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journal homepage: www.elsevier.com/locate/camwa



Fractional models, non-locality, and complex systems

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ARTICLE INFO

Keywords: Deterministic fractional models Fractional differential equations Caputo fractional derivative Dynamical systems Population dynamics Complex processes

ABSTRACT

In this paper, a new approach to the deterministic modelling of dynamics of certain processes in an anomalous environment is proposed. To this end, the standard assumptions that are usually justified by the experiments and led to the classical dynamics models are rewritten in the way that takes into consideration the non-local features of the anomalous environment. The new class of models obtained in this way is characterized by the memory functions that have to be properly determined for a concrete process. In particular, the so-called fractional dynamics models described in terms of the fractional differential equations are among particular cases of the general model. When a concrete process is observed and its characteristics are measured within a certain time interval, the memory functions that characterize the non-locality of the medium can be found by solving an inverse problem for a system of the Volterra integral equations. Special attention is given to the population dynamics examples to highlight the advantages of the new way to focus the model of the dynamics of complex processes compared with the classical ones.

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1. Introduction

It is well known that some complex systems and processes can show anomalous behaviour that is affected by the characteristics of a medium where the processes evolve. The classical models of such processes that are formulated with the linear ordinary or partial differential equations often do not provide a good enough description of this kind of dynamics.

In the literature, the problem mentioned above is usually addressed from two different perspectives. The first one makes use of stochastic methods (for example, the CTRW – Continuous Time Radon Walk – method, see e.g. [1,2]), whereas the second one employs the nonlinear ordinary or partial differential equations. The merits of the theory and applications of the nonlinear differential equations are well known. Still, as has been shown e.g. in [3], there exist processes that cannot be described with any model involving differential equations. Other approaches are thus required. During the last decade of the twentieth century, a clear connection between the sub-diffusive anomalous processes and the so-called fractional differential equations and/or Fractional Models was established (see e.g. [1]). This relation has led to a considerable interest of several research groups working in different branches of applied sciences and engineering toward using the Fractional Models for the adequate description and simulation of the complex systems and processes observed in their domains.

Motivated by the research activities mentioned above, this paper presents an approach to characterize the influence of the complex media on the anomalous dynamics of the processes evolving in this media just by using some deterministic reasoning and without any stochastic argumentation.

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^{0898-1221/\$ –} see front matter s 2009 Elsevier Ltd. All rights reserved. doi:10.1016/j.camwa.2009.05.018

The rest of the paper is divided into two sections. In the first section, the standard assumptions that are usually justified by the experiments and led to the classical dynamics models are rewritten and interpreted in the way that takes into consideration the non-local features of the anomalous environment. These new assumptions led to a new class of models that is characterized by the so-called memory functions. In particular, the fractional dynamics models described in terms of the fractional differential equations are among particular cases of the general model. To illustrate the advantages of the new models compared with the classical ones some population dynamics examples are discussed. In particular, a nonlinear system of two fractional differential equations is considered in details from the viewpoint of the theory of the dynamical systems. In the second section, the problem of determination of a proper memory function for a concrete process is addressed. When the process is observed and its characteristics are measured within a certain time interval, the memory functions that characterize the non-locality of the medium can be found by solving an inverse problem for a system of the Volterra integral equations. One simple algorithm for solving the inverse problem is introduced and illustrated with an example.

2. Fractional dynamics models and the control of population dynamics

Population dynamics like for instance coexistence of or competition between two species or a predator-prey system are usually modelled by the systems of differential equations as

$$\frac{\mathrm{d}x}{\mathrm{d}t} = a_1 x(t),\tag{1}$$

$$\frac{dy}{dt} = a_2 y(t) \tag{2}$$

(coexistence of two species in an ideal environment without any restrictions) or

$$\frac{dx}{dt} = x(a_1 - b_1 x - c_1 y),$$
(3)
$$\frac{dy}{dt} = y(a_2 - b_2 y - c_2 x)$$
(4)

(competition between two species in an environment with restricted resources), where x, y are the population densities of two different species at the time t and a_i , b_i , c_i (i = 1, 2) are positive real constants that characterize the processes under consideration.

These models have been extensive studied in the literature as the classical examples of the linear and nonlinear dynamical systems. The hypotheses that led to the models of this kind are well known:

1. In an ideal environment, the linear behaviour of the population dynamics is established experimentally, i.e., the velocity of the populations growth is proportional to their current sizes:

$$\frac{\mathrm{d}x}{\mathrm{d}t} = a_1 x(t),\tag{5}$$

$$\frac{\mathrm{d}y}{\mathrm{d}t} = a_2 y(t). \tag{6}$$

The formulae (5)–(6) can be rewritten in the form

$$x(t) = x(0) + \int_0^t a_1 x(s) ds = x(0) + (1 * a_1 x)(t),$$
(7)

$$y(t) = y(0) + \int_0^t a_2 y(s) ds = y(0) + (1 * a_2 y)(t).$$
(8)

On the other hand, they are equivalent to

1...

$$\begin{aligned} x(t) &= d_1 e^{a_1 t}, \\ y(t) &= d_2 e^{k_2 t}, \end{aligned} (10)$$

that is, the evolution of the population densities in the time follows a classical exponential law.

- 2. In reality, the population dynamics often shows a nonlinear behaviour that is usually described by the following two hypotheses:
 - An increase of the population density x causes a fall of the population density y, and vice versa (nonlinear terms xy).
 - The population densities cannot grow infinitely because they are limited by the environment restrictions (nonlinear terms x^2 and y^2).
- 3. In some cases, the additional delay terms are taken into consideration in the models for the population dynamics to account for the non-locality of the environment.

However, in the nature there exist many processes that cannot be adequate described with the classical exponential law. For example, the dynamics of the population densities can follow a law that behaves like the exponential one but changes slowly or faster than the classical exponential function does. Of course, in a real situation, the population dynamics must be measured experimentally to establish the corresponding laws. But let us suppose that it can be described by the Mittag-Leffler function that is a well-known generalization of the exponential function. Then the hypotheses (9)-(10) can be rewritten as

$$\mathbf{x}(t) = d_1 E_\alpha(a_1 t^\alpha),\tag{11}$$

$$y(t) = d_2 E_\beta(a_2 t^\beta), \tag{12}$$

where the Mittag-Leffler function is defined as follows:

$$E_{\alpha}(z) = \sum_{k=0}^{\infty} \frac{z^k}{\Gamma(\alpha k + 1)} \quad (\alpha > 0).$$
(13)

On the other hand, the functions (11)-(12) can be interpreted as the solution of the system of the fractional differential equations

$$\begin{pmatrix} ^{C}D_{0+}^{\alpha}x \end{pmatrix}(t) = a_{1}x(t), \tag{14}$$

$$\begin{pmatrix} ^{C}D_{0+}^{\beta}y \end{pmatrix}(t) = a_{2}y(t)$$
(15)

with the initial conditions $x(0) = d_1$ and $y(0) = d_2$ (see e.g. [2] or [4]), where d_1, d_2, a_1 and a_2 are real constants and $^{C}D_{0+}^{\alpha}$, $^{C}D_{0+}^{\beta}$ are Caputo fractional derivatives of order $0 < \alpha$, $\beta < 2$, respectively. The Caputo fractional derivative is defined by

$${}^{\left({}^{C}D_{a+}^{\gamma}f\right)}(x) = {}^{\left({}^{R}L_{a+}^{n-\gamma}D^{n}f\right)}(t) dt \quad (x > a).$$
(16)

The Riemman–Liouville fractional integral ${}^{RL}I_{a+}^{\gamma}$, $\gamma > 0$ and the Riemman–Liouville fractional derivative ${}^{RL}D_{a+}^{\gamma}$ are given by

$$\binom{RL}{a+f}(x) = \frac{1}{\Gamma(\gamma)} \int_{a}^{x} (x-t)^{\alpha-1} f(t) \, \mathrm{d}t \quad (x>a),$$
(17)

$$\binom{RL}{D_{a+}^{\gamma}}f(x) = D^{n} \binom{RL}{a_{a+}^{n-\gamma}}f(x),$$
(18)

where $n - 1 < \gamma < n (n \in \mathbb{N})$, $a \in \mathbb{R}$.

The Caputo and the Riemman-Liouville fractional derivatives are connected each to other:

$${}^{C}D_{a+}^{\gamma}f)(x) = D_{a+}^{\gamma}\left[f(x) - \sum_{j=0}^{n-1} f^{(j)}(a+) \frac{(x-a)^{j}}{j!}\right].$$
(19)

In the model (14)–(15), the orders of the fractional derivatives are nothing else than the additional parameters for the control of the growth velocity of the population densities x(t) and y(t). Let us assume now that the second hypothesis mentioned at the beginning of the section holds true, too. This leads to the following fractional model

$$^{C}D_{0+}^{\alpha}x = x(a_{1} - b_{1}x - c_{1}y),$$
(20)

$${}^{C}D_{0+}^{\beta}y = y(a_{2} - b_{2}y - c_{2}x), \tag{21}$$

where a_i, b_i, c_i (i = 1, 2) are positive real constants. The parameters α, β allow us to control the velocity of the populations growth that could be very useful as a new way to better model the population dynamics of many different species in the complex media, like e.g. bacteria, virus, certain kinds of lichens populations, etc. Moreover, this kind of fractional models could be employed to characterize the dynamical systems in an anomalous environment where the system behaviour is affected by the non-locality and the memory of the media have to be taken into consideration. It is worth mentioning that the fractional model was deduced and justified by using just the deterministic reasoning and without any stochastic argumentation.

Once the fractional operators have appeared in the equations describing the population dynamics, the convolution kernels that keep memory of the process were automatically introduced into the model. Moreover, it is important to remark that these phenomena cause a change in the velocity of the trajectories of the solutions and we get the control of these changes in our model by means of a suitable choice of the parameters α , β and the initial conditions, that is, of the size of the populations at the initial time.

As an illustrative example, let us consider the following fractional dynamics system:

$${}^{C}D_{0+}^{\alpha}x = x(1-y),$$

$${}^{C}D_{0+}^{\beta}y = y(-1+x),$$
(22)
(23)

where $0 < \alpha, \beta < 2$.



Fig. 1. Plots x versus t, y versus t and y versus x, respectively, for $\alpha = 0.8$, $\beta = 1.2$ and the initial conditions $x_0 = 1.2$, $y_0 = 0.1$

This system has two isolated critical points, (0, 0) and (1, 1), which were classified in [5] by means of the analysis of the fractional quasi-linear system (22)–(23). In this paper, we are interested in showing that the parameters α and β can be used in this kind of fractional dynamical systems like the controllers that led to the new freedom degrees compared with the classical case. This allows us to apply the fractional dynamical systems to simulate the dynamics of the real anomalous processes in the complex media, as we have mentioned above. The nonlinear system (22)–(23) is studied now by taking different values for the initial conditions to observe the behaviour of the trajectories of the solutions near the critical point (1, 1) that corresponds to a centre in the ordinary case $\alpha = \beta = 1$.

For the numerical solution of the initial-value problems for the nonlinear system (22)–(23) of the fractional differential equations, the FracPECE algorithm (fractional Predict-Evaluate-Correct-Evaluate algorithm) discussed in [6] is used. Some plots produced by this method as well as their discussion are presented below.

In the Fig. 1, it can be observed that for the initial conditions taken far from the critical point (1, 1) the periodicity of the trajectories decreases with the time while the velocity of the trajectories of *x* and *y* is controlled by the value of the parameters α and β .

In the Figs. 3 and 5, the different behaviour of the trajectories near the critical point (1, 1) in the fractional and ordinary cases can be compared with each other. In the ordinary case, the point (1, 1) is a centre (Fig. 5), but in the fractional case the centre disappears and we observe an ellipse-type trajectory that tends to the critical point with the velocity controlled by the values of α and β (Fig. 3).

In the examples above, the values of α and β that satisfy the relation $\alpha + \beta = 2$ were chosen. From the analysis of the plots the following conjecture can be set up:

Conjecture 1. Let $0 < \alpha$, $\beta < 2$ with $\alpha + \beta = 2 + \varepsilon$, ε being sufficiently small. Then the trajectories of the solutions of the system (22)–(23) can move to the critical point (1, 1) as slowly as desired. Moreover, the trajectories can show a limit cycle behaviour as long time as wanted.

Furthermore, the periodicity of the trajectories has a different character depending on the initial conditions. Fig. 1 shows that when the initial conditions are taken far from the point (1, 1) then the population densities *x* and *y* decrease very fast and in a different way for both populations. However, for the initial conditions taken near to the point (1, 1) both population densities have a similar behaviour. For $\alpha = \beta = 1$ (see Fig. 5), the densities of both populations remain constant with the time that leads to a centre in the point (1, 1). For $\alpha = 0.8$, $\beta = 1.2$ (Fig. 3), the periodicity behaviour of the trajectories is slightly different compared with the above case and now we observe the spirals around the point (1, 1). Still, the velocity of the spirals that tend to the critical point can be controlled with the parameters α , β .

Figs. 2, 4 and 6 present the trajectories of the solutions *x* and *y* in their own phase spaces and allow is to observe in detail their velocities. For any initial condition taken near the point 0, the velocity of the trajectories decreases very fast (Fig. 2), because of the strong influence of the nonlinear terms *xy*. On the other hand, for the initial conditions taken near the point (1, 1), the trajectories are periodic like the ones in the ordinary case (see Fig. 6). Still, in the fractional case (see Fig. 4) a small difference in the velocities of the trajectories appears that justifies the existence of the spirals. Thus the disappearance of the centre in the fractional case is caused by the difference in the velocities of both populations that are induced by the different parameters α and β .

As to the applications of the models considered above, there exist many real situations where these fractional models can be useful. For example, the plagues (common in the oceans or in the human or animal populations) follow a complex dynamics, which cannot be properly controlled with the systems of the ordinary differential equations.

Furthermore, the same technique can be applied to the situations that currently employ the partial differential equations, i.e., to describe the sub- or super-diffusion or waves spread out in the anomalous media, like media affected by the strong magnetic fields.

However, in practice an important problem while modelling of real situations with the equations discussed above, is how to choose the suitable parameters or, in the more general case, the convolution kernels or the memory functions to better describe the behaviour of the corresponding processes.

In the following section, an approach to solve this problem is suggested.



Fig. 2. Plots x' versus x and y' versus y, respectively, for $\alpha = 0.8$, $\beta = 1.2$ and the initial conditions $x_0 = 1.2$, $y_0 = 0.1$.



Fig. 3. Plots *x* versus *t*, *y* versus *t* and *y* versus *x*, respectively, for $\alpha = 0.8$, $\beta = 1.2$ and the initial conditions $x_0 = 1$, $y_0 = 1.2$.



Fig. 4. Plots *x'* versus *x* and *y'* versus *y*, respectively. for $\alpha = 0.8$, $\beta = 1.2$ and the initial conditions $x_0 = 1$, $y_0 = 1.2$.



Fig. 5. Plots *x* versus *t*, *y* versus *t* and *y* versus *x*, respectively, for $\alpha = 1$, $\beta = 1$ and the initial conditions $x_0 = 1$, $y_0 = 1.2$.

3. Identification of the memory functions

It was shown in the previous section, that the standard model for the population dynamics

$$\frac{dx}{dt} = f_1(t, x, y),$$

$$\frac{dy}{dt} = f_2(t, x, y)$$
(24)





together with the initial conditions

$$x(0) = x_0,
 y(0) = y_0
 (27)$$

$$y(0) = y_0 \tag{27}$$

can be rewritten in the integral form

$$x(t) = x_0 + \int_0^t f_1(\tau, x(\tau), y(\tau)) \,\mathrm{d}\tau,$$
(28)

$$y(t) = y_0 + \int_0^t f_2(\tau, x(\tau), y(\tau)) \,\mathrm{d}\tau.$$
⁽²⁹⁾

Taking into account the so-called memory effects, the model (28)-(29) can be generalized to the following one:

$$x(t) = x_0 + \int_0^t M_1(t, \tau) f_1(\tau, x(\tau), y(\tau)) \,\mathrm{d}\tau,$$
(30)

$$y(t) = y_0 + \int_0^t M_2(t, \tau) f_2(\tau, x(\tau), y(\tau)) \,\mathrm{d}\tau.$$
(31)

In particular, if $M_1(t, \tau) \equiv M_2(t, \tau) \equiv 1$ then the model (30)–(31) is reduced to the standard model (28)–(29) and if

$$M_1(t,\tau) := K_1(t-\tau) = \frac{(t-\tau)^{\alpha_1-1}}{\Gamma(\alpha_1)}, \quad 0 < \alpha_1 \le 1,$$
(32)

$$M_2(t,\tau) := K_2(t-\tau) = \frac{(t-\tau)^{\alpha_2 - 1}}{\Gamma(\alpha_2)}, \quad 0 < \alpha_2 \le 1,$$
(33)

then (30)–(31) can be interpreted as a system of fractional differential equations with the Caputo derivatives of order $0 < \alpha_1, \alpha_2 \le 1$:

$$(D_0^{\alpha_1} x)(t) = f_1(t, x, y), \tag{34}$$

$$(D_0^{\alpha_2}y)(t) = f_2(t, x, y)$$
(35)

with the initial conditions

$$x(0) = x_0,$$
 (36)

$$y(0) = y_0.$$
 (37)

Remark 1. In the case $1 < \alpha_1, \alpha_2 < 2$, the system (30)–(31) can be replaced by the following one:

$$x(t) = x_0 + tx'(0) + \int_0^t M_1(t, \tau) f_1(\tau, x(\tau), y(\tau)) \,\mathrm{d}\tau,$$
(38)

$$y(t) = y_0 + ty'(0) + \int_0^t M_2(t,\tau) f_2(\tau, x(\tau), y(\tau)) \,\mathrm{d}\tau.$$
(39)

The fractional population dynamics models like (34)–(35) were already considered in the literature from the mathematical viewpoint. Unfortunately, no reasonable motivation for such models has been given until now — they were introduced just formally. In this paper, we try to attack this problem.

As we have seen, the model (34)–(35) is just a very particular case of the more general model (30)–(31). For a concrete process like e.g. the population dynamics in a complex environment, it is almost impossible to a priori establish a reasonable model in the form (30)–(31) with the concrete kernel functions. That is why our approach would be rather to try to recover the "right" kernel functions that properly characterize the process under consideration from the experimental data.

In this case, we are dealing with the so-called inverse problem: Let a solution of the system (30)-(31) be known, e.g., by experimental measurements. The problem consists then in determination of the kernel functions M_1 and M_2 . These kernels are of course specific for each concrete problem and depend on the measurements of *x* and *y*. Because one can rarely obtain the problem data exactly, the solution of the inverse problem for a system of the Volterra integral equations of the first kind with perturbed data *x*, *y* is a severely ill-posed problem.

In this paper, we suppose that the functions f_1 and f_2 from the right-hand sides of the Eqs. (30)–(31) are known and the kernels M_1 and M_2 depend on the difference of the variables t and τ (then we name them K_1 and K_2 instead of M_1 and M_2), i.e. the class of the possible models has the following form:

$$x(t) = x_0 + \int_0^1 K_1(t-\tau) f_1(\tau, x(\tau), y(\tau)) \,\mathrm{d}\tau,$$
(40)

$$y(t) = y_0 + \int_0^t K_2(t-\tau) f_2(\tau, x(\tau), y(\tau)) \,\mathrm{d}\tau.$$
(41)

Further, we suppose that the functions *x* and *y* are known from an experiment (at least in the points of a certain greed on the interval [0, T]). The problem is now to determine the unknown kernels K_1 and K_2 . In fact, both the Eqs. (40)–(41) are the Volterra integral equations of the first kind for the unknown functions K_1 and K_2 . Once the functions *x* and *y* are known (e.g. from experimental data), the Eqs. (40)–(41) are independent of each other and we can restrict ourselves to the solution of just one equation in the form

$$\phi(t) = \int_0^t K(\tau) f(t - \tau) \, \mathrm{d}\tau, \quad t \in [0, T],$$
(42)

where the functions ϕ and f are known and the function K has to be determined. To get the representation (42) from (40)–(41) the commutative property of the Laplace convolution was used.

The theory of the numerical solution of the Volterra integral equations of the first kind is well developed (see e.g. [7–10]). In this paper, we suggest an approach based on discretization and the numerical integration rules and illustrate it by an example. Here we are not interested in the best numerical method, but just in a way to demonstrate how to solve the problem.

The idea behind the numerical methods for the Volterra integral equations of the first kind based on the integration rules is quite straightforward. The integral in Eq. (42) is replaced by a numerical quadrature and then it is required that the resulting equation be satisfied exactly at a finite number of points in [0, T]. Because the exact solution of Eq. (42) can be unbounded in the neighbourhood of the point t = 0 (see e.g. the model (34)–(35) where the kernel functions have the form (32)–(33)), we employ the simple midpoint integration rule for the numerical quadrature of the integral in (40) on the greed $t_i = i * h$, i = 1, ..., N, N * h = T (for the sake of convenience, we set here $t_0 = 0$):

$$\phi(t_i) = h * (K(t_i - h/2)f(t_1 - h/2) + K(t_{i-i} - h/2)f(t_2 - h/2) + \dots + K(t_1 - h/2)f(t_i - h/2)),$$

$$i = 1, \dots, N.$$
(43)

The system (43) of the linear equations has a triangular matrix and can be easily solved step by step.

Of course, one could modify the method by applying higher order integration rules to the integral in (42). But it is well known that other methods like e.g. the trapezoidal rule result in the methods that are numerically unstable. As mentioned in [10], the midpoint method is generally the best choice for the approximate solution of the Volterra integral equation of the first kind in the presence of noise-free data. Of course, the accuracy of the midpoint method may be improved using the standard Richardson extrapolation.

Let us now discuss an example to demonstrate the approach presented above. We consider the Volterra integral equation of the first kind

$$x(t) = x_0 + \int_0^t K(\tau) f(t - \tau, x(t - \tau)) \, \mathrm{d}\tau, \quad t \in [0, T],$$
(44)

where the function *f* is given by $f(t, x) := t + x^2$ and the function *x* is known numerically from the measurements and is given in Fig. 7.

The Volterra integral equation (44) of the first kind is solved by using the discretization with the midpoint integration rule that was implemented in the computer algebra system Mathematica. The result of the kernel identification obtained with this method is presented in Fig. 8. In a real situation, no information about the kernel function *K* is available a priori, but the obtained numerical values can give a hint about a possible analytical formula. In the case under consideration the analysis of Fig. 8 suggests to fit numerical values of the kernel *K* by the potential functions in the form

$$K(t) = Ct^{\beta}.$$
(45)

Doing this, the values C = 0.810633 and $\beta = -0.270437$ are obtained. The kernel K and its fit (45) are shown in Fig. 9.



Fig. 9. Plots *K* (line) and its fit (points) versus *t*.

The values for the constants C and β we obtained by our method are very close to $C_1 = \frac{1}{\Gamma(3/4)} = 0.816049$ and $\beta_1 = \frac{3}{4} - 1 = -0.25$. Therefore, in this case the integral equation (44) could be written as the fractional differential equation:

$${}^{C}D_{0+}^{\beta}x(t) = f(t, x(t))$$
(46)

with $f(t, x(t)) = t + (x(t))^2$ and $\beta = \frac{3}{4}$. As we see, the method gives the reasonable results in the case under consideration. Other numerical experiments showed that the method becomes instable for $t_0 \rightarrow 0$ or for large time intervals [0, *T*]. The instability can be managed, for example, to some extent through the appropriate choice of the step size h that has to be made smaller and smaller. Of course, because of the accumulation of the numerical errors, the step size *h* cannot be taken arbitrary small and there exits an optimal step size *h*^{*}. Finally, we remark that in this paper our main objective was not presenting the best numerical method to solve the problem, but just an illustration that the techniques introduce above can really work to model real complex processes.

Acknowledgements

The authors want to express their deep gratitude to Professors Cesar Palencia and Eduardo Cuesta, from the University of Valladolid, for the fruitful discussion that they had with the authors on the contents of this paper. In addition, the authors would like to express their deep gratitude to MICINN of Spain Government (Project MTM2007-60246 and Scholarship FPU of master Velasco, call order 19843/2007 of 25 of October), and to Technical University of Applied Sciences of Berlin.

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