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A pattern recognition approach to the solution of optimal singular control problems

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Abstract

A considerable number of algorithms have been proposed in the literature for the optimization of control policies of non-linear chemical systems. However, most algorithms do not seem to be flexible and robust enough for their application to be a matter of routine. Rather, each of them presents typical shortcomings that restrict applications to special classes of problems. In particular, bang–bang (or on–off) policies are difficult to optimize, due to control discontinuities.

In this paper we propose a strategy based on a combination of pattern recognition theory and non-linear mathematical programming for the computation of optimal singular control problems. © 1997 Published by Elsevier Science S.A.

Keywords: Optimal control; Singular arcs

1. Introduction

The optimization of dynamic systems with respect to one or more control variables and/or parameters has long been recognized as a fundamental problem in various areas of chemical engineering, such as batch process theory or start-up simulation.

The mathematical problem is given by the minimization of a suitable objective function

$$\Phi = J(\underline{x}_f, \underline{\theta}, t_f) + \int_0^{t_f} L(\underline{x}, \underline{\theta}, u, t)\, dt \qquad (1)$$

where $\underline{x}$ are the state variables of the system (i.e. the variables that define the system uniquely), $\underline{u}(t)$ the control variables that are to be optimized, $\underline{\theta}$ the finite dimensional vector of time independent parameters to be optimized, whereas the index f indicates values at the final time t_f.

The optimization procedure is subject to equality differential-algebraic constraints given by:

$$\frac{d\underline{x}}{dt} = \underline{f}(\underline{x}, \underline{u}, \underline{\theta}, t) \quad \underline{x}(0) = \underline{x}_0$$
$$\underline{g}(\underline{x}, \underline{u}, \underline{\theta}, t) = 0 \qquad (2)$$

which represent the dynamic behaviour of the system, to inequality constraints on the control variables of the type:

$$\underline{u}_l \le \underline{u} \le \underline{u}_p$$

which represent the physical impossibility of using a control outside a certain range, and to general inequality constraints on both control and state variables of the type:

$$\underline{h}(\underline{x}, \underline{u}, \underline{\theta}, t) \le 0 \qquad (3)$$

which eliminate mathematical solutions void of physical meaning (such as negative temperatures) or corresponding to unsatisfactory values of state variables (such as temperatures above the melting point of apparatuses).

The differential terms in system (1) are generally given by mass and/or energy balance equations and are linear in the command variables $\underline{u}$ (i.e. $\underline{f}(\underline{x}, \underline{u}, \underline{\theta}, t) = \underline{f}_1(\underline{x}, \underline{u}, \underline{\theta}, t) + \underline{u}^T \underline{f}_2(\underline{x}, \underline{u}, \underline{\theta}, t)$), which represent flow-rates or heat supplies, to which the accumulation terms are proportional.

This gives rise to a typical on–off optimal control, with the command variables taking up either the upper or the lower limit, according to whether $\underline{p}^T \underline{f}_2(\underline{x}, \underline{u}, \underline{\theta}, t)$ (which are the coefficients of $\underline{u}$ in the Hamiltonian function to be optimized with respect to $\underline{u}$ at every time, with $\underline{p}$ being the adjoint vector to be defined later in this section) is negative or positive.

A special case turns up when $\underline{p}^T \underline{f}_2(\underline{x}, \underline{u}, \underline{\theta}, t)$ is equal to zero over a certain finite interval. In these intervals, which are generally referred to as singular arcs, the control variables $\underline{u}$

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can take up values different from either the upper or the lower bound. An accurate description of the analytical theory for computing the values of $\underline{u}$ over singular arcs can be found in Aly [1].

Most numerical methods fall into one of three different classes of algorithms.

(a) Methods based on Pontryagyne's maximum principle [2].

A maximum of the Hamiltonian function

$$H = L + \underline{p}^{\mathrm{T}} \underline{f} \tag{4}$$

is searched, where the adjoint variables $\underline{p}$ are determined by the system of differential equations:

$$\dot{\underline{p}} = -\frac{\partial H}{\partial \underline{x}} \tag{5}$$

Since the values of $\underline{p}$ are available at the final time t_f, the simultaneous integration of

$$\begin{aligned} \dot{\underline{p}} &= -\frac{\partial H}{\partial \underline{x}} \\ \dot{\underline{x}} &= -\frac{\partial H}{\partial \underline{p}} \end{aligned} \tag{6}$$

give rise to a two-point boundary system of equations with considerable convergence difficulties.

Furthermore, the presence of constraints on the state variables requires the introduction of additional variables [3] which can add considerably to convergence difficulties. Finally, the simultaneous optimization with respect to the finite dimensional vector $\underline{\theta}$ can be carried out only using a two-step procedure with a prohibitive computational burden.

(b) Methods base on dynamic programming or variations of it (such as iterative dynamic programming [4] or differential dynamic programming [5]).

While very efficient at dealing with constraints on both control and state variables, this class of algorithms can encounter some difficulties in locating discontinuity points (due to the very large number of elements necessary to describe them accurately) and in the identification of time independent parameters, which has to be carried out in a two-step procedure which needs optimizing [6] for computational efficiency.

(c) Methods based on mathematical programming.

In these methods the control variables are parametrized as functions of time with unknown coefficients [7], which are then determined, along with the original parameters $\underline{\theta}$ by means of mathematical programming algorithms.

The state variables can also be parametrized. In this case the model equations are satisfied only at convergence and we have to use a general unfeasible path algorithm [8].

This class of methods is very efficient at dealing with constraints on both state and control variables. Furthermore, the presence of time-independent parameters is taken care of by simply adding them to the finite dimensional vector of the unknown time coefficients.

However, discontinuities are difficult to describe and the introduction of elements and super elements with adjustable boundaries, as proposed by Vasantharajan and Biegler [9], for locating the points at which the continuity conditions can be dropped, can lead to the determination of a large number of local minima.

The aim of this work is to describe a method that keeps the determination of optimal control policies over each time interval separate from the determination of the times at which control variables are not continuous.

The former task can be accomplished by any one of the algorithms described in (b) and (c). In this work the method proposed by Vassiliadis et al. [7] based on a feasible path successive quadratic programming algorithm has been chosen, due to its simpler implementation within the framework of the overall procedure.

The determination of discontinuities is carried out using a pattern recognition approach based on interval analysis, which will be described in the next section along with the structure of the global algorithm.

A detailed example will be examined in the final section to evaluate the robustness and efficiency of the method proposed.

2. Description of the algorithm

The first step in the overall algorithm serves the purpose of approximately locating the time intervals over which each control variable takes up the lower or the upper value or corresponds to a singular arc.

To this purpose, the entire time interval is divided into a certain number (say N_0) of elements with fixed boundaries, over which a first-order parametrization of the control variables is carried out. In other words, each command u_i is supposed piecewise constant over the entire interval. If the final time is not fixed, it is also subject to optimization.

The resulting optimization problem is:

$$\Phi = J(\underline{x}_f, \underline{\theta}, t_f) + \sum_{k=1}^{N_0} \int_{t_{k-1}}^{t_k} L(\underline{x}, \underline{\theta}, \underline{u}_k, t)\, \mathrm{d}t = \min \tag{7}$$

$$\frac{\mathrm{d}\underline{x}}{\mathrm{d}t} \overset{s.t.}{=} \underline{f}(\underline{x}, \underline{u}_k, \underline{\theta}, t) \quad t_{k-1} \le t \le t_k \tag{8}$$

$$\underline{g}(\underline{x}, \underline{u}_k, \underline{\theta}, t) = 0$$

$$\underline{u}_{l,k} \le \underline{u}_k \le \underline{u}_{p,k}$$

$$\underline{h}(\underline{x}, \underline{u}_k, \underline{\theta}, t) \le 0$$

with respect to the vector $\{\underline{\xi}\} = \{\underline{u}_k\}_{k=1,..,N_0} \oplus \{\underline{\theta}\}$.

The derivatives of both the objective function and inequality constraints (which are needed for the implementation of the minimization algorithm) require the availability of $(\partial \underline{x})/(\partial \underline{\xi})$, which can be computed by means of the sensitivity equations of system (8).

Once this problem has been solved, it is possible to locate off–on and singular arc intervals as well as the transition regions for each control variable.

To this purpose the following rules seem to work satisfactorily.

1. Locate by simple inspection the regions where the control variables attain their maximum or minimum values.
2. If the control variables are different from their upper and lower bounds over three or more consecutive intervals, regard the region defined by them as a singular arc.
3. Regard the one- or two-interval regions between maxima, minima and singular arcs as transition regions.

The optimization procedure is now repeated using a full parametrization (i.e. fourth-order Lagrangian interpolation) for the control variables over the regions where the control variables are described by singular arcs, keeping them fixed in the intervals where they had attained their lower or upper bounds, and dividing the transition regions into two equal parts, in each of which the control variables are supposed constant.

As a result of the new optimization step, each control variable in one of the two subdivisions of the transition regions will be close to its adjoining (maximum, minimum or singular arc) interval, if the discontinuity point lies in the other subdivision. Thus, merging one of the two subdivisions with its adjoining interval halves the transition region at each iteration.

An alternative strategy for the subdivision and progressive reduction of transition regions is provided by interval analysis [10].

To this purpose, let us define:

(a) the interval vectors $B_i = [\underline{B}_i, \bar{B}_i]$ such that the ith discontinuity time t_i lies in the range $\underline{B}_i \le t_i \le \bar{B}_i$;

(b) the functions

$$sign(B_i) = \begin{cases} 1 & \underline{B}_i > 0 \\ 0 & \underline{B}_i \le 0 \le \bar{B}_i \\ -1 & \bar{B}_i < 0 \end{cases}$$

$$Q(i,b) = \{\underline{t} \mid \underline{t} \in B, t_i = b\} = (B_1, B_2, ..b.., B_n) \qquad (9)$$

It has been demonstrated by Dussel [11] that in convex programming (as successive quadratic programming can be assumed to be) $f(\underline{\tau}) = \min f(\underline{t})$, $t \in Q(i,b)$ implies $sign(f_i'(\underline{\tau})) = sign(b - t_i^*)$ where t_i^* is the unknown optimal value of t_i and f_i' is the derivative of f with respect to t_i at its current value (i.e. $(\partial f)/(\partial b_i)$).

On the other hand, $f_i'(\underline{\tau})$ (i.e. $(\partial \Phi)/(\partial b_k)$), where b_k is the mid point of the current kth transition region) can easily be obtained by noting that $(\partial \underline{u}(t))/(\partial b_k) = (\underline{u}_{r,k} - \underline{u}_{l,k})\,\delta(t - b_k)$ where δ is the Dirac improper function and $\underline{u}_{rk}$ and $\underline{u}_{lk}$ are the values of $\underline{u}$ on the right and on the left of the discontinuity point b_k. Thus, knowing the value of $sign(f_i'(\underline{\tau}))$ and consequently of $sign(b - t_i^*)$ enables us to select the right or left part of the transitions regions as the one containing the sought after discontinuity point.

We can now set up the following global optimization strategy.

1. Carry out the first optimization step using piecewise constant values for the control variables and identify maxima, minima, singular arcs and transition regions.
2. Each transition region is subdivided into two equal parts.
3. Carry out a new optimization step keeping the values of control variables fixed in the regions where they have already been identified as maxima or minima, letting them vary according to a fourth-order polynomial law in the singular arcs and assuming piecewise constant values in each part of the transition regions.
4. Attach the left or the right part of each transition region to its neighbour interval according to the functional form of u over each subdivision or to the value of $sign(b - t_i^*)$ and bisect the remaining transition region.
5. If all transition regions are less than a predetermined quantity ϵ then stop, otherwise goto (3).

The presence of more than one command can be handled within the framework of the procedure described by simply applying it to all the control variables.

However in the cases examined, i.e.

(a) fed batch reactors with variable profiles of heat supplies;

(b) fed batch reactors with two time-dependent feed streams;

(c) plug–flow reactors with variable profiles of catalyst composition and heat supply;

no singular arc was detected even by using a very high number of initial intervals.

Furthermore, we have encountered, in the chemical engineering literature, no singular control in the presence of more than one command. While this can be the result of a failure in locating the global optimal profile, it is more likely to be due to the more stringent theoretical conditions required for the presence of singular arcs in multicontrol processes. A complete description can be found by Goh [12]. Let us briefly mention here the main difference to the single control optimization.

The presence of a singular arc in the jth control variables implies that its coefficient $K_j(t)$ in the Hamiltonian function is zero, along with its first time derivative $\dot{K}_j(t)$. The equation resulting from setting the second time derivative $\ddot{K}_j(t)$ to zero provides the unknown value of the singular control, provided it contains it explicitly and satisfies the Legendre–Clebsch condition

$$\frac{\partial[\ddot{K}_j(t)]}{\partial u_j} \ge 0$$

In the case of a single control process, both $K_j(t)$ and $\dot{K}_j(t)$ do not depend on any control variable. This makes the conditions for a singular arc less stringent, because the absence of control variables allows us to neglect the requirement that the Hamiltonian be at an optimum with respect to them.

Admittedly, the question whether, in spite of these more stringent conditions and the difficulties of numerically locating them, singular arcs do exist in various chemical engineering problems, where they have not yet been detected, is open.

The initial number of intervals does not affect the robustness and the efficiency of the procedure, provided it is sufficiently large. In all the cases examined we have used 36 intervals, which has turned out to be the most effective choice for control profiles with one singular arc and one or two bang–bang intervals, which is a very frequent situation when there are linear control variables. The number of iterations necessary to reduce the width of transition regions to 10^{-k} times the original value is:

$$k \ln_2 10 = 3.322\, k$$

Thus the order of magnitude of the iterations is typically ~ 10.

This increased computational burden is approximately offset by the reduced effort in each optimization step, due to the lower number of independent variables with respect to which each optimization step is actually carried out.

In the next section a numerical example will illustrate efficiency and robustness of the method described.

3. A numerical example

To illustrate the method described we have considered the problem of evaluating the optimal control of a fed-batch reactor. This kind of problem is generally considered difficult to solve numerically, due to the presence of bang–bang control policies. However, there are a few cases that can be solved analytically or semi-analytically [13]. One of these is the biosynthesis of penicillin which can be described by the following system of differential equations:

$$\frac{dX}{dt} = \mu(X,S)X - \left(\frac{X}{S_F V}\right)U \quad X(0) = 1.5$$

$$\frac{dP}{dt} = \rho(S)X - K_{deg}P - \left(\frac{P}{S_F V}\right)U \quad P(0) = 0$$

$$\frac{dS}{dt} = \mu(X,S)\left(\frac{X}{Y_{X/S}}\right) - \rho(S)\left(\frac{X}{Y_{P/S}}\right) - \left(\frac{m_s S}{K_m + S}\right)X + (1 - S/S_F)\frac{U}{V} \quad S(0) = 0$$

$$\frac{dV}{dt} = \frac{U}{S_F}$$

$$\mu(X,S) = \mu_{max}\left(\frac{S}{K_x X + S}\right)$$

$$\rho(S) = \rho_{max}\left(\frac{S}{K_p + S(1 + S/K_{in})}\right) \qquad (10)$$

$0 \le X(t) \le 40$, $0 \le S(t) \le 100$, $0 \le V(t) \le 10$, $0 \le U(t) \le 50$, $72 \le t_f \le 200$.where X is the biomass contained in the reactor, S the substrate, P the product, V the volume and U the feedrate of substrate. The constants present in the equations have been assigned the values provided in [14].

The final amount of product is the sought-after objective function to be maximized, i.e.

$$\max_{(t),t_f} \Phi = P(t_f)V(t_f)$$

The semianalytical solution by Lim et al. [13] predicts the correct shape of the control profile (one maximum interval, one minimum interval and one singular arc), whereas switching times are to be computed by trial and error. Their results, after some correction so as to take account of different values assigned to the variables, are reported in Table 1, whereas those obtained by Cuthrell and Biegler [14] are reported in Table 2.

The method described in this paper was also applied to the solution of this problem. To this purpose the whole range was initially divided into 36 time intervals. The first iteration provided the optimal piecewise constant control, using a starting value of 10 for the control over the entire time range. The relevant parameters are reported in Table 3. As can be noted, the objective function is higher than that provided by the semi-analytical approach, but it is still lower than that obtained by Cuthrell and Biegler.

Similarly, the results obtained in the second iteration are reported in Table 4. The objective function is now very close to the value obtained by Cuthrell and Biegler and it keeps going down very slowly as the widths of the transition regions

Table 1
Semianalytical solution

Objective function	87.08
1st switching time	11.21 (h)
2nd switching time	28.79 (h)
Final time	124.9 (h)

Table 2
Numerical solution provided by the unfeasible path mathematical programming algorithm

Objective function	87.77
1st superelement boundary	11.46 (h)
2nd superelement boundary	29.29 (h)
Final time	128.29 (h)

Table 3
Results after the first iteration (this work)

Objective function	87.11
1st switching time	10.5 (h)
Width of 1st transition region	3.5 (h)
2nd switching time	24.5 (h)
Width of 2nd transition region	7.0 (h)
Final time	128.29 (h)

Table 4
Results after the second iteration (this work)

Objective function	87.63
1st switching time	10.5 (h)
Width of 1st transition region	1.75 (h)
2nd switching time	28.0 (h)
Width of 2nd transition region	3.5 (h)
Final time	129.2 (h)

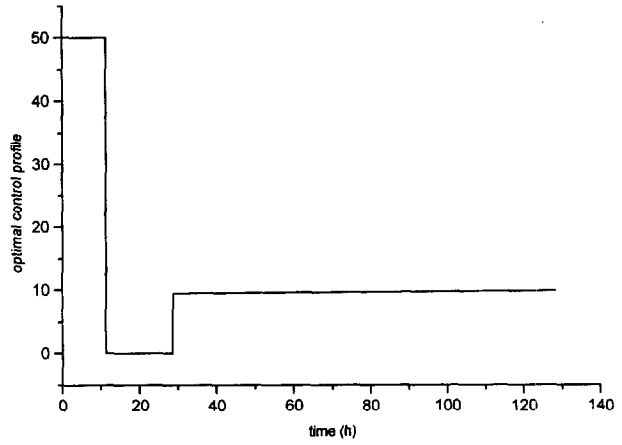

Fig. 1. Optimal feedrate of substrate.

Table 5
Final results (this work)

Objective function	87.84
1st switching time	11.3 (h)
2nd switching time	28.6 (h)
Final time	128.7 (h)

are reduced. The final control profile (corresponding to widths inferior to 10^{-3}) is plotted in Fig. 1 and the relevant parameters are reported in Table 5. The shape of the profile obtained is very close to that predicted semi-analytically, except for the slope of the singular arc which is now close to zero. As can be seen, the objective function is now slightly better than that obtained by Cuthrell and Biegler, although their control profile is not bang–bang. This seems to confirm their assumption about the objective function being flat in the vicinity of the optimal solution. On the other hand this makes the numerical determination of the correct profile by traditional non-linear techniques difficult. Hence the convenience of using algorithms that select the functional form of control profiles non-uniquely by means of numerical methods.

4. Conclusions

The pattern recognition approach to the determination of optimal control seems to provide a convenient algorithm in those cases in which the shape of the control profile, due to the presence of discontinuities, is difficult to obtain by numerical methods alone.

While the number of iterations necessary to attain the convergence is decidedly higher (typically ten times as high, as discussed previously), each of them is considerably more efficient due to the starting points getting closer and closer to the final optimal solution. Thus the increased price in the computational burden is typically four to five times the amount required by other methods. This price seems, in these times of cheap computational power, a modest one.

5. Notation

b	mid-point of transition region
B	interval element
f	differential state equations
g	algebraic state equations
h	inequality constraints
H	Hamiltonian
J	term of objective function that depends on final values
K_{deg}	kinetic constant ($0.01\ h^{-1}$)
K_{in}	kinetic constant ($0.1\ g\ S\ l^{-1}$)
K_m	kinetic constant ($0.0001\ g\ S\ l^{-1}$)
K_p	kinetic constant ($0.0001\ g\ S\ l^{-1}$)
K_x	kinetic constant ($0.006\ g\ S\ g^{-1}\ X$)
L	integrand function of objective function
m_s	kinetic constant ($0.029\ g\ S\ g^{-1}\ X\ h^{-1}$)
N_0	initial number of subintervals
p	adjoint variables
P	product ($g\ l^{-1}$)
Q	function defined by Eq. (9)
S	substrate ($g\ l^{-1}$)
t	time
u	control variable
U	feed rate
V	reactor volume l
x	state variables
X	feed rate ($g\ h^{-1}$)
$Y_{P/S}$	kinetic constant ($1.2\ g\ X\ g^{-1}\ s$)
$Y_{X/S}$	kinetic constant ($0.47\ g\ X\ g^{-1}\ s$)

Greek symbols

δ	Dirac's function
ξ	extended set of parameters
θ	parameters
μ	growth rate of biomass (h^{-1})
ρ	production rate of penicillin ($g\ P\ g-1\ X\ h^{-1}$)
Φ	objective function

Subscripts

f	related to final time
F	related to feed conditions
l	related to lower bound
p	related to upper bound
0	related to initial conditions

Superscripts

*	related to optimal conditions
·	time derivative

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