In the above derivation, \( a_{j,n+1} \) and \( b_{j,n+1} \) are given as follows:

\[
a_{j,n+1} = \begin{cases} 
\frac{n^{\alpha+1} - (n - \alpha)(1 + n)}{\alpha}, & j = 0, \\
(n + 2 - j)^{\alpha+1} - 2(n + 1 - j)^{\alpha+1} & + (n - j)^{\alpha+1} & 1 \leq j \leq n, \\
1, & j = n + 1,
\end{cases}
\]

and

\[
b_{j,n+1} = \frac{\Gamma(\alpha)}{\alpha}(n + 1 - j)^{\alpha} - (n - j)^{\alpha}, \quad 0 \leq j \leq n.
\]

4.1 Strategy A: using parameter values fitted for integer-order model

Now we check the behavior of the Chlamydia fractional-order mathematical model (2) at different fractional orders \( \alpha \) by using all the specified parameter values fitted for integer-order mathematical model (1), which are listed in the first column of Table 1.

Figure 4 illustrates the dynamics of the Chlamydia model compartments in the terms of the Caputo fractional derivative with orders \( \alpha = 1, 0.95, 0.90, \) and 0.85. In this group, Fig. 4a explains the behavior of susceptible unvaccinated individuals \( S(t) \), Fig. 4b illustrates the characteristics of susceptible individuals \( V(t) \) who have received vaccinations, and Figs. 4c and d show the dynamics of exposed humans \( E(t) \) and infected humans \( I(t) \) and Figs. 4e and f describe the nature of treated and recovered individuals \( T(t) \) and \( R(t) \), respectively. Here the time scale has been extended from \([0, 30]\) to \([0, 50]\) which actually provides the forecasting of disease for the next 20 years (because 1 unit is equal to 1 year). The fractional-order outputs justifying the memory effects in the model are clearly visible from the plots.

4.2 Strategy B: using \( \alpha \) as the optimal parameter to be estimated

Most of the time, the researchers use the same integer-order parameter values to perform the fractional-order simulations for checking how the model behaves at various fractional orders with the inclusion of memory effects (that is what we have just done in the previous section). Here to produce more degrees of freedom in the graphical simulations and the estimation of parameters, we treat our fractional order \( \alpha \) as the optimal parameter to be estimated. In this case, by using the aforementioned parameter estimation algorithms, we get the optimal value of the fractional order \( \alpha = 0.9839 \) (Column 5, Table 1). The fitting performance of the given model (2) for \( \alpha = 0.9839 \) is clearly visible in Fig. 5.
Fig. 6 Outputs of the fractional-order model for $\alpha = 0.9839$
The nature of the fractional-order model classes at $\alpha = 0.9839$ can be seen from Fig. 6. Where Fig. 6a explains the behavior of susceptible unvaccinated individuals $S(t)$, Fig. 6b illustrates the characteristics of susceptible individuals $V(t)$ who have received vaccinations, Figs. 6c and d show the dynamics of exposed peoples $E(t)$ and infected individuals $I(t)$, and Figs. 6e and f describe the nature of treated and recovered individuals $T(t)$ and $R(t)$, respectively.

From Fig. 7, we can clearly see the dynamics of the infectious class $I(t)$ in the case of integer- and fractional-order fittings. In integer-order case (Fig. 7a), the infectious peak occurs at $t \approx 34$ but for the fractional-order case (Fig. 7b), it exists at $t \approx 36$.

For more clarity in the given data fittings, we plot the curve of the infectious class $I(t)$ at optimal value of the fractional-order $\alpha = 0.9839$ by using the parameters values of the optimal value case (column 5, Table 1) and integer-order case (column 2, Table 1). Here we notice from Fig. 8, in the case of optimal-value parameters, the infectious peak occurs at $t \approx 37$ but for the integer-order value case, it exists at $t \approx 35$.

Therefore, it is clearly visible that as per the given integer- and fractional-order model fittings with the real data of the yearly infectious cases of chlamydia in the United States from the year 1989 ($t = 0$) to 2019 ($t = 30$), the duration 2023 ($t = 34$) to 2026 ($t = 37$) is the time when the spread of chlamydia will be on peak. We notice that the predictive strength of both integer- and fractional-order models is just similar but the property of capturing memory effects in a system makes the fractional order outcomes more reliable than the integer-order ones.

5 Conclusions

In this research work, we have simulated a nonlinear mathematical model of the transmission of Chlamydia in the United States by using real data from 1989 to 2019. Firstly, we represented an integer-order model and estimated the relative parameter values with the
help of some efficient fitting algorithms. Therefore, we generalized the integer model into a fractional-order form using the well-known Caputo fractional derivatives. We have simulated several figures for the various possible cases of the given parameters to explore the future outbreaks of chlamydia in the United States. The presence of fractional derivatives provided more degrees of freedom to explore the given disease dynamics. From our observations, we conclude that the time span of 2023 to 2026 will be the time when the spread of chlamydia can touch its peak. This study will be very useful for the research organizations that are working in the medical area. In the future, our real data oriented estimated parameter values can be used to forecast chlamydia outbreaks by using different models. Also, some optimal controls can be introduced in the same model by using the proposed data.

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Declarations

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