

Detection and exploitation of the control switching structure in the solution of dynamic optimization problems

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Abstract

In this paper we present a novel method for the numerical solution of dynamic optimization problems. After obtaining a first solution at a coarse resolution of the control profiles with a direct sequential approach, the structure of the control profiles is analyzed for possible switching times and arcs. Subsequently, the problem is reformulated automatically and solved as a multi-stage problem, with each stage corresponding to a potential arc. Order and resolution of the control parameterization are adapted to the type of the particular arc. By means of some case studies we show that accurate solutions with only few degrees of freedom can be obtained.

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1. Introduction

The optimization of the operation of batch processes or transient phases in continuous processes for either off-line or on-line applications requires the solution of dynamic optimization problems. It is still a challenge to obtain a high-quality solution for such problems efficiently, especially when the problem formulation contains large-scale models, e.g., those stemming from industrial applications. However, even for problems with just small models where the computation time is not an issue, the solution quality, which can be obtained by numerical methods, is not always satisfactory.

One important reason for this fact is that the analytical solution of a dynamic optimization problem consists of one or more intervals, the so-called *arcs* [3]. The control variables to be optimized are continuous and differentiable within each interval, but can jump from one interval to the next at the so-called *switching times*. This

inherent discontinuous nature of optimal control profiles may pose problems to numerical solution methods, because the quality of the solution depends on the chosen parameterization order and resolution of the control variables. The solution quality can be insufficient if the parameterization does not properly reflect the switching structure. This is illustrated in Fig. 1. It shows the result of a dynamic optimization problem (which will be discussed in more detail in Section 6) for three different choices for the control parameterization.

Obviously, the control profiles are not the same, although they are supposed to be the solution of the same original problem. Nevertheless, the principle shape of the solution, the solution structure in terms of arcs, is the same in all three cases. However, the sequence and nature of the arcs is typically not known beforehand.

In practice, these problems are usually dealt with by either accepting the often limited accuracy of the numerical solution, or by trying to interpret and to subsequently improve the solution manually. The latter approach typically involves human interaction such as visual inspection of the numerical solution for finding the type and sequence of the arcs and often also requires

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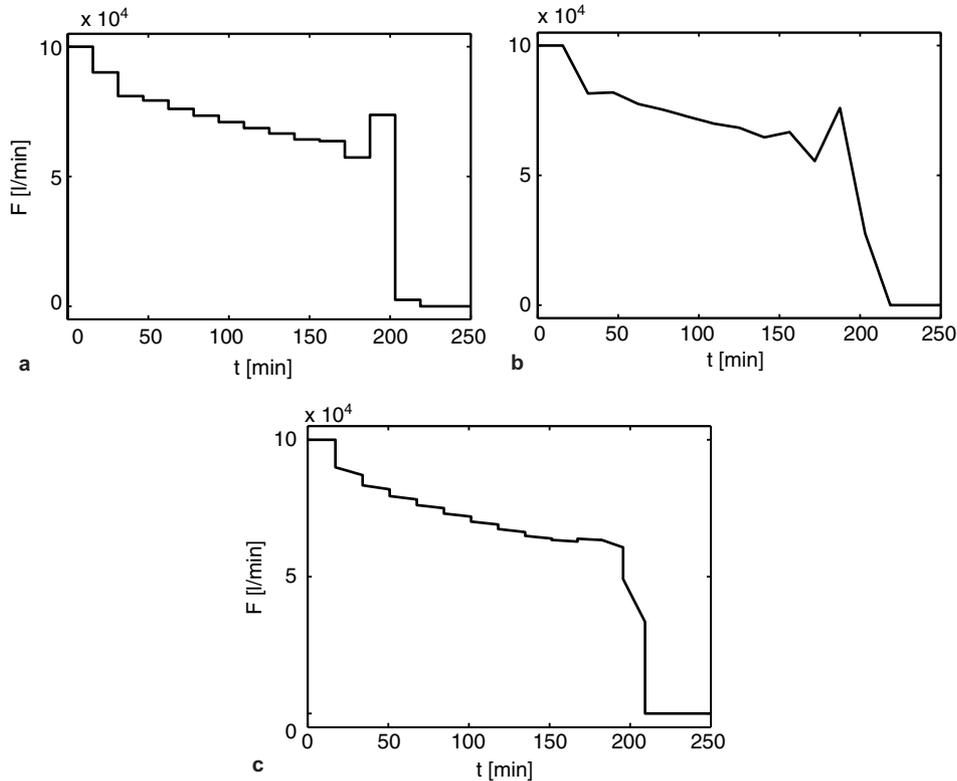


Fig. 1. Solution profiles for 16 intervals with different approximation orders: (a) equidistant piecewise constant, (b) equidistant piecewise linear, and (c) piecewise linear with free interval length.

the use of physical insight [20]. Adaptive refinement of the control profile discretization [19] can lead to solutions with higher accuracy at a lower computational expense, but the switching structure is not considered explicitly.

A characterization of such nominal solution structures and a survey of various numerical solution methods for dynamic optimization problems has been presented by Srinivasan et al. [20] in the context of batch and semi-batch process optimization. In this class of processes, discontinuous control profiles can be found quite often. For example, the optimal feed rate of a semi-batch reactor may be first at its upper operational limit and later jump to the lower bound or some intermediate value, if some constrained process variables such as the reactor volume reach their specific limits.

To the authors' knowledge there has been only one previous attempt to try to determine the sequence of arcs in the solution structure automatically. Winderl and Büskens [23] mention an algorithm for this purpose, though no details are presented. Some solution methods like the one of Vassiliadis et al. [21] allow free interval lengths for control profile discretization, but the switching structure is not explicitly considered there, either.

In this paper, we present the combination of a direct sequential solution approach for dynamic optimization

with an automatic structure detection method. This procedure allows to solve a problem with a control variable parameterization specifically tailored to reflect the sequence and nature of the different arcs. It results in a high solution quality involving only relatively few degrees of freedom. This is accomplished by an automatic reformulation and subsequent solution of the problem as a *multi-stage problem*, where each stage corresponds to an arc of the solution structure as determined by the detection algorithm.

The paper is organized as follows: After a description of some fundamentals (Section 2) and the numerical solution technique employed (Section 3), we will present a detailed description of the proposed structure detection and reparameterization method in Section 4. Some technical details are presented in Section 5. In Section 6, two numerical case studies will be presented, before we conclude the paper in Section 7.

2. Preliminaries

2.1. Problem formulation

The general formulation of a dynamic optimization problem used in this paper reads as

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