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Exploitation of the control switching structure in multi-stage optimal control problems by adaptive shooting methods

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ABSTRACT

The adaptive switching structure approach is generalized from single-stage problems and single-shooting to multi-stage problems and multiple-shooting. This generalization is based on previous work on the exploitation and detection of the control switching structure and wavelet-based control grid refinement for single-stage problems. Here, single-shooting is employed to transcribe the multi-stage optimal control problem (OCP) into a nonlinear programming problem. The proposed multi-stage formulation is also capable to represent the transcription of single-stage OCP stemming from multiple-shooting. Thus, the previously reported adaptive multiple-shooting approach is extended by an adaptation of the switching structure. Finally, a new stopping criterion is introduced that measures the intermediate constraint violation at the optimal solution.

The proposed adaptive switching structure detection is illustrated for a multi-stage and a multiple-shooting problem using the Williams–Otto semi-batch reactor. A solution of user-specified accuracy in the objective and the path-constraints can be obtained using only few decision variables.

1. Introduction

The optimal operation of chemical processes often requires the solution of multi-stage control problems. The scientific and industrial interest in multi-stage optimal control problems (OCP) has been increasing steadily in process systems engineering (Barton and Pantelides, 1994; Vassiliadis et al., 1994a,b; Avraam et al., 1998; Bonvin, 1998; Biegler and Grossmann, 2004). Generally, multi-stage OCP can be divided into two classes. The first class assumes that the number of stages the system goes through is unknown, while the second class requires a priori knowledge of the number and type of stages (Avraam et al., 1998). The first class often consists of multiple stages, where each stages is described by a different DAE system. The stages are connected by state transitions, which are triggered by some logical constraint. These systems are also referred to as non-smooth systems.[1] Typically, the non-smooth systems of interest are continuous in the state but with discontinuous right-hand side. These systems are modeled using if-else-clauses in the modeling environments. Technical examples for non-smooth systems include the model of a reactive three-phase batch distillation column by Brüggemann et al. (2004) or just the model of a bouncing ball (Hannemann-Tamás et al., 2014).

Typical examples of the second class of multi-stage problems include the operation of batch and semi-batch reactors, which rely on recipe-driven operation (Bonvin, 1998). Recipes are subdivided hierarchically into process stages, process operations and process actions (ISA, 2010). These operational modes usually result in a planned sequence of chemical or physical changes of the state of material being processed. Thus, a batch process normally comprises various stages, e.g., a batch reactor is first cleaned, then charged, the reaction is enabled, and the reactor is finally drained. Depending on the process, the reaction can be further subdivided into additional stages, e.g., adding catalyst and reactants separately, withdrawing material, heating and cooling (Bonvin, 1998). Thus, industrial semi-batch processes always result in multi-stage OCPs with a known number of stages. An example of particular industrial interest is the optimal control of (fed-batch) bioreactors (Balsa-Canto et al., 2000; Ramkrishna, 2003), which are used to manufacture specialty chemicals, pharmaceuticals, and bio-chemicals. Even continuous processes can experience transient operational stages (Barton and Pantelides, 1994) such as multiple grade changes. Further, chemical processes may include different modes of operation requiring different process models (e.g., adsorption, regeneration, pressurization, in a dynamic cycle (Nilchan and Pantelides, 1998)). For

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[1] For a detailed classification of non-smooth systems the reader is referred to the work of Leine and Nijmeijer (2004).

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these applications, each stage is described by separate state variables and models, which are linked by incorporating transitions between those dynamic stages (Biegler and Grossmann, 2004). A multi-stage OCP may also arise in a control context, e.g., if an infinite horizon problem is formulated (Würth and Marquardt, 2014).

This paper deals with the formulation and optimization of multi-stage OCPs arising in process engineering with a known number of stages. The case of state transition networks is not discussed in this work, however; the algorithm presented could be also generalized for this particular case. The formulation of a multi-stage OCP with a given number of stages requires setting up a sequence of operational modes (e.g. process stages, process operations and process actions) with a varying set of controls, objectives, constraints, and even model equations with complicated state transitions between the stages. Here, the stages of a multi-stage OCP are defined as either *physical stages*, which are either enforced by state transition networks of the underlying nonlinear process, or by *algorithmic stages*, which are due to the formulation of the OCP (Schlegel and Marquardt, 2006a). To the best of author's knowledge, multi-stage OCP in the literature consists of either *physical* or *numerical stages*. In this work, a generalized formulation that simultaneously comprises both *physical* and *numerical stages* is presented which results in a nested multi-stage problem.

Typically, multi-stage OCPs are solved after approximating the continuous problem by a finite-dimensional optimization problem by some kind of transcription. The control profiles are typically parameterized uniformly relying on a pragmatically chosen grid. However, it is important to note that in such an approach the computed solution may not properly resolve the qualitative structure of the optimal control profile (switching structure), which is determined by a series of (continuous) arcs delimited by discontinuous jumps (Bryson and Ho, 1975). Localizing the switching points between continuous arcs exactly not only improves the solution accuracy but, more importantly, increases process insight. For example, this insight allows applying NCO (necessary conditions of optimality) tracking control (Srinivasan et al., 2003a) only using the solution structure determined by off-line optimization (Kadam et al., 2007). A straightforward approach allows to optimize the location of the grid points for a fixed number of control intervals. Cuthrell and Biegler (1987) and von Stryk (1995) have applied this idea in the context of full discretization methods. Vassiliadis et al. (1994a) have used a similar concept, but apply it in the context of single shooting. The major drawback of such relocation methods is that the resulting nonlinear programming problem (NLP) tends to be strongly nonlinear and tough to solve. In particular, even a linear optimal control problem results in an NLP after parameterization if relocation methods are used. This drawback can be compensated by introducing a bi-level approach, where the optimization is solved on a fixed grid in an inner loop, while the lengths of the discretization intervals are determined in an outer loop (Tanartkit and Biegler, 1997).

To the best of authors' knowledge, multi-stage OCPs cannot be tackled directly by commercial software packages (e.g. gPROMS,[2] Aspen Custom Modeler[3]).

In this paper, we generalize the adaptive switching structure approach introduced by Schlegel and Marquardt (2006b) for single-stage to multi-stage problems. This generalization is based on previous work on the exploitation and detection of the control switching structure (Schlegel and Marquardt, 2006a) and wavelet-based control grid refinement (Schlegel et al., 2005) for single-stage problems. Here, we employ direct single-shooting (Sargent and Sullivan, 1978) to transcribe the continuous dynamic multi-stage OCP into an NLP. Further, the proposed multi-stage formulation is capable to represent the transcription of a single-stage OCP into an NLP by multiple-shooting[4] (Morrison et al., 1962; Bock and Plitt, 1984). Thus, we also extend the adaptive multiple-shooting approach introduced by Assassa and Marquardt (2014) by the adaptive switching structure approach in this paper. Further, we introduce a new measure to evaluate the intermediate constraint violation (ICV), which can be used as a stopping criterion for both refinement approaches.

The adaptive switching structure approach of Schlegel and Marquardt (2006b) generalized to multi-stage and multiple-shooting problems comprises two steps: first, a problem-dependent discretization is generated using the wavelet-based control grid refinement (Schlegel et al., 2005; Assassa and Marquardt, 2014) to avoid an unnecessarily fine control grid. The iterative refinement procedure is terminated if the detected control switching structure for all stages remains unchanged in two consecutive iterations. In the second step, the multi-stage problem is reformulated to incorporate the detected switching structure (Schlegel and Marquardt, 2006a) by introducing a second layer of stages, the so-called *algorithmic stages*. In particular, every *physical stage* is subdivided by some *algorithmic stages*. Each *algorithmic stage* has the same type of controls, objective, constraints and model as its associated *physical stage*. These *algorithmic stages* allow to capture the control switching structure behavior with only few optimization parameters combining control grid adaptation and switching structure detection. The control grid of the reformulated problem is again refined using wavelet-based grid refinement until a satisfactory solution quality is obtained. The stopping criterion either relies on a measure of the ICV and/or a change in the objective function. A change in the switching structure leads to a reformulation of the underlying problem with subsequent control grid refinement.

We illustrate adaptive control grid refinement and adaptive switching structure detection for a multi-stage problem and a multiple-shooting strategy using the Williams–Otto semi-batch reactor (Williams and Otto, 1960). The proposed algorithm successfully detects the control switching structure in both cases. A solution of user-specified accuracy in the objective and the path-constraints can be obtained using only few decision variables.

The paper is structured as follows. Section 2 first introduces the multi-stage problem formulation and the necessary conditions of optimality. The theoretical background of the suggested approach and the applied solution method are presented in Section 3. It concludes with a summary of the unified automatic structure detection approach. In Section 4, we give an overview on the solvers used and the implementation of the optimization strategy. Section 5 introduces an exemplary multi-stage and single-stage problem of the Williams–Otto semi-batch reactor. The multi-stage problem is solved using single-shooting, while the single-stage problem is discretized by the multiple-shooting strategy. Both examples are analyzed and compared to an equidistant discretization of the controls with respect to performance and solution accuracy. Finally, in Section 6, we conclude the paper with a summary and future perspectives.

2. Problem formulation

First, the multi-stage OCP is formulated and generalized by introducing a second level of stages, so-called *algorithmic stages*. Second, the theoretical framework to reformulate the multi-stage

[2] http://www.psenterprise.org/.
[3] http://www.aspentech.org/.

[4] Multiple-shooting explicitly addresses OCP problems embedding unstable initial value problems, which often cannot be solved successfully by single-shooting.