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Initial guess of the solution of dynamic optimization of chemical processes

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Abstract

1 Introduction

Obtaining the accurate solution of optimal control problems is a crucial aspect in many areas of applied science. In this paper we shall focus especially on problems that arise in chemical engineering. There is a vast array of numerical methods and software packages for solving dynamic optimization or optimal control problems numerically, such as: SOCS, RIOTS_95, DIRCOL, MISER3, MINOPT, NDOT, DIDO, GPOCS, DYNOPT or Bryson's Matlab code. Unfortunately, these packages require an initial guess of the solution to start the iterations. Sometimes, in cases when convergence is not obtained, it is likely that the initial guess is such that convergence to the true solution is impossible. In such cases, users of these packages are accordingly advised to try different sets of initial guesses.

In this paper we shall concentrate on the special structure that appears in numerous problems of chemical reactors; more specifically, in the nonlinear Continuous Stirred Tank Reactor (CSTR). We shall present a very simple method to obtain an initial guess for the solution for this complex system. Moreover, we shall show that, for the chemical processes tested, the initial guess is very close to the solution and that our initial guess is attracted to a global minimum. We shall show that the theory allows us to address a wide range of problems: constrained, unconstrained, nondifferentiable, etc., while employing a very short computation time in all cases.

2 Mathematical Formulation

A Lagrange type Optimal Control Problem (OCP) can be formulated as follows:

$$\min_{\mathbf{u}(t)} I = \int_0^{t_f} F\left(t, \mathbf{x}(t), \mathbf{u}(t)\right) dt \tag{1}$$

subject to satisfying:

$$\dot{\mathbf{x}}(t) = f\left(t, \mathbf{x}(t), \mathbf{u}(t)\right) \tag{2}$$

$$\mathbf{x}(0) = \mathbf{x}_0 \tag{3}$$

$$\mathbf{u}(t) \in U(t),\ 0 \leq t \leq t_f \tag{4}$$

where I is the performance index, F is an objective function, $\mathbf{x} = (x_1(t), ...,x_n(t)) \in \mathbb{R}^n$ is the *state vector*, with initial conditions $\mathbf{x}_0$, $\mathbf{u} = (u_1(t), ...,u_m(t)) \in \mathbb{R}^m$ is the *control vector* bounded by $\mathbf{u}_{\min}$ and $\mathbf{u}_{\max}$, U denotes the set of admissible control values, and t is the operation time that starts from 0 and ends at t_f. The *state variables* (or simply the *states*) must satisfy the *state equation* (2) with given initial conditions (3). In this statement, we consider that the final instant is fixed and the final state is free. Let H be the Hamiltonian function associated with the problem

$$H(t, \mathbf{x}, \mathbf{u}, \lambda) = F\left(t, \mathbf{x}, \mathbf{u}\right) + \lambda \cdot f\left(t, \mathbf{x}, \mathbf{u}\right) \tag{5}$$

where $\lambda = (\lambda_1(t), ...,\lambda_n(t)) \in \mathbb{R}^n$ is called the *costate vector*. The classical approach involves the use of Pontryagin's Minimum Principle (PMP), which results in a two-point boundary value problem (TPBVP). In order for $\mathbf{u} \in U$ to be optimal, a nontrivial function λ must necessarily exist, such that for almost every $t \in [0, t_f]$

$$\dot{\mathbf{x}} = H_\lambda = f \tag{6}$$

$$\dot{\lambda} = -H_{\mathbf{x}} \tag{7}$$

$$H(t, \mathbf{x}, \mathbf{u}, \lambda) = \min_{\mathbf{v}(t) \in U} H(t, \mathbf{x}, \mathbf{v}, \lambda) \tag{8}$$

$$\mathbf{x}(0) = \mathbf{x}_0; \lambda(t_f) = \mathbf{0} \tag{9}$$

In this paper we deal with various chemical models whose dynamic equations present a particular structure (we present the two dimensional case for the sake of simplicity):

$$\min_{u_1(t)} I = \int_0^{t_f} F\left(x_1(t), x_2(t), u_1(t)\right) dt \tag{10}$$

$$\dot{x_1}(t) = f\left(x_1(t), x_2(t), u_1(t)\right) \tag{11}$$

$$\dot{x_2}(t) = f\left(x_1(t), x_2(t)\right) \tag{12}$$

The principal characteristic of this system is the absence of the control u_2 in equations (10-12). In several previous papers [1,2], the authors have presented a very simple method that is able to solve, for a known x_2, the problem formed by the equations (10-11). We now adapt this method to obtain an initial guess for the solution of the system (10-11-12).

The idea consists in constructing x_1 in an approximate and similar way to how it is constructed in [1,2] and in simultaneously constructing x_2 using Euler's (or Euler's improved) method in (12). In the discretization process, the values of x_2 obtained at the prior nodes are used to calculate x_1 at each node, and the values obtained for x_1 are used to calculate x_2. The method that we have developed to obtain x_1 is based on the use of an integral form of the Euler equation, combined with the simple shooting method. In the next section we shall see the excellent behavior of our approach by means of several examples.

3 Examples

We analyze three cases. In Example 3.1 we first consider the nonlinear CSTR as being unconstrained. In Example 3.2, we generalize the previous example, considering the constrained case with bounded control. Finally, in Example 3.3. we present a nondifferentiable case. We now present only the first case.

3.1 Unconstrained CSTR

Let us consider the system consisting of the dynamic optimization of a first-order irreversible chemical reaction carried out under non-isothermal conditions in a CSTR. The equations describing the chemical reactor are

$$\frac{dx_1}{dt} = -(2+u)(x_1+0.25) + (x_2+0.5)\exp(\frac{25x_1}{x_1+2}) \tag{13}$$

$$\frac{dx_2}{dt} = 0.5 - x_2 - (x_2+0.5)\exp(\frac{25x_1}{x_1+2}) \tag{14}$$

The control variable $u(t)$ represents the manipulation of the flow-rate of the cooling fluid. Here $x_1(t)$ represents the deviation from the dimensionless steady-state temperature, and $x_2(t)$ represents the deviation from the dimensionless steady-state concentration. In this section, we consider the case in which the control u is unbounded, and the initial conditions $x_1(0) = 0.09$ and $x_2(0) = 0.09$ are used. The optimal control problem is to determine u in the time interval $0 \leq t < t_f$ that will minimize the quadratic performance index

$$I = \int_0^{t_f} (x_1^2 + x_2^2 + 0.1u^2)dt \tag{15}$$

subject to the nonlinear dynamic constraints, where the dimensionless final time t_f is specified as 0.78.

Using a control vector iteration procedure, Luus and Cormack [3] showed that there exists a local optimum of $I = 0.244425$ and a global optimum of $I = 0.133094$. This optimal control problem provides a good test problem for optimization procedures and is a member of the list of benchmark problems [4]. It has been used by Luus [5] to evaluate his Iterative Dynamic Programming (IDP) algorithm, and by Luus and Galli [6] to examine the multiplicity of solutions. Ali et al. [7] solved this problem using eight stochastic global optimization algorithms, the results obtained varying between $I = 0.135$ and $I = 0.245$. The CPU time used was quite high, in some case more than 2382 s .

We apply our simple method and present the results below. The minimum value of $I = 0.1334$ was obtained very rapidly. The computation time for 15 iterations, with a discretization of 100 subintervals, was 2.5 s .

Our method presents numerous advantages: It is very easy to programme, the theory allows us to address a wide range of problems, the computation time is very short, the initial guess is very close to the solution, and the initial guess is attracted to

a global minimum. The resulting initial guess for the optimal control policy is given in Figure 1 and for the state trajectories in Figure 2.

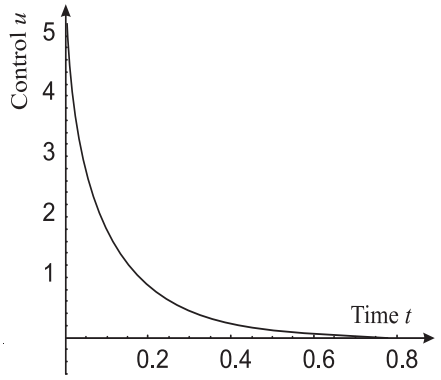

Fig. 1. Optimal control.

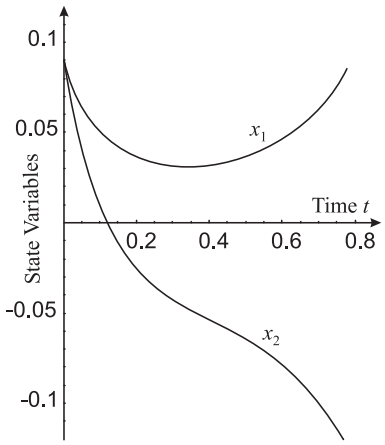

Fig. 2. Trajectories of the state variables.

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