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A fractional calculus approach to the dynamic optimization of biological reactive systems. Part II: Numerical solution of fractional optimal control problems

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HIGHLIGHTS

- Fractional optimal control problems are formulated for biological reactive systems.
- Combines numerical/analytical strategies are proposed for solving FOCP.
- One approach combines optimality conditions for a FOCP and the gradient method.
- Second approach combines an NLP solver, shooting method and Laplace transformation.
- Resulting profiles show the effect of the fractional orders in the optimal results.

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ABSTRACT

This second paper of our series is concerned with the formulation and solution strategies of fractional optimal control problems (FOCP). Given the sets of fractional differential equations representing the behavior of fermentation and thermal hydrolysis reactive systems, here we formulate the corresponding FOCP's and describe suitable techniques for solving them. An analytical/numerical strategy that combines the optimality conditions and the gradient method for FOCP as well as the predictor–corrector fractional integrator is used to obtain optimal dilution rate profiles for the fermentation case-study. For the case of the thermal hydrolysis, the strategy involves discretization of the FOCP to formulate it as a Non-Linear Programming problem; then, the solution algorithm involves the use of an NLP solver and the shooting technique coupled to an inverse Laplace transformation subroutine. The optimal profiles show the performance of the numerical solution approaches proposed and the effect of the fractional orders in the optimal results.

1. Introduction

Optimal control problems (OCP) have been extensively studied in the literature. Several references and classical books provide the theoretical basis and fundamentals of this area (see for instance the books by Stengel, 1994; Sethi and Thompson, 2000; Diwekar, 2008 and the work by Poznyak, 2002).

In summary, an OCP is defined by the system of Eqs. (1)–(4):

$$\underset{u}{\text{Optimize}} \quad J=\phi(x(t_f),t_f)+\int_{t_0}^{t_f} L(x(t),u(t),t)dt \tag{1}$$

Subject to:

$$\frac{d(t)x}{dt}=f(x(t),u,t) \quad x(0)=x_0 \tag{2}$$

$$h(x,u,t)=0 \tag{3}$$

$$g(x,u,t)\le 0 \tag{4}$$

Solution techniques for an OCP involve the use of calculus of variation, dynamic programming and the maximum principle of

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Pontryagin. The use of the calculus of variations provides the optimality conditions for an OCP (also known as Euler–Lagrange equations). The optimality conditions involve a two-point boundary value problem whose solution provides the optimal profiles for the state and control variables.

1.1. A fractional optimal control problem (FOCP)

If the system dynamics of an OCP (Eq. (2)) is represented instead in terms of a set of differential equations of fractional order α,

$$ {}_0^C D_t^\alpha y(x) = f(x(t), u(t), t) \tag{5}$$

the resulting optimization problem is then a fractional optimal control problem (FOCP). Eq. (5) represents the fractional dynamics of a system in terms of the Caputo definition.

Interesting and promising applications of fractional calculus have been proposed in the area of process control (Moreau et al., 2002; Podlubny, 1999, 2002; Delavari et al., 2013), mostly related to the design and tuning of controllers. However, in the area of dynamic optimization or optimal control, the fractional calculus literature is limited. Still, recent advances propose numerical solution approaches to the solution of FOCP's. Agrawal (2002, 2004) uses calculus of variations and the formula for fractional integration by parts to derive the optimality conditions of an FOCP; the author provides the Euler–Lagrange equations for FOCP based on the Riemann–Liouville definition of a fractional derivative and developed an approximate numerical solution based on the transformation of the problem into a set of algebraic equations (by using Legendre polynomials). In later works, Agrawal (2008), Agrawal et al. (2010) also derived the optimality conditions when the Caputo definition for the fractional derivatives is used and proposed numerical solution techniques based on the Grünwald–Letnikov approximation. Numerical schemes for the solution of FOCP are also proposed in Tangpong and Agrawal (2009) and in Tricaud and Chen (2010). Tricaud and Chen (2010) solved classical FOCP's by using the Oustaloup recursive approximation to reformulate an FOCP as an OCP. These authors then used the RIOTS95 (Schwartz et al., 1997) solution algorithm for solving the resulting OCP.

1.1.1. Optimality conditions (Euler–Lagrange equations) for an FOCP (Agrawal, 2004)

The derivation of the optimality conditions for an FOCP is described in detail on the work of Agrawal (2004). The author used a simplified formulation of an FOCP as follows:

$$ \underset{u}{\text{Minimize}} \quad J(u) = \int_0^1 F(x, u, t)\, dt \tag{6}$$

subject to:

$$ {}_a D_t^\alpha\, x = G(x, u, t) \quad x(0) = x_0 \tag{7}$$

where the fractional derivative in Eq. (7) corresponds to the left hand side Riemann–Liouville definition. The goal is finding an optimal control profile $u(t)$ to minimize the integral Eq. (6); F and G are arbitrary continuous functions. Also notice that the integration limits have been set to 0 and 1 and it is further assumed that $0 < \alpha < 1$; these considerations do not affect the generalization of the derivation procedure. The derivation includes a calculus of variations approach and the formula for fractional integration by parts developed by Riewe (1996) and Samko et al. (1993). Agrawal (2004) demonstrates that the minimization of the Lagrangean objective function requires:

$$ {}_0 D_t^\alpha x = G(x, u, t) \quad x(0) = x_0 \tag{8}$$

$$ {}_t D_1^\alpha \lambda = \frac{\partial F}{\partial x} + \lambda \frac{\partial G}{\partial x} \quad \lambda(1) = 0 \tag{9}$$

and

$$ \frac{\partial F}{\partial u} + \lambda \frac{\partial G}{\partial u} = 0 \tag{10}$$

The fractional boundary value system of fractional Eqs. (8)–(10) are the Euler–Lagrange optimality conditions for FOCP's based on the left hand side Riemann–Liouville definitions for fractional derivatives. Following a similar procedure, Agrawal (2008) derived the Euler–Lagrange optimality conditions for FOCP's based on the Caputo definition for the fractional derivatives. The result of the derivations is given by Eqs. (11)–(13):

$$ {}_0^C D_t^\alpha x = G(x, u, t) \quad x(0) = x_0 \tag{11}$$

$$ {}_t^C D_1^\alpha \lambda = \frac{\partial F}{\partial x} + \lambda \frac{\partial G}{\partial x} \quad \lambda(1) = 0 \tag{12}$$

$$ \frac{\partial F}{\partial u} + \lambda \frac{\partial G}{\partial u} = 0 \tag{13}$$

If the order of the fractional derivatives, α, becomes 1, the system of Eqs. (11)–(13) reduces to the classical optimality condition equations for an OCP.

In the following sections, the fractional models developed for the biological reactive systems described in Toledo-Hernandez et al. (2014) will be reformulated as FOCP's. Then analytical/numerical solution strategies will then be proposed to solve those problems. Finally, results are presented and a final discussion is provided.

2. Case studies: Formulation of illustrative FOCP's

This section presents three illustrative examples of FOCP's. The first example is the fractional version of the classical time invariant problem (Agrawal, 2004); this case is used to test the numerical strategy that we have implemented to solve the fractional boundary value problem (optimality conditions) based on Caputo definitions for the fractional derivatives. The second and third examples correspond to the fermentation and thermal hydrolysis reactive systems described in Toledo-Hernandez et al. (2014); a performance index was incorporated to those fractional dynamic formulations, resulting in two FOCP's.

2.1. Fractional time invariant problem

The fractional version of the classical time invariant problem was proposed by Tricaud and Chen (2010) and Agrawal (2004); in those references, such formulation was approached by considering the Riemann–Liouville definition of fractional derivative. In this paper, however, we will consider the alternative approach based on the Caputo fractional derivative definition presented by Agrawal (2008).

The time invariant problem consists of finding the optimal control, $u(t)$, that minimizes the function:

$$ J(u) = \frac{1}{2} \int_0^1 [x^2(t) + u^2(t)] dt \tag{14}$$

subject to:

$$ {}_0^C D_t^\alpha x = -x + u \quad x(0) = 1 \tag{15}$$

The Hamiltonian functions for this problem is given by:

$$ \mathscr{H} = 1/2(x^2 + u^2) + \lambda(-x + u)$$

By obtaining the optimality conditions defined by Eqs. (11)–(13), the Euler–Lagrange equations for the fractional time invariant