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GLOBAL SOLUTION OF MIXED-INTEGER DYNAMIC OPTIMIZATION PROBLEMS

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Abstract — This paper presents a decomposition approach for a quite general class of mixed-integer dynamic optimization problems that is capable of guaranteeing the global solution despite the nonconvexities inherent to the dynamic optimization subproblems. A case study is presented in connection to the optimal design and operation of a batch process consisting of a series reaction followed by a separation with no intermediate storage. The developed algorithms demonstrate efficiency and applicability in solving this problem.

Key words: mixed-integer dynamic optimization, global optimization, batch process design

1 Introduction

Recent advances in process synthesis, design, operations and control have created an increasing demand for efficient numerical algorithms capable of optimizing a dynamic system coupled with discrete decisions; these problems are termed Mixed-Integer Dynamic Optimization (MIDO). Areas of application for MIDO include batch process synthesis and development, design of batch distillation columns, solvent design in batch processes, simultaneous design and control, and optimization of hybrid discrete/continuous systems.

In contrast to dynamic optimization problems, for which direct solution methods (including global dynamic optimization methods) are capable of solving a broad class of problems, only limited progress has been made in addressing MIDO problems. In particular, no general procedure has yet been proposed that guarantees convergence to the global solution of MIDO problems.

In this contribution, building upon recent developments in both deterministic global optimization for Mixed-Integer NonLinear Programs (MINLPs) and relaxation techniques for optimization problems with ODEs embedded, we develop a decomposition approach for a quite general class of MIDO problems that is capable of guaranteeing the global solution despite the nonconvexities inherent to the dynamic optimization subproblems, while still potentially avoiding total enumeration of the discrete alternatives.

2 Theoretical Background

Let $P = \left[\mathbf{p}^L, \mathbf{p}^U\right] \subset \mathbb{R}^{n_p}$, $Y = \{0,1\}^{n_y}$ and $X \subseteq \mathbb{R}^{n_x}$ be such that $\mathbf{x}(\mathbf{p},\mathbf{y},t) \in X$, $\forall (\mathbf{p},\mathbf{y},t) \in P \times Y \times [t_0, t_f]$. We consider the class of MIDO problems that conform to the following formulation:

$$
\begin{array}{rrcl}
 & \displaystyle\min_{\mathbf{p},\mathbf{y}} \mathcal{J} & = & \phi_0\left(\mathbf{x}\left(\mathbf{p},\mathbf{y},t_f\right),\mathbf{p},\mathbf{y}\right) + \displaystyle\int_{t_0}^{t_f} \psi_0\left(\mathbf{x}\left(\mathbf{p},\mathbf{y},t\right),\mathbf{p},\mathbf{y},t\right) dt \\
\text{s.t.} & 0 & \geq & \phi_k\left(\mathbf{x}\left(\mathbf{p},\mathbf{y},t_f\right),\mathbf{p},\mathbf{y}\right) + \displaystyle\int_{t_0}^{t_f} \psi_k\left(\mathbf{x}\left(\mathbf{p},\mathbf{y},t\right),\mathbf{p},\mathbf{y},t\right) dt \ , \ k = 1,\ldots,n_c \\
 & \dot{\mathbf{x}}\left(\mathbf{p},\mathbf{y},t\right) & = & \mathbf{f}\left(\mathbf{x}\left(\mathbf{p},\mathbf{y},t\right),\mathbf{p},\mathbf{y},t\right) \ , \ \forall t \in [t_0, t_f] \\
 & \mathbf{x}\left(\mathbf{p},\mathbf{y},t_0\right) & = & \mathbf{h}\left(\mathbf{p},\mathbf{y}\right) \\
 & \mathbf{p} & \in & P \\
 & \mathbf{y} & \in & Y
\end{array}
\qquad \text{(P)}
$$

where $\mathbf{p}$ denotes the continuous time-invariant parameters; $\mathbf{y}$ is a special set of time invariant parameters that can only take $0-1$ values; t_0 and t_f denote the initial and final time, respectively; $\mathbf{x}$ are the continuous variables describing the state of the process. Also note that in this formulation, ϕ_k and ψ_k, $k = 0,\ldots,n_c$ are potentially nonconvex mappings.

The methodology adopted to solve MIDO problems as specified in (P) to guaranteed global optimality consists of extending the outer approximation algorithms originally developed by Kesavan and co-workers [1, 2] for nonconvex MINLPs. Two distinct algorithms are considered. On finite termination, the first algorithm guarantees finding the global solution of (P) within finite tolerance, while the second algorithm finds rigorous bounds bracketing the global solution of (P) (and a potentially suboptimal solution). The advantage of the second algorithm is a substantial reduction in computational expense as will be illustrated by the case study. These algorithms are both based on construction of the following subproblems:

- **Primal problem:** a nonconvex dynamic optimization problem obtained by fixing the binary variables $\mathbf{y}$ in (P), any feasible solution of which yields a rigorous upper bound to the solution of MIDO problem (P),

- **Lower Bounding Convex MIDO problem:** a convex MIDO problem, the solution of which yields a valid lower bound to the global solution of problem (P),

- **Relaxed Master problem:** a MILP, the solution of which represents a valid lower bound on that subset of Y not yet explored by the algorithm,

- **Primal Bounding problem:** a convex dynamic optimization problem, the solution of which provides a valid and tighter lower bound to the Primal problem for each fixed binary realization $\mathbf{y}$ than that provided by the Relaxed Master problem that generates $\mathbf{y}$.

A prerequisite for constructing any of these subproblems, excluding the Primal problem, is a convexity theory for dynamic optimization and the ability to build valid convex relaxations for the functions in Problem (P). Here, valid convex relaxations for the nonconvex functions with state variable participating are constructed by applying the convexity theory and relaxation techniques developed in [3, 4] according to the following three-step procedure:

1. Compute time varying enclosures for the solution of the embedded dynamic system by applying any suitable state bounding technique.

2. Construct convex underestimators and concave overestimators for the solution of the embedded differential system.

3. Derive convex underestimators for the terms with state variables participating, *e.g.*, by applying McCormick's technique for relaxing factorable functions [5]. Concerning integral terms, valid convex/concave relaxations are derived by exploiting the monotonicity of the Lebesgue integral as demonstrated in [6].

A thorough description of the different subproblems, as well as a complete statement of the Algorithms, are presented in [7].

3 Case Study

The application of the MIDO algorithms is demonstrated with an example based on the batch process shown in Fig. 1. It consists of a series reaction ($A \rightarrow B \rightarrow C$) followed by separation with no intermediate storage (NIS). The objective is to select the optimal process design and operation that minimizes the overall manufacturing cost subject to a fixed production amount of B in given time. The interested reader is referred to [7] for a complete statement of the problem objective and constraints. The model equations are derived by assuming that the process operates at a cyclic steady state. The concentration profiles of the reactant A and products B, C are governed by a set of ODEs, assuming first-order kinetics, whereas a perfect split of components is assumed for the batch distillation. The inventory of equipment, their rental cost and their characteristics, as well as the physical properties of the pure components A, B and C, are the same as those specified in [8].

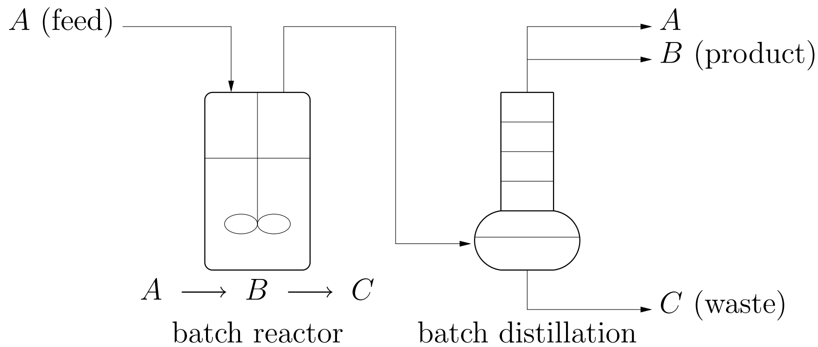

Figure 1: Task network of a 2-stage batch process.

The resulting problem is a nonconvex MIDO problem that contains 1 control variable (reactor temperature), 4 design parameters (length of the manufacturing campaign, batch reactor cycle time, batch distillation cycle time, and reactor volume), 39 binary variables (equipment selection), and 1 integer variable (total number of batches). By accounting for the existing SOS1 sets of binary variables, the total number of discrete alternatives in this problem is 8,316.

Table 1: Results for the case study problem.

Heuristics	Iterations	CPU time (sec)			
		primal	primal bounding	relaxed master	overall
MIDO algorithm 1:					
without domain reduction	1,305/1,266	53,631	272	1,584	55,656
with domain reduction	1,082/1,062	50,416	235	703	51,465
with domain reduction & screening model cuts	512/482	12,243	303	420	13,020
MIDO algorithm 2:					
without domain reduction	1,305/1,266	334	269	1,587	2,357
with domain reduction	1,082/1,062	371	234	703	1,417
with domain reduction & screening model cuts	512/482	66	298	421	839

The computational times for solving this problem are reported in Table 1. The application of Algorithm 1 provides the global solution to the problem in about 14.3 hours and 15.5 hours depending on whether or not domain reduction is applied; in both cases, total enumeration of the process structure alternatives is avoided as only 1,082 binary realizations out of 8,316 were visited in the former case, and 1,305 in the latter. As expected, the major computational expense derives from the solution of Primal problems to ε-optimality.

Roughly, the more promising binary realizations are visited early by the outer approximation algorithm, and the upper bound rapidly reaches the global minimum of the problem (found after about 200 iterations); this can be seen from Fig. 2 (left plot), which depicts the solutions of the Primal and Relaxed Master problems versus the iteration count. By using the current upper bound as an incumbent in the branch-and-bound procedure, the computational expense for subsequent Primal problems is then progressively reduced as it becomes faster to detect whether a given binary realization will yield a worse upper bound or is infeasible. These considerations are illustrated on the right plot in Fig. 2, which depicts the computational expense versus the iteration count.

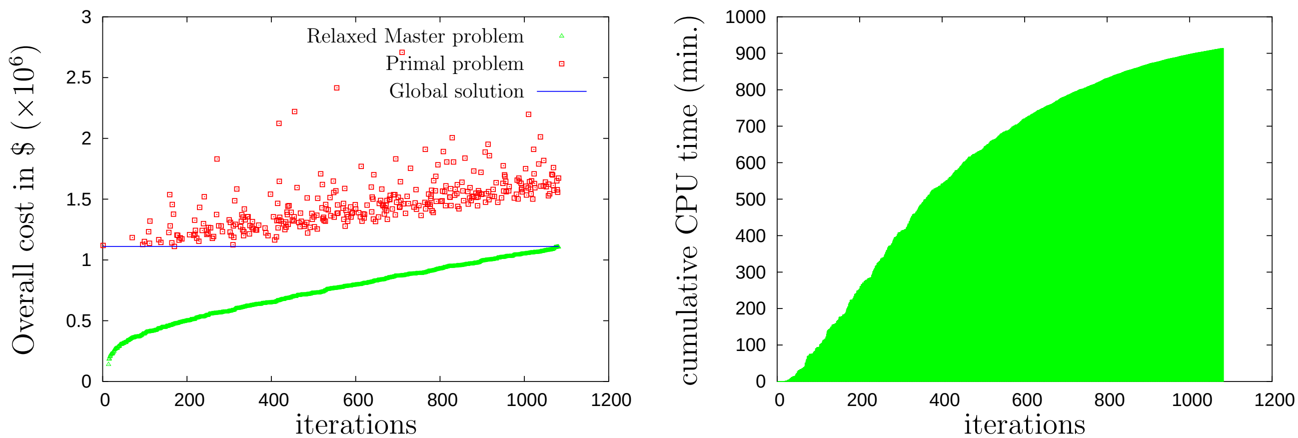

Figure 2: Case study problem — *left plot*: MIDO iterations; *right plot*: CPU time (with domain reduction).

The application of Algorithm 2 was also considered to solve this problem. It is worth noting that this simplified algorithm finds the global solution despite the fact that no theoretical guarantee can be given. In addition, the CPU time required to solve the problem is dramatically reduced, for Algorithm 2 terminates in approximately 40 minutes and 24 minutes without and with the application of domain reduction techniques, respectively.

In order to enhance the convergence of the algorithms, a link has been established with the screening model approach developed in [9]. More specifically, valid cuts derived from the screening model are added to the Lower Bounding Convex MIDO problem to tighten the relaxations. The results obtained are also reported in Table 1 for Algorithms 1 and 2. One sees that the addition of screening model cuts significantly reduces the overall number of iterations, and correlatively the overall CPU time, for the use tighter relaxations allows the algorithms to exclude a larger number of binary realizations. These results therefore demonstrate that large benefits can be realized by considering screening models for batch process development purposes.

4 Conclusion

In this paper, we presented an algorithm for solving MIDO problems to guaranteed global optimality that potentially avoids total enumeration of the discrete alternatives. The algorithm implements an outer-approximation method for nonconvex MIPs in combination with a relaxation technique for constructing convex underestimators of functions with state variables participating. Two variants of the algorithm were considered.

A case study was presented in connection to batch process development. The process considered consists of a series reaction followed by a separation with no intermediate storage. The objective is to select the optimal process design and operation that minimizes the overall manufacturing cost subject to either a fixed production rate constraint or a fixed amount of product in given time. The developed algorithms demonstrate efficiency and applicability in solving either problem. Several heuristics, such as bounds tightening techniques, were considered to enhance the convergence of the algorithms. A link was also established with the screening model approach by introducing additional cuts to tighten the MIDO problem relaxations. These cuts provide large reductions in terms of the number of iterations and the overall computational time.

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