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An optimization method for the best fractional order to estimate real data analysis

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Abstract

In this paper we consider fractional differential equations, with dependence on a Caputo fractional derivative of real order. Using real experimental data of Blood Alcohol Level we obtain a system of fractional differential equations that model the problem. A numerical optimization approach based on least squares approximation is used to determine the order of the fractional operator that better describes real data as well as other related parameters. We prove that it describes better the dynamics than the classical one.

Key words: Fractional calculus, fractional differential equation, numerical optimization

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1 Introduction

We start with a review on fractional calculus, as presented in e.g. [4, 9, 10]. Fractional calculus is an extension of ordinary calculus, in a way that derivatives and integrals are defined for arbitrary real order. In a famous letter dated 1695, L'Hopital's asked to Leibniz

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what would be the derivative of order $\alpha = 1/2$, and the responde of Leibniz "An apparent paradox, from which one day useful consequences will be drawn" became the birth of fractional calculus. Along the centuries, several attempts were made to define fractional operators. For example, in 1730, using the formula

$$\frac{d^n x^m}{dx^n} = m(m-1)\dots(m-n+1)x^{m-n} = \frac{\Gamma(m+1)}{\Gamma(m-n+1)}x^{m-n},$$

Euler obtained the following expression

$$\frac{d^{1/2}x}{dx^{1/2}} = \sqrt{\frac{4x}{\pi}}.$$

Here, Γ denotes the Gamma function,

$$\Gamma(t) = \int_0^\infty s^{t-1}\mathrm{e}^{-s}\,ds, \quad t \in \mathbb{R}\setminus\mathbb{Z}_0^-,$$

which is an extension of the factorial function to real numbers. Two of the basic properties of the Gamma function are

$$\Gamma(m) = (m-1)!, \quad \text{for all } m \in \mathbb{N},$$

and

$$\Gamma(t+1) = t\Gamma(t), \quad t \in \mathbb{R}\setminus\mathbb{Z}_0^-.$$

However, the most famous and important definition is due to Riemann. Starting with Cauchy's formula

$$\int_a^t ds_1 \int_a^{s_1} ds_2 \dots \int_a^{s_{n-1}} y(s_n)\,ds_n = \frac{1}{(n-1)!}\int_a^t (t-s)^{n-1}y(s)ds,$$

Riemann defined a fractional integral type of order $\alpha > 0$ of a function $y : [a,b] \to \mathbb{R}$ as

$${}_aI_t^\alpha y(t) = \frac{1}{\Gamma(\alpha)}\int_a^t (t-s)^{\alpha-1}y(s)ds.$$

Fractional derivatives are defined using the fractional integral idea. The Riemann–Liouville fractional derivative of order $\alpha > 0$ is given by

$${}_aD_t^\alpha y(t) = \left(\frac{d}{dt}\right)^n {}_aI_t^{n-\alpha}y(t) = \frac{1}{\Gamma(n-\alpha)}\left(\frac{d}{dt}\right)^n \int_a^t (t-s)^{n-\alpha-1}y(s)ds$$

where $n \in \mathbb{N}$ is such that $\alpha \in (n-1,n)$. These definitions are probably the most important with respect to fractional operators, and until the $20th$ century the subject was relevant in pure mathematics only. Nowadays, this is an important field not only in mathematics

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but also in other sciences, engineering, economics, etc. In fact, using these more general concepts, we can describe better certain real world phenomena which are not possible using integer-order derivatives. For example, in mechanics [1], engineering [6], viscoelasticity [7], dynamical systems [11], ect. For real applications, another fractional operator, called the Caputo fractional derivative, has proven its applicability due to two reasons: the fractional derivative of a constant is zero and for initial value problems, it dependes on integer-order derivatives only. The Caputo fractional derivative of a function $y : [a, b] \to \mathbb{R}$ of order $\alpha > 0$ is defined by

$$ {}_a^C D_t^\alpha y(t) = {}_a I_t^{n-\alpha} y^{(n)}(t) = \frac{1}{\Gamma(n-\alpha)} \int_a^t (t-s)^{n-\alpha-1} y^{(n)}(s) ds, $$

where $n = [\alpha] + 1$. In particular, when $\alpha \in (0, 1)$, we obtain

$$ {}_a^C D_t^\alpha y(t) = \frac{1}{\Gamma(1-\alpha)} \int_a^t (t-s)^{-\alpha} y'(s) ds. $$

This article is organized as follows. Next section solves a real application related to Blood Alcohol Level using integer-order derivatives. Section 3 analyzes the same problem but modeled by fractional derivatives. The MATLAB numerical experiments to find the model parameters as well as the non-integer derivatives that fits better in the model are carried out in Section 4. Finally the last section presents the conclusions of this work.

2 Blood Alcohol Level problem

In [5] we find a simple model to determine the level of Blood Alcohol, described by a system of two differential equations. Let A represents the concentration of alcohol in the stomach and B the concentration of alcohol in the blood. The problem is described by the following Cauchy system:

$$ \begin{cases} A'(t) = -k_1 A(t) \\ B'(t) = k_1 A(t) - k_2 B(t) \\ A(0) = A_0 \\ B(0) = 0, \end{cases} $$

where A_0 is the initial alcohol ingested by the subject and k_1, k_2 some real constants. The solution of this system is given by the two functions

$$ A(t) = A_0 \mathrm{e}^{-k_1 t} $$

and

$$ B(t) = A_0 \frac{k_1}{k_2 - k_1} (\mathrm{e}^{-k_1 t} - \mathrm{e}^{-k_2 t}). $$

Also, in [5] some experimental data is obtained in order to determine the arbitrary constants. The Time is in minutes and the Blood Alcohol Level (BAL) in mg/l.

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Time	0	10	20	30	45	80	90	110	170
BAL	0	150	200	160	130	70	60	40	20

Using the data from the table, the values that minimize the Mean Absolute Error when the values from B are fitted with the experimental data are:

$$A_0 = 245.8769, \quad k_1 = 0.109456, \quad k_2 = 0.017727,$$

and the error is this approximation is

$$E_{classical} = 775.2225,$$

and for comparison, and get the following results:

Time	0	10	20	30	45	80	90	110	170	Error
BAL (Experiment)	0	150	200	160	130	70	60	40	20	
BAL (Model - classical)	0.0000	147.5379	172.9499	161.3813	130.0021	71.0018	59.4910	41.7418	14.4100	775.2225

3 Fractional Blood Alcohol Level problem

In this case we show that, if we consider the problem modeled by fractional derivatives, we obtain a curve that fits better in the experimental results.

Let $\alpha, \beta \in (0,2)$ and consider the system of fractional differential equations

$$\begin{cases} {}_0^C D_t^\alpha A(t) = -k_1 A(t) \\ {}_0^C D_t^\beta B(t) = k_1 A(t) - k_2 B(t) \\ A(0) = A_0 \\ B(0) = 0 \end{cases}$$

Using the formula (cf. Lemma 2.23 [4])

$${}_0^C D_t^\gamma E_\gamma(\lambda t^\gamma) = \lambda E_\gamma(\lambda t^\gamma), \quad \lambda \in \mathbb{R}, \quad \gamma > 0$$

where E_γ is the Mittag–Leffler function

$$E_\gamma(t) = \sum_{k=0}^{\infty} \frac{t^k}{\Gamma(\gamma k + 1)}, \; t \in \mathbb{R},$$

we obtain that

$$A(t) = A_0 E_\alpha(-k_1 t^\alpha)$$

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is the solution with respect to A, for any $\alpha > 0$. To determine B, it can be found as the solution of the fractional linear equation

$$ {}_0^C D_t^\beta B(t) + k_2 B(t) = k_1 A_0 E_\alpha(-k_1 t^\alpha). \tag{1} $$

First, let $\beta \in (0,1)$, and consider the α-exponential function

$$ \mathrm{e}_\alpha^{\lambda(t-a)} = (t-a)^{\alpha-1} \sum_{k=0}^{\infty} \frac{\lambda^k (t-a)^{k\alpha}}{\Gamma((k+1)\alpha)}. $$

By Theorem 5 in [2] (or Theorem 7.2 in [3]), and using the initial condition $B(0) = 0$, we get that the solution is given by

$$ B(t) = \int_0^t \mathrm{e}_\beta^{-k_2(t-s)} k_1 A_0 E_\alpha(-k_1 s^\alpha) ds. $$

We remark that, considering $\alpha, \beta \to 1^-$, the Mittag–Leffler function and the α-exponential function are simply the exponential function and thus the solutions of the fractional differential system coincide with the solutions of the ordinary system of differential equations.

Let us re-write the function B. By definition,

$$ B(t) = k_1 A_0 \sum_{n=0}^{\infty} \sum_{m=0}^{\infty} \frac{(-k_2)^n (-k_1)^m}{\Gamma((n+1)\beta)\Gamma(\alpha m + 1)} \int_0^t (t-s)^{n\beta+\beta-1} s^{m\alpha} ds. $$

Using the Beta function,

$$ B(a,b) = \int_0^1 t^{a-1}(1-t)^{b-1} dt, \quad a, b > 0, $$

the following property

$$ B(a,b) = \frac{\Gamma(a)\Gamma(b)}{\Gamma(a+b)}, $$

and doing the change of variables $u = s/t$, we obtain

$$ \int_0^t (t-s)^{n\beta+\beta-1} s^{m\alpha} ds = t^{n\beta+\beta+m\alpha} \int_0^1 (1-u)^{n\beta+\beta-1} u^{m\alpha} du $$

$$ = t^{n\beta+\beta+m\alpha} B(n\beta+\beta, m\alpha+1) = \frac{\Gamma(n\beta+\beta)\Gamma(m\alpha+1)}{\Gamma(n\beta+\beta+m\alpha+1)} t^{n\beta+\beta+m\alpha} $$

and so

$$ B(t) = k_1 A_0 \sum_{n=0}^{\infty} \sum_{m=0}^{\infty} \frac{(-k_2)^n (-k_1)^m}{\Gamma(n\beta+\beta+m\alpha+1)} t^{n\beta+\beta+m\alpha}, \quad \beta \in (0,1). $$

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Consider now $\beta \in (1,2)$. Using the relation (cf. Eq. (2.4.6) in [4])

$$ {}_0^C D_t^\beta B(t) = {}_0 D_t^\beta B(t) - \frac{B'(0)}{\Gamma(2-\beta)} t^{1-\beta}, $$

where ${}_0 D_t^\beta B(t)$ stands for the Riemann-Liouville fractional derivative of B of order β, we obtain that the fractional differential equation (1) is equivalent to

$$ {}_0 D_t^\beta B(t) + k_2 B(t) = k_1 A_0 E_\alpha(-k_1 t^\alpha) + \frac{B'(0)}{\Gamma(2-\beta)} t^{1-\beta}. $$

By Theorem 7.2 in [3], we obtain the solution with respect to B:

$$ \begin{aligned} B(t) \quad &= B'(0) \int_0^t E_\beta(-k_2 s^\beta) + \beta \frac{(t-s)^{1-\beta}}{\Gamma(2-\beta)} s^{\beta-1} E'_\beta(-k_2 s^\beta) ds \\ &+\beta k_1 A_0 \int_0^t E_\alpha(-k_1(t-s)^\alpha) s^{\beta-1} E'_\beta(-k_2 s^\beta) ds. \end{aligned} $$

With similar calculations as done before, we arrive at the expression

$$ \begin{aligned} B(t) \quad &= k_1 A_0 \sum_{n=0}^\infty \sum_{m=0}^\infty \frac{(-k_2)^n(-k_1)^m}{\Gamma(n\beta+\beta+m\alpha+1)} t^{n\beta+\beta+m\alpha} \\ &+2B'(0) \sum_{n=0}^\infty \frac{(-k_2)^n}{\Gamma(n\beta+2)} t^{n\beta+1}. \end{aligned} \tag{2} $$

Differentiating both sides of Eq. (2) and putting $t = 0$, we get $B'(0) = 0$. In conclusion, for any $\beta \in (0,2)$, the solution of the fractional differential equation is

$$ B(t) = k_1 A_0 \sum_{n=0}^\infty \sum_{m=0}^\infty \frac{(-k_2)^n(-k_1)^m}{\Gamma(n\beta+\beta+m\alpha+1)} t^{n\beta+\beta+m\alpha}. \tag{3} $$

4 Numerical experiments

The numerical experiments were done in MATLAB [8] using the routine `lsqcurvefit` that solves nonlinear data-fitting problems in least-squares sense. This routine is based on an iterative method with local convergence, *i.e.*, depending on the initial approximation to the parameters to estimate. In the computational tests the trust-region-reflective algorithm was selected. For computational purposes we consider the upper bound $n = m = 45$ in (3).

Using the available data, we obtain

$$ A_0 \approx 373.0295, \quad k_1 \approx 0.0643, \quad k_2 \approx 0.0088, $$

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with fractional orders

$$\alpha \approx 1.1771, \quad \beta \approx 1.0052,$$

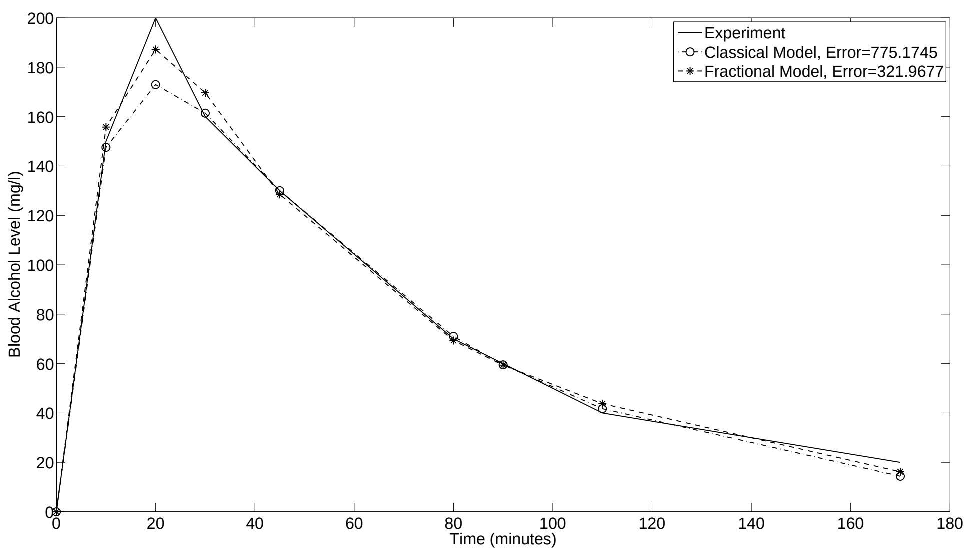
and the error in this approximation is

$$E_{fractional} \approx 321.9677.$$

In the following table we sumarize the results, comparing the standard approach, using first-order derivatives, with ours using fractional-order derivatives.

Time	0	10	20	30	45	80	90	110	170	Error
BAL (Experiment)	0	150	200	160	130	70	60	40	20	
BAL (Model - classical)	0.0000	147.5379	172.9499	161.3813	130.0021	71.0018	59.4910	41.7418	14.4100	775.1745
BAL (Model - fractional)	0.0000	155.7458	187.1950	169.6587	128.4871	69.3254	59.3669	43.7670	16.2108	321.9677

The graph of figure below illustrates the blood alcohol level with experimental data, classical model and fractional model.



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5 Conclusions

Fractional differential equations can describe better certain real world phenomena. This is understandable since systems are not usually perfect, and can be perturbed (like friction, manipulation, external forces, etc) and because of it integer-order derivatives may not be adequate to understand the trajectories of the state variables. By considering fractional derivatives, we have an infinite choices of derivative orders that we can choose, and with it determine what is the best fractional differential equation that fits better in the model. We have seen this in our experimental data, where non-integer derivatives allow the solution curve to fit better with the available data.

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