

Design of process operations using hybrid dynamic optimization

Paul I. Barton*, Cha Kun Lee

Department of Chemical Engineering, Massachusetts Institute of Technology, Cambridge, MA 02139, USA

Abstract

Accurate nonlinear dynamic models of process operations such as start-ups and shut-downs include state-dependent events that trigger discrete changes to the describing equations, and are best analyzed within a hybrid systems framework. The automated design of an optimal process operation can thus be formulated as a dynamic optimization problem with a hybrid system embedded. This paper describes recent progress on the development of suitable deterministic algorithms for the global solution of these problems. A method for constructing convex relaxations of general nonconvex nonlinear programming (NLP) problems with linear dynamic systems embedded is presented. These convex relaxations are then extended to multistage problems with model switches between the stages. Finally, integer variables are introduced to represent alternative sequences of model switches. The ability to construct convex relaxations enables existing nonconvex mixed nonlinear programming (MINLP) algorithms to be applied to find the global solution of the resulting mixed integer dynamic optimization (MIDO) problems.

© 2003 Elsevier Ltd. All rights reserved.

Keywords: Global optimization; Linear hybrid systems; Convex relaxations; Dynamic optimization

1. Introduction

Economic, environmental, safety and quality considerations all motivate careful study and optimization of process operations. Of particular interest in this paper will be the design and optimization of major process transients such as start-up, shut-down and changeover procedures, and the design and formal verification of logic-based controllers for abnormal situation management. In addition, a majority of chemical and biological products are manufactured in processes that are operated in an inherently transient manner rather than at some nominal steady state. Examples include batch and semi-continuous processes, and periodic processes that operate at a cyclic steady state, such as pressure swing adsorption units and reverse flow reactors. The design of such systems is in essence an exercise in optimal process operation.

All of these applications call for detailed dynamic models that can predict accurately process transients that depart significantly from the nominal steady state (if it exists). In addition to time dependence and nonlinearity, these models will most likely embed discontinuities, or *discrete events*,

superimposed on the continuous state dynamics. These discrete phenomena belong to one of two categories (Barton & Pantelides, 1994): (a) physico-chemical discontinuities that arise from descriptions of the physics, chemistry and biology of the system in question (often abstractions of phenomena that are too complex and/or fast to model in detail at the scale of interest); and (b) external discontinuities caused by control actions and disturbances. Examples of physico-chemical discontinuities include (thermodynamic) phase changes, flow reversals and transitions, the saturation of control valves, irregularities in the geometry of vessels, etc. Examples of external discontinuities include the starting/stopping of a pump, the action of an interlock system (logic-based controller), equipment failures, the opening/closing of control loops, etc. In general, these discrete phenomena are modeled by switches in the functional form of the model equations and/or instantaneous jumps in the values of the continuous state variables. In many cases, the events that trigger these discontinuities are *state dependent*, i.e., the timing of the discontinuity is not known a priori, instead the event occurs whenever some condition involving the values of the state variables is satisfied. For example, an interlock system may implement a discrete control action whenever a threshold in reactor temperature is exceeded.

Over the past 10 years, it has become widely accepted that the most natural framework for the analysis of such process transients is that of hybrid (discrete/continuous)

* Corresponding author. Tel.: +1-617-253-6526;
fax: +1-617-258-5042.

E-mail addresses: pib@mit.edu (P.I. Barton), chakun@mit.edu (C.K. Lee).

systems theory. In general, hybrid systems theory encompasses time-dependent, nonlinear dynamic models that exhibit model switching and state jumps as a consequence of both time- and state-dependent events. Much progress has been made in the past decade in the development of robust, large-scale dynamic simulation software for such models, e.g., DAEPACK (Tolsma & Barton, 1999, 2000), and ABACUSS II (Clabaugh, Tolsma, & Barton, 1999; Tolsma, Clabaugh, & Barton, 2002).

Given robust and accurate dynamic models, the automated design of optimal process operations can often be formulated as open loop optimal control (or dynamic optimization) problems, where we search a priori for the input profiles and/or real and integer valued parameters for a dynamic system that will optimize a given performance metric over a finite time interval (Barton, Allgor, Feehery, & Galán, 1998). Given the progress in hybrid simulation technology, it is natural to consider embedding hybrid system models in dynamic optimization problems in order to design major process transients exhibiting discontinuities. However, with a hybrid system model embedded, reliable solution of the resulting optimization problem becomes a formidable task, especially when the timing and sequence of model switches and jumps vary over the decision space of interest (as a consequence of state-dependent events). A continuous time partial discretization approach to this optimization problem, where the controls are discretized using control parameterization (e.g., see Teo, Goh, & Wong, 1991), is presented in Galán and Barton (1998), and shown in Fig. 1. For a given approximate problem, the numerical solution of the resulting parameter optimization problem can be obtained by a decomposition into two subproblems:

1. an initial value (IVP) subproblem in which the hybrid system model is solved for given values of the time invariant parameters using robust hybrid simulation technology, e.g., DAEPACK, and ABACUSS II;
2. a nonlinear programming (NLP) master problem that searches in the Euclidean parameter space using function and gradient information furnished by the IVP subproblem.

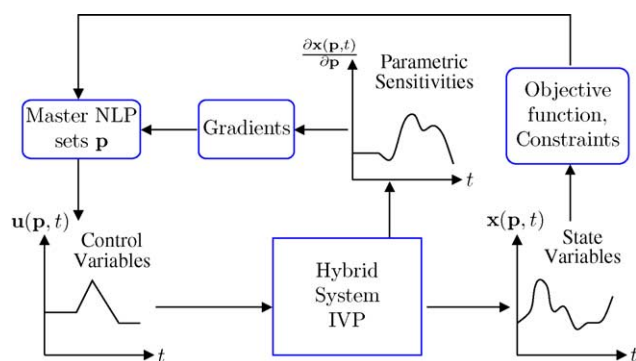


Fig. 1. Control parameterization.

The utility of such a method hinges on the existence and uniqueness of the parametric sensitivities of the hybrid system (or the related adjoints), which are used to calculate the gradients of the objective and constraint functions in the master problem (Feehery, Tolsma, & Barton, 1997; Tolsma & Barton, 2002). Sufficient conditions for the existence and uniqueness of these sensitivities are developed in Galán, Feehery, and Barton (1999), and these imply a classification of problems for which gradient-based methods can be applied (Galán & Barton, 1998). These results indicate that the sensitivity trajectories of a hybrid system will usually exist almost everywhere in the parameter space. Subject to the key restriction that the temporal sequence of model switches and jumps (or modes), is fixed throughout the parameter space (the timing of switches may still vary), the resulting Master NLP is smooth and existing gradient-based methods can be used to find local solutions. On the other hand, if the temporal sequence of model switches and jumps can vary as a function of the optimization parameters, then it appears that most resulting Master NLPs will exhibit some degree of nonsmoothness (Galán & Barton, 1998).

As a practical example of the application of hybrid optimal control in the automated design of safe operating procedures, consider the hybrid dynamic model of a pressure vessel located in a chemical plant that is shown in Fig. 2 (Barton, Banga, & Galán, 2000). The tank may be supplied with oxygen, nitrogen and/or methane via three separate lines, and gas mixtures may be withdrawn from the vessel through a fourth line. The flow in each line is regulated by an open/close non-return valve. Discontinuities in the solution trajectories occur because the non-return valves are modeled using three distinct modes: zero, laminar/turbulent and choked flow regimes.

It is evident that the equations describing the flow/pressure relationships will differ in each mode. Consider now a scenario in which we wish to design a minimum time operating policy for a tank changeover operation, where we want to find the sequence of valve openings and closings that will bring the system from a steady state where pure methane is flowing through the system, to the next steady state where pure oxygen is flowing through the system. This has to be achieved without forming a dangerous explosive mixture within the pressure vessel, as shown in Fig. 2(b). As mentioned above, solution of this optimization problem involves finding the optimal sequence and timings of the mode transitions (Barton, Banga, & Galán, 2000).

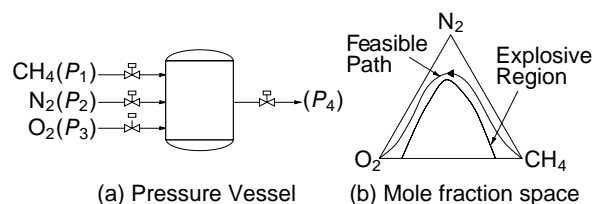


Fig. 2. Pressure vessel and mole fraction space.

Currently, it is possible to mitigate the implications of nonconvexities and nonsmoothness in the Master NLP by utilizing a direct stochastic search (see Barton, Banga, & Galán, 2000). However, such a method can, in general, only provide ad hoc improvements to the operating procedure design, because stochastic searches cannot guarantee location of the global solution within a finite number of iterations. Furthermore, applications such as formal safety verification of logic-based controllers, taking into account the continuous dynamics of the underlying process, optimization problems, when formulated as dynamic demand that the global solution be located. For example, a local solution could falsely indicate that all safety specifications are met, leading to disastrous consequences if, in actuality, a global solution exists which provides a counter example (or certificate) that violates some safety specification. These considerations motivate the development of deterministic global optimization algorithms for nonconvex, nonsmooth dynamic optimization problems with embedded hybrid systems. The methods described in this paper will serve as an important foundation on which general hybrid dynamic optimization problems (e.g., the tank changeover example described above) can be solved via control parameterization in the continuous time domain.

At this point, it is worthwhile to mention other approaches for optimal control of hybrid systems that have been proposed in the literature. It is beyond the scope of this paper to provide a comprehensive review, however, we note that active research areas include discrete time approaches (e.g., Bemporad, Borrelli, & Morari, 2000; Cuzzola & Morari, 2001), total discretization approaches (e.g., Avraam, Shah, & Pantelides, 1998), and reachability analysis approaches based on the formal definition of the hybrid automaton (e.g., Alur et al., 1995; Shakernia, Pappas, & Sastry, 2000; Trontis & Spathopoulos, 2001). The hybrid automaton in Alur et al. (1995) incorporates a stochastic element in the timings of events, of which our modeling framework is a special case of. For related work on linear switched systems with quadratic objective functions, see Xu and Antsaklis (2001), where the sequence of modes is fixed, the timings of the transitions are parameterized, and the gradients to the local NLP solver are obtained by solving the Hamilton–Jacobi–Bellman (HJB) equations using the dynamic programming approach. The ideas and methods outlined in this paper differ from the other approaches in that global mathematical programming techniques (described below) are utilized to solve the control-parameterized optimization problem in the continuous time domain.

Many modern, general methods for deterministic global optimization in Euclidean spaces rely on the notion of a convex relaxation of a nonconvex function (McCormick, 1976). This is a convex function which underestimates a nonconvex function on the set of interest. The convex programs that result from convex relaxation of all nonconvex objective and constraint functions in an optimization problem can (in principle) be solved to guaranteed global optimality, which, for example, can be used to generate rigorous lower bounds

on the solution of the nonconvex problem for a branch and bound (B&B) algorithm. In B&B, the feasible set is first relaxed and subsequently split into partitions (*branching*) over which rigorous lower and upper bounds on the nonconvex problem can be determined (*bounding*). If the lower bound on a partition of the feasible space is greater than the current best upper bound, that partition is removed from the search space since the minimum can never be attained there (*fathomed*). A number of established methods (McCormick, 1976; Adjiman, Dallwig, Floudas, & Neumaier, 1998) exist for the construction of convex relaxations of elementary functions on Euclidean spaces.

Recently, a convexity theory has been developed that enables the well-known convex relaxations of elementary functions on Euclidean spaces (described above) to be harnessed in the construction of convex relaxations of general, nonconvex Bolza-type functionals subject to an embedded linear time-varying (LTV) dynamic system (Singer & Barton, 2003b). This key result can be extended to linear time-varying hybrid systems when the transition times are fixed, and the sequence of modes is known (Lee, Singer, & Barton, 2002). The resulting master problem in control parameterization is smooth, and a deterministic B&B framework can be applied to find the global solution.

In this paper, we will describe an extension to problems in which the transition times (events) of the linear time-varying hybrid system are fixed, but the temporal sequence of modes is allowed to vary. Binary variables are introduced into the problem formulation to represent all possible sequences of modes. Once the binary variables are fixed, the sequence of modes is fixed, and the aforementioned nonsmoothness in the master problem is eliminated. Our continuous time approach has a number of advantages over that in Avraam, Shah, & Pantelides (1998), where a total discretization approach (i.e., discretization of both controls and states) is taken. Firstly, the major difficulty with any discretization approach for solving dynamic optimization problems is the size of the resulting NLP/mixed nonlinear programming (MINLP) that can be solved practically. Compared to discrete time (Bemporad, Bovelli, & Morari, 2000; Cuzzola & Morari, 2001), and total discretization approaches, control parameterization yields a much smaller Master optimization problem that is often within the capabilities of existing global optimization algorithms. Secondly, and perhaps more importantly, the standard methods employed by Avraam, Shah, & Pantelides (1998) for the solution of the resulting mixed integer nonlinear programming problems rely on the assumption that the participating functions and constraints are convex. If these conditions are not satisfied, standard MINLP algorithms will most likely converge to arbitrary suboptimal points (Kocis & Grossmann, 1989; Sahinidis & Grossmann, 1991; Bagajewicz & Manousiouthakis, 1991; Floudas, 1995). Deterministic global optimization algorithms for MINLPs have begun to emerge in recent years (Adjiman, Androulakis, & Floudas, 2000; Kesavan, Allgor, Gatzke, & Barton, 2001; Ryoo & Sahinidis, 1996).

However, the size of problem that can be solved is still quite small, so that only very small hybrid optimal control problems can potentially be solved via discrete time or total discretization approaches.

The outline and contributions of this paper are as follows. In Section 2, we introduce the hybrid systems modeling framework used, the problem formulation, and review the convexity theory that has been developed (Lee, Singer, & Barton, 2003) for these systems. Section 3 illustrates how a deterministic branch and bound framework can be utilized to solve the global optimization problem via application to an illustrative example. In Section 4, we consider problems where the sequence of modes is no longer fixed, and has to be determined by the optimization procedure. We present a novel reformulation of the general problem that retains the linear structure of the embedded system. This enables the aforementioned convexity theory for continuous systems (Singer & Barton, 2003b) to be utilized for the application of nonconvex outer approximation (OA) (Kesavan, Allgor, Gatzke, & Barton, 2001) to solve the resulting mixed integer dynamic optimization (MIDO) problem. The application of the new approach to an illustrative example is also presented. In Section 5, we discuss the challenges involved in locating the global optimum when the transition times of the hybrid system are allowed to vary, and present some preliminary ideas for tackling that problem. Section 6 concludes the paper and includes some of our suggestions for future research.

2. Continuous time linear hybrid systems

The modeling framework of Barton and Lee (2002) is used to define the linear hybrid system of interest. The time horizon is partitioned into contiguous intervals called *epochs*. We define a *hybrid time trajectory*, T_τ , as a finite sequence of epochs $\{I_i\}$ terminating with epoch I_{n_e} , where n_e is the total number of epochs. Each epoch is a closed time interval $I_i = [t'_i, t_i] \subset \mathbb{R}$, $t'_i = t_{i-1}$ and $t_{i-1} \leq t_i$ for all $i = 1, \dots, n_e$ with $t_0 = t'_1$. For the epoch I_i , the system evolves continuously in time if $t'_i < t_i$, and it evolves discretely by making an instantaneous transition if $t'_i = t_i$. The continuous state subsystems are called *modes* and the corresponding sequence of modes for T_τ is called the *hybrid mode trajectory*, T_μ . At the end of epoch I_i , a transition is made from the *predecessor* mode in I_i to a *successor* mode in epoch I_{i+1} , also called an *event*.

Definition 1. The linear time-varying ODE hybrid system of interest is defined by the following statements:

- (a) A fixed $T_\mu = m_1, \dots, m_{n_e}$, with $m_i \in M$, where $M = \{1, \dots, n_m\}$ is an index set of modes, and a fixed T_τ with given time events (i.e., explicit transition times) $t_0, t_1, \dots, t_{n_e} = t_f$. The use of the superscript (m) will refer to any mode in M , while superscript (m_i) will refer to the active mode in epoch I_i .

- (b) An invariant structure system where the number of real valued state and control variables are constant in each mode, $V = \{\mathbf{x}(\mathbf{p}, t), \mathbf{u}(\mathbf{p}, t), \mathbf{p}, t\}$, where $\mathbf{u}(\mathbf{p}, t) \in \mathbb{R}^{n_u}$ for all $\mathbf{p} \in P \subset \mathbb{R}^{n_p}$, $t \in [t_0, t_f]$; and $\mathbf{x}(\mathbf{p}, t) \in \mathbb{R}^{n_x}$ for all $(\mathbf{p}, t) \in P \times [t'_i, t_i]$, $i = 1, \dots, n_e$. Note that $\mathbf{x}(\mathbf{p}, t)$ can take multiple values at the events.

- (c) The parameterization of the bounded real-valued controls

$$\mathbf{u}(\mathbf{p}, t) = \mathbf{S}(t)\mathbf{p} + \mathbf{v}(t), \quad (1)$$

$$\mathbf{u}^L \leq \mathbf{u}(\mathbf{p}, t) \leq \mathbf{u}^U \quad \forall t \in [t_0, t_f], \quad (2)$$

where $\mathbf{S}(t)$ and $\mathbf{v}(t)$ are piecewise continuous on $[t_0, t_f]$, and defined at any point of discontinuity.

- (d) The LTV ODE system for each mode $m \in M$, which is given by

$$\dot{\mathbf{x}}(\mathbf{p}, t) = \mathbf{A}^{(m)}(t)\mathbf{x}(\mathbf{p}, t) + \tilde{\mathbf{B}}^{(m)}(t)\mathbf{u}(\mathbf{p}, t) + \mathbf{C}^{(m)}(t)\mathbf{p} + \tilde{\mathbf{q}}^{(m)}(t), \quad (3)$$

where $\mathbf{A}^{(m)}(t)$ is continuous on $[t_0, t_f]$; $\tilde{\mathbf{B}}^{(m)}(t)$, $\mathbf{C}^{(m)}(t)$ and $\tilde{\mathbf{q}}^{(m)}(t)$ are piecewise continuous on $[t_0, t_f]$, and defined at any point of discontinuity, for all $m \in M$. After control parameterization, we have

$$\dot{\mathbf{x}}(\mathbf{p}, t) = \mathbf{A}^{(m)}(t)\mathbf{x}(\mathbf{p}, t) + \mathbf{B}^{(m)}(t)\mathbf{p} + \mathbf{q}^{(m)}(t), \quad (4)$$

where $\mathbf{B}^{(m)}(t) \equiv \tilde{\mathbf{B}}^{(m)}(t)\mathbf{S}(t) + \mathbf{C}^{(m)}(t)$ and $\mathbf{q}^{(m)}(t) \equiv \tilde{\mathbf{B}}^{(m)}(t)\mathbf{v}(t) + \tilde{\mathbf{q}}^{(m)}(t)$ are piecewise continuous on $[t_0, t_f]$, defined at any point of discontinuity, for all $m \in M$.

- (e) The transition conditions for the transitions between epochs I_i and I_{i+1} , for all $i = 1, \dots, n_e - 1$, which are trivial since all events are explicit time events:

$$L^{(m_i)} := (t = t_i), \quad (5)$$

indicating the transition from mode m_i in epoch I_i to mode m_{i+1} in epoch I_{i+1} at time t_i .

- (f) The system of transition functions, which is given by

$$\mathbf{x}(\mathbf{p}, t'_{i+1}) = \mathbf{D}_i\mathbf{x}(\mathbf{p}, t_i) + \mathbf{E}_i\mathbf{p} + \mathbf{k}_i, \quad (6)$$

$$i = 1, \dots, n_e - 1,$$

for the transition from mode m_i in epoch I_i to mode m_{i+1} in epoch I_{i+1} at time t_i .

- (g) A given initial condition for mode m_1 ,

$$\mathbf{x}(\mathbf{p}, t_0) = \mathbf{E}_0\mathbf{p} + \mathbf{k}_0. \quad (7)$$

A solution, $\mathbf{x}(\mathbf{p}, t)$, $t \in [t'_i, t_i]$, $i = 1, \dots, n_e$, will exist and be unique for all $\mathbf{p} \in P$, at least in the weak or extended sense (Coddington & Levinson, 1955, Chapter 2). Note that the control parameterization in Eq. (1) can be used to approximate the controls with piecewise Lagrange polynomials of arbitrary order, which include piecewise constant and piecewise linear controls. The advantage of using Lagrange polynomials as the basis functions lies in the straightforward translation of the natural bounds on the controls, \mathbf{u}

(see Eq. (2)), to bounds on the parameters, \mathbf{p} , since the coefficients of the Lagrange polynomials correspond to values of the controls at specific points in time. In most cases, this results in the Euclidean parameter space P (see Definition 1(b)) being a hyper-rectangle, ensuring its compactness.

2.1. The problem formulation

The following is the problem that we are interested in solving to ε optimality within a finite number of iterations. The setting is an embedded hybrid system with fixed T_μ and T_τ , in order to illustrate the convexity theory that has been developed. In the sequel, we will discuss how these restrictions can be relaxed.

Problem 1. Consider the following problem:

$$\begin{aligned} \min_{\mathbf{p} \in P} F(\mathbf{p}) = & \phi(\dot{\mathbf{x}}(\mathbf{p}, t_f), \mathbf{x}(\mathbf{p}, t_f), \mathbf{p}) \\ & + \sum_{i=1}^{n_e} \int_{t'_i}^{t_i} f_i(\dot{\mathbf{x}}(\mathbf{p}, t), \mathbf{x}(\mathbf{p}, t), \mathbf{p}, t) dt, \end{aligned} \quad (8)$$

such that

$$\begin{aligned} G(\mathbf{p}) = & \eta(\dot{\mathbf{x}}(\mathbf{p}, t_f), \mathbf{x}(\mathbf{p}, t_f), \mathbf{p}) \\ & + \sum_{i=1}^{n_e} \int_{t'_i}^{t_i} \mathbf{g}_i(\dot{\mathbf{x}}(\mathbf{p}, t), \mathbf{x}(\mathbf{p}, t), \mathbf{p}, t) dt \leq 0, \end{aligned} \quad (9)$$

where $\mathbf{x}(\mathbf{p}, t)$ is given by the solution of the embedded LTV ODE hybrid system described in Definition 1.

Fig. 3 shows a schematic of a hybrid automaton, illustrating the hybrid system framework.

The objective function in Eq. (8) and the inequality constraints in Eq. (9) are written in the form of Bolza functionals, e.g., the sum of an (end) point and isoperimetric term. The advantage of expressing the objective function and constraints in their *canonical form* (Teo, Goh, & Wong, 1991) is that they are all treated in the same way in as far as the computations of their values, convex relaxations, and respective gradients are concerned in the numerical solution of the optimization problem. In addition, there exist constraint transcriptions (Teo, Goh, & Wong, 1991) that will transform general constraints, e.g., equality or inequality path constraints, into the canonical form shown in Eq. (9).

In the next section, we will present the convexity theory that will enable us to construct convex relaxations of general Bolza-type functionals (and hence, the objective and constraints in Problem 1) subject to the LTV ODE hybrid system described in Definition 1. There exist formal technical conditions on the properties of the functions, f_i , ϕ , \mathbf{g} and η , which will not be discussed here for brevity. The interested reader is directed to Lee, Singer, & Barton (2003) instead. Before we proceed, it will be useful to define the following sets, which will be used in the next section.

Definition 2. Let P be a nonempty compact convex subset of \mathbb{R}^{n_p} . We define the following sets for all $i = 1, \dots, n_e$ where \underline{t} denotes fixed t :

$$\begin{aligned} \mathcal{X}^{(i)}(\underline{t}) &\equiv \{\mathbf{x}(\mathbf{p}, \underline{t}) | \mathbf{p} \in P, \underline{t} \in [t'_i, t_i]\}, \\ \dot{\mathcal{X}}^{(i)}(\underline{t}) &\equiv \{\dot{\mathbf{x}}(\mathbf{p}, \underline{t}) | \mathbf{p} \in P, \underline{t} \in [t'_i, t_i]\}, \\ \mathcal{X}^{(i)} &\equiv \bigcup_{\underline{t} \in [t'_i, t_i]} \mathcal{X}^{(i)}(\underline{t}), \quad \dot{\mathcal{X}}^{(i)} \equiv \bigcup_{\underline{t} \in [t'_i, t_i]} \dot{\mathcal{X}}^{(i)}(\underline{t}). \end{aligned}$$

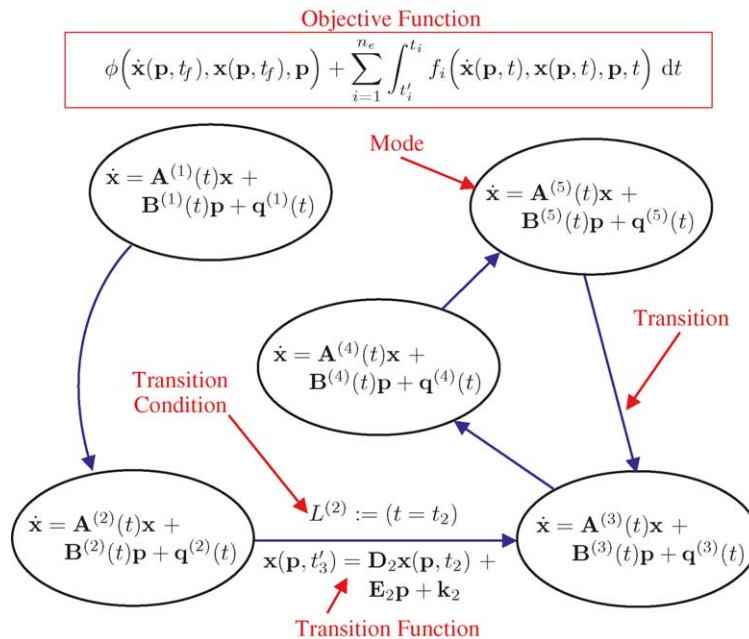


Fig. 3. Hybrid automaton.

These sets represent various images of the parameter space under the solution of the linear hybrid system.

2.2. Constructing convex relaxations

In this section, we shall describe the extension of the convexity theory developed in Singer and Barton (2003b) to the linear hybrid systems described above. The proofs for the following results are presented in Lee, Singer, & Barton (2003).

Consider first the objective function $F(\mathbf{p})$ in Eq. (8). It can be shown that if the following conditions are satisfied:

1. $f_i(\dot{\mathbf{x}}(\mathbf{p}, \underline{t}), \mathbf{x}(\mathbf{p}, \underline{t}), \mathbf{p}, \underline{t})$ is convex on $\dot{\mathcal{X}}^{(i)}(\underline{t}) \times \mathcal{X}^{(i)}(\underline{t}) \times P$ for all $\underline{t} \in [t'_i, t_i]$, $i = 1, \dots, n_e$;
2. $\phi(\dot{\mathbf{x}}(\mathbf{p}, t_f), \mathbf{x}(\mathbf{p}, t_f), \mathbf{p})$ is convex on $\dot{\mathcal{X}}^{(n_e)}(t_f) \times \mathcal{X}^{(n_e)}(t_f) \times P$,

then $F(\mathbf{p})$ is convex on P . In other words, if the functions ϕ and f_i are convex pointwise in time on their respective domains (see Definition 2) and P , the resulting Bolza functional is convex on P . The corollary of this result can be stated as follows.

Corollary 1. *If we have the following functional,*

$$U(\mathbf{p}) = \psi(\dot{\mathbf{x}}(\mathbf{p}, t_f), \mathbf{x}(\mathbf{p}, t_f), \mathbf{p}) + \sum_{i=1}^{n_e} \int_{t'_i}^{t_i} u_i(\dot{\mathbf{x}}(\mathbf{p}, t), \mathbf{x}(\mathbf{p}, t), \mathbf{p}, t) dt, \quad (10)$$

and if the following conditions are satisfied,

1. $\psi(\cdot) \leq \phi(\cdot) \forall \mathbf{p} \in P$;
2. $u_i(\cdot) \leq f_i(\cdot) \forall (\mathbf{p}, \underline{t}) \in P \times [t'_i, t_i]$, $i = 1, \dots, n_e$;
3. $u_i(\dot{\mathbf{x}}(\mathbf{p}, \underline{t}), \mathbf{x}(\mathbf{p}, \underline{t}), \mathbf{p}, \underline{t})$ is convex on $\dot{\mathcal{X}}^{(i)}(\underline{t}) \times \mathcal{X}^{(i)}(\underline{t}) \times P$ for all $\underline{t} \in [t'_i, t_i]$, $i = 1, \dots, n_e$;
4. $\psi(\dot{\mathbf{x}}(\mathbf{p}, t_f), \mathbf{x}(\mathbf{p}, t_f), \mathbf{p})$ is convex on $\dot{\mathcal{X}}^{(n_e)}(t_f) \times \mathcal{X}^{(n_e)}(t_f) \times P$,

then $U(\mathbf{p})$ is convex on P such that

$$U(\mathbf{p}) \leq F(\mathbf{p}), \forall \mathbf{p} \in P.$$

So far, we have focused on constructing convex relaxations for the objective function. It is clear that the exact same technique can be applied for the point and isoperimetric inequality constraints in Eq. (9). Corollary 1 is a powerful result that is the key basis on which convex relaxations of the objective function and constraints can be constructed, because well-known methods for constructing convex relaxations of elementary functions on Euclidean spaces (Adjiman, Dallwig, Floudas, & Neumaier, 1998; McCormic, 1976) can be harnessed to construct the relevant convex relaxations, $\psi(\cdot)$ and $u_i(\cdot)$ in Eq. (10), from $\phi(\cdot)$ and $f_i(\cdot)$ in Eq. (8). This is important as it enables us to construct convex relaxations required for the B&B and OA algorithms in the sequel. In turn, this will enable rigorous

lower bounds to be obtained in the bounding step of the B&B algorithm, and the lower bounding convex MINLP to be constructed in the nonconvex OA algorithm.

2.3. Implied state bounds

A final piece of information is needed to utilize the well-known symbolic convex underestimators in Euclidean spaces, namely, bounds on the state variables (i.e., the sets $\mathcal{X}^{(i)}(\underline{t})$ and $\dot{\mathcal{X}}^{(i)}(\underline{t})$ in Definition 2). For example, consider the simple univariate concave function,

$$f(x) = -x^2,$$

where $f: \mathbb{R} \rightarrow \mathbb{R}$. In order to construct a convex relaxation, one has to define the set of interest as some finite real interval $x \in [x^L, x^U]$. Once the bounds x^L and x^U are set, the convex relaxation is simply given by the secant of the function,

$$u(x) = (x^L + x^U)(x^L - x) - (x^L)^2.$$

Corollary 1 enables us to apply the same technique for dynamic systems, but now pointwise in time. Recall that conditions 3 and 4 in the corollary require convexity on the sets $\mathcal{X}^{(i)}(\underline{t})$ and $\dot{\mathcal{X}}^{(i)}(\underline{t})$. This is where the implied state bounds come in. We can think of the implied state bounds as the dynamic analogue of the bounds x^L and x^U described above. These time-varying state bounds, $\mathbf{x}^L(t)$ and $\mathbf{x}^U(t)$, can be obtained by performing interval analysis on the supplied bounds on the parameters, $[\mathbf{p}^L, \mathbf{p}^U]$ (hence, the term *implied*), because the structural form of the solution to the linear hybrid system is *affine* in \mathbf{p} (Lee, Singer, & Barton, 2003),

$$\mathbf{x}(\mathbf{p}, t) = \mathbf{M}_i(t)\mathbf{p} + \mathbf{n}_i(t), \quad \forall t \in [t'_i, t_i], \quad i = 1, \dots, n_e. \quad (11)$$

Differentiating with respect to \mathbf{p} , Eq. (11) reveals that the matrix $\mathbf{M}_i(t)$ represents the parametric sensitivities of the hybrid system, which will be described in the next section. This enables us to calculate the implied state bounds for the real valued state variables pointwise in time from the following natural interval extension:

$$[\mathbf{x}](\mathbf{p}, \underline{t}) = \mathbf{M}_i(\underline{t})[\mathbf{p}] + \mathbf{n}_i(\underline{t}), \quad \underline{t} \in [t'_i, t_i], \quad \forall i = 1, \dots, n_e. \quad (12)$$

Further, the implied bounds for $\dot{\mathbf{x}}(\mathbf{p}, t)$ are given pointwise in time by the following interval equation:

$$[\dot{\mathbf{x}}](\mathbf{p}, \underline{t}) = (\mathbf{A}^{(m_i)}(\underline{t})\mathbf{M}_i(\underline{t}) + \mathbf{B}^{(m_i)}(\underline{t}))[\mathbf{p}] + \mathbf{A}^{(m_i)}(\underline{t})\mathbf{n}_i(\underline{t}) + \mathbf{q}^{(m_i)}(\underline{t}), \quad \underline{t} \in [t'_i, t_i], \quad \forall i = 1, \dots, n_e. \quad (13)$$

3. Global optimization with fixed T_τ and T_μ

A B&B algorithm (Falk & Soland, 1969; McCormick, 1976; Ryoo & Sahinidis, 1996) will be employed to obtain

a global solution, within ε tolerance, of **Problem 1** with a finite number of iterations. The hybrid system described in **Definition 1** is embedded in the optimization problem, reducing the otherwise infinite dimensional search space (containing $\mathbf{x} \in (\hat{C}^1[t'_i, t_i])^{n_x}$, $i = 1, \dots, n_e$) to a finite dimensional one in the parameter space P . The upper bounding problem can be solved using any local gradient-based method, utilizing the parametric sensitivities of the hybrid system to deliver the required gradients.

It is shown in Lee, Singer, & Barton (2003) that the parametric sensitivities of the LTV ODE hybrid system in **Definition 1** exist (at least in the weak sense), $\partial \mathbf{x}(\mathbf{p}, t) / \partial \mathbf{p} \in \mathbb{R}^{n_x \times n_p}$, $t \in [t'_i, t_i]$, $i = 1, \dots, n_e$ for all $\mathbf{p} \in P$, and are given by the solution of the following equations:

$$\frac{\partial}{\partial t} \left(\frac{\partial \mathbf{x}}{\partial \mathbf{p}} \right) = \mathbf{A}^{(m_i)}(t) \frac{\partial \mathbf{x}}{\partial \mathbf{p}} + \mathbf{B}^{(m_i)}(t), \quad \forall t \in (t'_i, t_i],$$

$$i = 1, \dots, n_e, \quad (14)$$

$$\frac{\partial \mathbf{x}(\mathbf{p}, t_0)}{\partial \mathbf{p}} = \mathbf{E}_0, \quad (15)$$

$$\frac{\partial \mathbf{x}(\mathbf{p}, t'_{i+1})}{\partial \mathbf{p}} = \mathbf{D}_i \frac{\partial \mathbf{x}(\mathbf{p}, t_i)}{\partial \mathbf{p}} + \mathbf{E}_i, \quad i = 1, \dots, n_e - 1. \quad (16)$$

It is further shown, subject to mild conditions, that the objective function $F(\mathbf{p})$ in **Problem 1** is continuously differentiable on P , and that there exists a minimum to the problem.

To generate rigorous lower bounds in the B&B algorithm, we must construct convex relaxations for the Bolza-type objective $F(\mathbf{p})$, and constraints $\mathbf{G}(\mathbf{p})$, which are provided by **Corollary 1**. The resulting convex program can be solved globally to obtain a lower bound on the solution using any suitable gradient-based NLP algorithm. After obtaining upper and lower bounds on the global solution in a given partition of the parameter search space, the B&B algorithm terminates if the bounds are within ε tolerance, otherwise, the search space is further partitioned using a branching heuristic, and the bounding process is repeated. If the lower bound on a given partition is greater than the current best upper bound, that region of the parameter search space is fathomed. A B&B algorithm utilizing the convex relaxations constructed from **Corollary 1** is shown to be infinitely convergent in Lee, Singer, & Barton (2003). Since we require ε optimality, such an algorithm is guaranteed to terminate in a finite number of iterations.

Example 1. Consider the following problem

$$\min_p F(p) = \int_0^3 -x(p, t)^2 dt,$$

where $p \in P = [-4, 4]$, and $x(p, t)$ is given by the solution to the following hybrid system

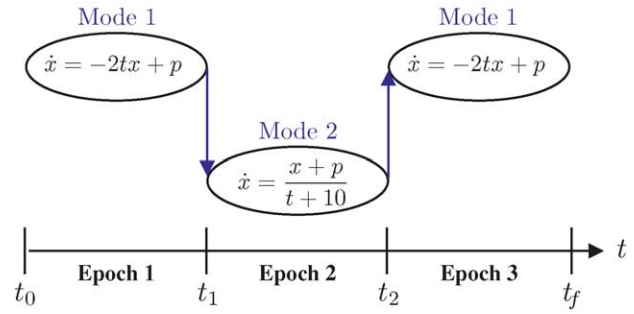


Fig. 4. Hybrid system for **Example 1**.

$$\text{Mode 1 : } \dot{x}(p, t) = -2tx(p, t) + p,$$

$$\text{Mode 2 : } \dot{x}(p, t) = \frac{x(p, t) + p}{t + 10},$$

with $x(p, 0) = 1$ and $T_\mu = 1, 2, 1$. State continuity is enforced at the explicit transitions at $t_1 = 1$ and $t_2 = 2$,

$$L^{(m_1)} := (t = t_1), \quad T^{(m_1)} = x(t'_2) - x(t_1),$$

$$L^{(m_2)} := (t = t_2), \quad T^{(m_2)} = x(t'_3) - x(t_2).$$

The hybrid system for this example is illustrated in **Fig. 4**.

We can solve this problem with a global deterministic B&B algorithm utilizing the theory described above. The convex relaxation for the objective function, $U(p)$, is simply the secant of the univariate concave function,

$$\int_0^3 (x^L(t) + x^U(t))(x^L(t) - x(p, t)) - x^L(t)^2 dt.$$

The implied state bounds constructed from **Eq. (12)**, $x^L(t)$ and $x^U(t)$, are shown in **Fig. 5(a)**. The nonconvex objective function, $F(p)$, and its constructed convex underestimator, $U(p)$, over the entire feasible region P are shown in **Fig. 5(a)**. The lower bound (LB) at the first iteration will be obtained at $p = 4$. Depending on the initial guess for p , the upper bound (UB) at the first iteration will be obtained at either $p = 4$, in which case we have found the global solution, since $UB - LB < \varepsilon$, or $p = -4$, for which we have to branch.

To illustrate the concept of fathoming, suppose that the feasible region is partitioned into three partitions of $[-4, -2]$, $[-2, 2]$ and $[2, 4]$ in that order (usually, the partition space is bisected). Each of these partitions imply new tightened state bounds, which update the convex underestimator. The constructed convex underestimators for these regions are shown in **Fig. 5(c)**. In the first iteration, the lower and upper bounds on $[-4, -2]$ are attained at $p = -4$, which is the global solution in that partition. At the second iteration, the lower bound on $[-2, 2]$ is attained at $p = 2$. Since this lower bound on $[-2, 2]$ is greater than the current best upper bound at $p = -4$, the partition $[-2, 2]$ is fathomed. The algorithm terminates at the global solution of $p = 4$, $F(4) = U(4) = -15.360$ in the third iteration.

In the general multi-parameter case, branching heuristics are employed to decide which variable to branch on. For

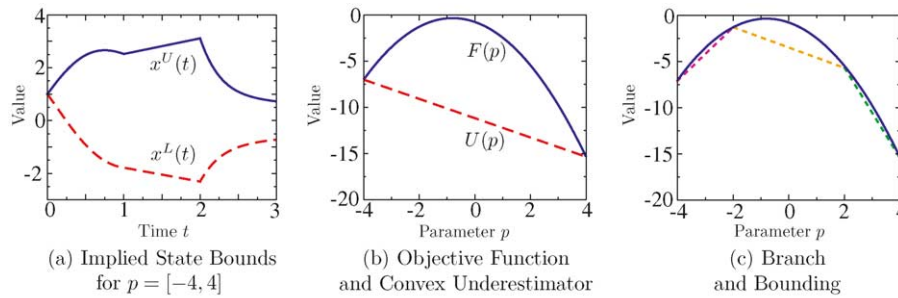


Fig. 5. State bounds and convex relaxations for Example 1.

example, one simple heuristic is to select the parameter with the largest interval to branch on, i.e., choose p_j , where $j = \arg \max_{1 \leq i \leq n_p} (p_i^U - p_i^L)$. The parameter space can then be partitioned by a simple bisection procedure.

4. Global optimization with fixed T_τ and varying T_μ

In the preceding sections, we have considered the global solution of problems where T_μ was fixed. In general, we might be interested in solving problems where the sequence of modes is not known a priori and/or might change as a function of the optimization parameters. In order to take sequencing decisions into account in the solution of the global optimization problem, the most common approach is to introduce integer or binary variables into the model. In this section, we shall present a novel reformulation of the resulting MIDO problem. Nonconvex OA is then used to solve the resulting nonconvex MINLP after control parameterization. The key advantage in the new formulation is that the convexity theory presented above can be used to construct the required convex relaxations for nonconvex OA.

4.1. Nonconvex outer approximation

Before we proceed, it is worthwhile to summarize the OA algorithm for nonconvex MINLPs. Outer approximation as a decomposition approach has been employed very successfully for convex MINLPs (Duran & Grossmann, 1986; Fletcher & Leyffer, 1994). The extension to nonconvex MINLPs hinges on the ability to construct convex relaxations of the objective function and constraints to form a lower bounding convex MINLP (Kesavan & Barton, 2000; Kesavan, Allgor, Gatzke, & Barton, 2001). The decomposition then consists of three main subproblems:

1. the *primal problem*, $NLP(Y^k)$, which is the nonconvex NLP obtained by fixing the binary variables, Y^k , in the nonconvex MINLP,
2. the *primal bounding problem*, $NLPB(Y^k)$, which is the convex NLP obtained by fixing the binary variables, Y^k , in the lower bounding convex MINLP,

3. the *relaxed master problem*, which is the relaxation of the equivalent mixed integer linear programming (MILP) master problem for the lower bounding convex MINLP.

The algorithm solves for the global solution by alternating finitely between the primal problem, the primal bounding problem, and relaxations of the master problem, as shown in Fig. 6. Because the solution of the relaxed master problem provides a non-decreasing sequence of rigorous lower bounds, and the solution of the primal problem provides a sequence of upper bounds, the algorithm terminates finitely either when the lower bound crosses the best upper bound, or the relaxed master problem becomes infeasible.

The primal bounding problem provides a valid and tighter lower bound to the primal problem for each binary realization, Y^k , then that provided by the current relaxed master problem. Hence, if the solution to $NLPB(Y^k)$ is greater than the best upper bound, $NLP(Y^k)$ need not be solved for iteration k . This is important, since the convex primal bounding problem is the least expensive to solve, followed by the relaxed master problem, while the nonconvex primal problem, which requires global deterministic methods to solve,

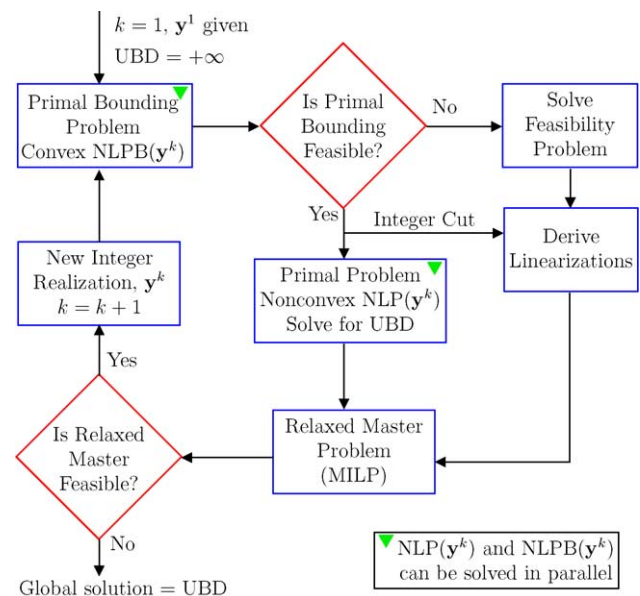


Fig. 6. Outer approximation for nonconvex MINLPs.

is usually the most expensive, unless a special structure is exhibited once the binary variables are fixed.

4.2. The revised problem, with varying T_μ

Consider [Example 1](#), with the relaxation that T_μ is not fixed.

Example 2. Consider the following problem

$$\min_{p, T_\mu} F(p, T_\mu) = \int_0^3 -x(p, T_\mu, t)^2 dt,$$

where $p \in P = [-4, 4]$, $T_\mu = m_1, m_2, m_3$; $m_i=1, \dots, 3 \in \{1, 2\}$, and $x(p, T_\mu, t)$ is given by the solution to the following hybrid system

$$\text{Mode 1: } \dot{x}(p, T_\mu, t) = -2tx(p, T_\mu, t) + p,$$

$$\text{Mode 2: } \dot{x}(p, T_\mu, t) = \frac{x(p, T_\mu, t) + p}{t + 10},$$

with $x(p, T_\mu, 0) = 1$. State continuity is enforced at the explicit transitions at $t_1 = 1$ and $t_2 = 2$,

$$L^{(m_1)} := (t = t_1), \quad T^{(m_1)} = x(t'_2) - x(t_1),$$

$$L^{(m_2)} := (t = t_2), \quad T^{(m_2)} = x(t'_3) - x(t_2).$$

Here, we wish to determine the optimal sequence of modes, T_μ , in addition to the optimal value of the parameter, that will minimize the objective function. A possible method to calculate the global solution would be to explicitly enumerate all $n_m^{n_e}$ possible combinations of T_μ . However, it is apparent that such a method quickly becomes intractable, especially when we have a large number of modes and epochs in the hybrid system. A more attractive method would be to introduce binary decision variables to represent all possible sequences of modes.

Example 3. Consider the following problem

$$\min_{p, Y} F(p, Y) = \int_0^3 -x^2(p, Y, t) dt,$$

such that

$$y_{11} + y_{21} = 1, \quad y_{12} + y_{22} = 1, \quad y_{13} + y_{23} = 1, \quad (17)$$

where $x(p, Y, t)$ is given by the solution to the following hybrid system,

$$\text{Epoch 1: } \dot{x}(p, Y, t) = y_{11}(-2tx + p) + y_{21} \left(\frac{x + p}{t + 10} \right),$$

$$\text{Epoch 2: } \dot{x}(p, Y, t) = y_{12}(-2tx + p) + y_{23} \left(\frac{x + p}{t + 10} \right),$$

$$\text{Epoch 3: } \dot{x}(p, Y, t) = y_{13}(-2tx + p) + y_{23} \left(\frac{x + p}{t + 10} \right),$$

$$x(p, 0) = 1,$$

$p \in P = [-4, 4]$, $Y \in Y^b = \{0, 1\}^{n_m \times n_e}$, and state continuity is enforced at $t_1 = 1$ and $t_2 = 2$.

Here, we have introduced $n_m n_e$ binary variables y_{mk} , $m = 1, \dots, n_m$, $k = 1, \dots, n_e$, which are treated as additional optimization parameters. [Eq. \(17\)](#) ensure that only one mode is active in each epoch. If m_k^* is the active mode in epoch I_k , then $y_{m_k^*, k} = 1$ and $y_{m \neq m_k^*, k} = 0$, for all $k = 1, \dots, n_e$. In other words, if mode m is in epoch I_k , $y_{mk} = 1$, else $y_{mk} = 0$. The resulting hybrid superstructure is illustrated in [Fig. 7](#). If certain transitions are forbidden by the structure of the hybrid automaton, these can be excluded by the inclusion of logical constraints between the binary variables y_{mk} .

Note that the form of the underlying hybrid system is no longer linear, due to the presence of multiple bilinear terms $y_{mk}x$ and $y_{mk}p$ in every differential equation. Hence, the above convexity theory can no longer be used to construct the required convex relaxations of the objective function. Work is in progress to explore methods to construct convex relaxations of functions with nonlinear dynamic systems embedded, extending the convexity theory that has been developed ([Singer & Barton, 2003a](#)). However, it is possible to retain the linearity of the underlying dynamic system in the formulation that follows.

Example 4. Consider the following problem

$$\begin{aligned} \min_{p, Y} F(p, Y) &= \int_0^1 y_{11}(-x_{11}^2(p, t)) + y_{21}(-x_{21}^2(p, t)) dt \\ &+ \int_1^2 y_{12}(-x_{12}^2(p, t)) + y_{22}(-x_{22}^2(p, t)) dt \\ &+ \int_2^3 y_{13}(-x_{13}^2(p, t)) + y_{23}(-x_{23}^2(p, t)) dt, \end{aligned} \quad (18)$$

such that

$$y_{11} + y_{21} = 1, \quad y_{12} + y_{22} = 1, \quad y_{13} + y_{23} = 1,$$

$$p_2 = y_{11}x_{11}(p, t_1) + y_{21}x_{21}(p, t_1), \quad (19)$$

$$p_3 = y_{12}x_{12}(p, t_2) + y_{22}x_{22}(p, t_2), \quad (20)$$

where $x_{mk}(p, t)$ are given by the solution of the following linear systems:

$$\begin{aligned} \dot{x}_{11} &= -2tx_{11} + p_1, \quad \dot{x}_{12} = -2tx_{12} + p_1, \quad \dot{x}_{13} = -2tx_{13} + p_1, \\ \dot{x}_{21} &= \frac{x_{21} + p_1}{t + 10}, \quad \dot{x}_{22} = \frac{x_{22} + p_1}{t + 10}, \quad \dot{x}_{23} = \frac{x_{23} + p_1}{t + 10}, \\ x_{11}(p, 0) &= 1, \quad x_{12}(p, t_1) = p_2, \quad x_{13}(p, t_2) = p_3, \\ x_{21}(p, 0) &= 1, \quad x_{22}(p, t_1) = p_2, \quad x_{23}(p, t_2) = p_3, \end{aligned}$$

$Y \in Y^b = \{0, 1\}^{n_m \times n_e}$, $p = (p_1, p_2, p_3) \in P = [-4, 4] \times [p_2^L, p_2^U] \times [p_3^L, p_3^U]$, and $t_1 = 1$, $t_2 = 2$.

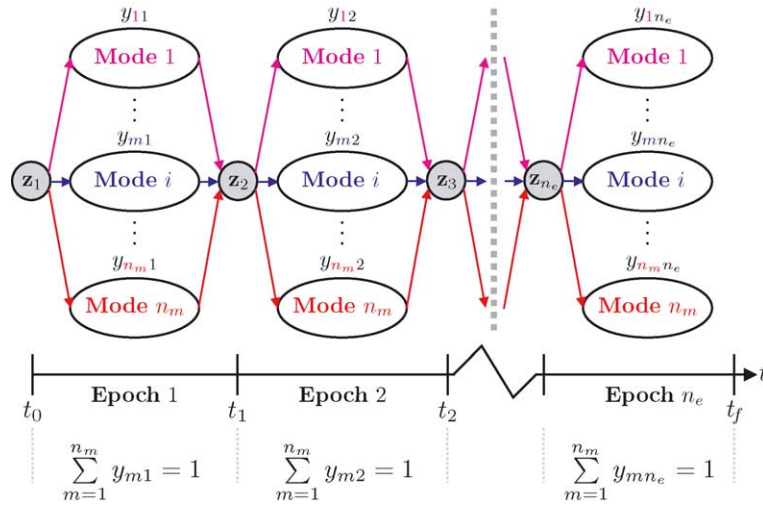


Fig. 7. Hybrid superstructure with binary variables.

Example 4 is a nonconvex MINLP with dynamic systems embedded. The same binary variables y_{mk} are introduced as in **Example 3**, resulting in the superstructure seen in Fig. 7. The key difference, however, is the introduction of the additional continuous parameters, p_2 and p_3 (shown as the variables z_i in Fig. 7, representing the initial conditions for each epoch), which transform the hybrid system into $n_m n_e$ equivalent linear dynamic systems. Eqs. (19) and (20) ensure that the correct transition functions are active at the events. This enables the application of the convexity theory presented to construct the lower bounding convex MINLP. In general, $n_x(n_e - 1)$ additional parameters need to be introduced into the nonconvex MINLP. However, these parameters will not affect the size of the primal or primal bounding problems. In addition, since MILP algorithms tend to scale linearly with the number of continuous variables and exponentially with the number of binary variables, these additional variables will usually not have a significant effect on the cost of solving the relaxed master problem. The bounds on these variables, $[p_2^L, p_2^U]$ and $[p_3^L, p_3^U]$, can be obtained from the original bounds on p_1 , as will be discussed below.

4.3. The primal problem

The primal problem, $NLP(Y^k)$, for **Example 4** is simply **Example 1** with the corresponding T_μ . The global solution is obtained using the B&B framework described in the preceding sections, and so the introduction of p_2 and p_3 does not affect the size of $NLP(Y^k)$.

4.4. The lower bounding convex MINLP

To construct the lower bounding convex MINLP, we need convex relaxations of Eqs. (18)–(20). We shall first treat the bilinear terms in Eqs. (19) and (20). Consider the following

constraints,

$$\begin{aligned} w &= yx, \\ y &\in \{0, 1\}, \\ x^L &\leq x \leq x^U. \end{aligned}$$

It is straightforward to obtain the following exact linearizations (Glover, 1975),

$$\begin{aligned} x^U(y - 1) + x &\leq w \leq x^L(y - 1) + x, \\ x^L y &\leq w \leq x^U y, \end{aligned}$$

which enables an exact linear reformulation of the bilinear terms in Eqs. (19) and (20) to be obtained. For example, Eq. (19) can be written as $p_2 = z_{11} + z_{21}$, where the exact linear reformulation for $z_{11} = y_{11}x_{11}(p, 1)$ can be obtained as

$$\begin{aligned} x_{11}^U(1)(y_{11} - 1) + x_{11}(p, 1) &\leq z_{11} \\ &\leq x_{11}^L(1)(y_{11} - 1) + x_{11}(p, 1), \end{aligned} \quad (21)$$

$$x_{11}^L(1)y_{11} \leq z_{11} \leq x_{11}^U(1)y_{11}, \quad (22)$$

and similarly for z_{21} . It is clear that when $y_{11} = 0$, Eq. (22) is active and $z_{11} = 0$; and when $y_{11} = 1$, Eq. (21) is active and $z_{11} = x_{11}(p, 1)$. Eqs. (21) and (22) are affine on $[0, 1] \times P$ because $x_{11}(p, 1)$ is affine in p . These linearizations for the relaxed master problem require $x_{11}^U(1)$, $x_{11}^L(1)$ and $x_{11}(p, 1) = m_{11}(1)^T p + n_{11}(1)$. The state bounds, as well as the parametric sensitivities and $n_{11}(1)$, can be obtained in a single preprocessing stage, which will be described below.

To treat the objective function, consider the following problem,

$$\min_{p, y} F(p, y) = y \int_0^1 -x^2(p, t) dt, \quad (23)$$

where $y \in \{0, 1\}$, $p \in [-4, 4]$ and $x(p, t)$ is given by the solution to the following linear system,

$$\begin{aligned}\dot{x} &= -2tx + p, \\ x(0) &= 1.\end{aligned}$$

Let an arbitrary $t \in [0, 1]$ be fixed. We have the following bounds,

$$\begin{aligned}x^L(t) &\leq x(p, t) \leq x^U(t), \\ v^L(t) &\leq -x^2(p, t) \leq v^U(t),\end{aligned}$$

where

$$v^L(t) = \min(-x^{L^2}(t), -x^{U^2}(t)), \quad (24)$$

$$v^U(t) = \begin{cases} -x^{L^2}(t) & \text{if } x^L(t) > 0, \\ -x^{U^2}(t) & \text{if } x^U(t) < 0, \\ 0 & \text{otherwise.} \end{cases} \quad (25)$$

The bounds in Eqs. (24) and (25) are constructed pointwise in time from the original objective function. We can then apply the convexification methods in McCormick (1976), together with Corollary 1, to obtain the following convex relaxation,

$$\min_{p, y, w} w, \quad (26)$$

$$(y - 1)w^U + c_w(p) - w \leq 0, \quad (27)$$

$$yw^L - w \leq 0, \quad (28)$$

where

$$w^L \equiv \int_0^1 v^L(t) dt, \quad w^U \equiv \int_0^1 v^U(t) dt, \quad (29)$$

$$c_w(p) \equiv \int_0^1 (x^L(t) + x^U(t))(x^L(t) - x(p, t)) - x^{L^2}(t) dt. \quad (30)$$

The constructed convex relaxations are shown in Fig. 8. Note that the expression for $c_w(p)$ has exactly the same form as

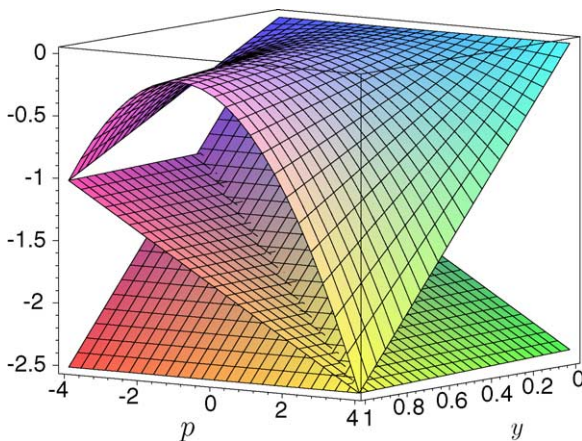


Fig. 8. Constructed convex relaxations for example objective function.

that obtained in Example 1. When $y = 0$, Eqs. (27) and (28) become

$$\begin{aligned}c_w(p) - w^U &\leq w, \\ 0 &\leq w,\end{aligned}$$

the second constraint is active, since $c_w(p) - w^U < 0$, and it is clear that the solution is $w = 0$. When $y = 1$, Eqs. (27) and (28) become

$$\begin{aligned}c_w(p) &\leq w, \\ w^L &\leq w,\end{aligned}$$

and either constraint can be active depending on the value of $c_w(p)$. These convex relaxations for the objective function require the bounds, w^L and w^U , which are obtained in the preprocessing stage described below.

The lower bounding convex MINLP can now be expressed as follows.

Example 5. Consider the following problem

$$\min_{p, Y, w, z} w_{11} + w_{21} + w_{12} + w_{22} + w_{13} + w_{23}$$

such that

$$y_{11} + y_{21} = 1, \quad y_{12} + y_{22} = 1, \quad y_{13} + y_{23} = 1,$$

$$\left. \begin{aligned} (y_{mk} - 1)w_{mk}^U + c_{mk}(p) - w_{mk} &\leq 0, \\ y_{mk}w_{mk}^L - w_{mk} &\leq 0, \end{aligned} \right\} \forall m = 1, 2; \\ k = 1, 2, 3$$

$$p_2 = z_{11} + z_{21}, \quad p_3 = z_{12} + z_{22},$$

$$\left. \begin{aligned} x_{mk}^U(t_k)(y_{mk} - 1) + x_{mk}(p, t_k) &\leq z_{mk}, \\ z_{mk} &\leq x_{mk}^L(t_k)(y_{mk} - 1) + x_{mk}(p, t_k), \\ x_{mk}^L(t_k)y_{mk} &\leq z_{mk}, \\ z_{mk} &\leq x_{mk}^U(t_k)y_{mk}, \end{aligned} \right\} \forall m = 1, 2; \\ k = 1, 2$$

where $x_{mk}(p, t)$ are given by the solution of the following linear systems:

$$\dot{x}_{11} = -2tx_{11} + p_1, \quad \dot{x}_{12} = -2tx_{12} + p_1, \quad \dot{x}_{13} = -2tx_{13} + p_1,$$

$$\dot{x}_{21} = \frac{x_{21} + p_1}{t + 10}, \quad \dot{x}_{22} = \frac{x_{22} + p_1}{t + 10}, \quad \dot{x}_{23} = \frac{x_{23} + p_1}{t + 10},$$

$$x_{11}(p, 0) = 1, \quad x_{12}(p, t_1) = p_2, \quad x_{13}(p, t_2) = p_3,$$

$$x_{21}(p, 0) = 1, \quad x_{22}(p, t_1) = p_2, \quad x_{23}(p, t_2) = p_3,$$

$Y \in Y^b = \{0, 1\}^{n_m \times n_e}$, $p = (p_1, p_2, p_3) \in P = [-4, 4] \times [p_2^L, p_2^U] \times [p_3^L, p_3^U]$, $w \in [w^L, w^U]$, $z_{mk} \in [\min(0, x_{mk}^L(t_k)), \max(0, x_{mk}^U(t_k))]$, $\forall m = 1, 2, k = 1, 2$, and $t_1 = 1, t_2 = 2$.

Table 1
Bounds for w , p , and x for Example 5

Variable	Lower	Upper
p_2	−1.784	2.520
p_3	−2.310	3.113
w_{11}	−5.195	−0.082
w_{21}	−1.583	−0.730
w_{12}	−3.545	0
w_{22}	−7.962	0
w_{13}	−2.203	0
w_{23}	−11.653	0
x_{11}	−1.784	2.520
x_{21}	0.700	1.500
x_{12}	−1.187	1.224
x_{22}	−2.310	3.113

The expressions for w_{mk}^L , w_{mk}^U , and $c_{mk}(p)$ are the corresponding versions of Eqs. (29) and (30) and are not included in the example above for clarity. The required bounds for this lower bounding convex MINLP can be calculated in the preprocessing stage, described below.

4.5. The preprocessing stage

In the preprocessing stage, we extract the bounds needed for the lower bounding convex MINLP, as well as the expression for $x_{mk}(p, t_k)$. First, we integrate the n_m sets of linear systems through the first epoch. We have already shown how to calculate the implied state bounds, $x_{mk}^L(t)$ and $x_{mk}^U(t)$, and the parametric sensitivities, $m_{mk}(t)$, $n_{mk}(t)$, as well as w_{mk}^L and w_{mk}^U . At the end of the first epoch, we can determine the bounds for p_2 , from the implied state bounds at time t_k , in this case,

$$p_2^L = \min[x_{11}^L(1), x_{21}^L(1)], \quad p_2^U = \max[x_{11}^U(1), x_{21}^U(1)].$$

With these bounds on p_2 , we can then integrate the next n_m sets of linear systems through the second epoch, and repeat the procedure to the last epoch. The bounds obtained for our example are shown in Table 1.

4.6. The primal bounding problem

When Y^k is fixed, the underlying dynamic system for the primal bounding problem simplifies to the equivalent hybrid system with T_μ fixed. As mentioned above, only the convex relaxations of the objective function with $y_{mk} = 1$ are active, and only these terms enter the convex NLPB(Y^k).

4.7. The relaxed master problem

The relaxed master problem is derived from the lower bounding convex MINLP by constructing linearizations of the constraints at the solution obtained from the primal

bounding problem. The following are some important points to note about the relaxed master problem:

1. The majority of the constraints are linear in the relaxed Master problem. Additional linearizations only have to be constructed for the nonlinear constraints introduced in the convex relaxations of the original objective function and constraints.
2. The form of Eq. (17) in the relaxed master problem will enable the special structure of SOS1 sets (Type 1 Special Ordered Sets) to be exploited in the solution of the MILP.
3. In constructing the linearizations, it suffices to add only the *active* constraints (Fletcher & Leyffer, 1994), from the primal bounding problem. Although it is possible that the lower bounds generated might become weaker, this is attractive because the $n_m n_e$ sets of sensitivity systems do not have to be integrated after every primal bounding problem to furnish the gradients of all the nonlinear constraints in the lower bounding MINLP, as the gradients of the active constraints can be directly obtained from the solution of the primal bounding problem.

In this example, the OA algorithm terminates at the second iteration, for a global solution of $T_\mu = 1, 2, 2$, $p = 4$, with an objective function of $F(4) = -24.810$.

5. Global optimization with varying T_τ and T_μ

In the preceding sections, we have developed deterministic algorithms for the global optimization of linear hybrid systems with fixed T_τ . We are interested in extending it further to the case where T_τ is allowed to vary, i.e., the transition times are optimization parameters. This seemingly simple extension turns out to be quite difficult and nontrivial. We shall present some preliminary ideas on treating the single stage version of this problem in this section.

Problem 2. Consider the following problem

$$\min_{p \in P, \xi \in \Xi} F(p, \xi) = \phi(\dot{x}(p, \xi), x(p, \xi), p, \xi) + \int_0^\xi f(\dot{x}(p, t), x(p, t), p, t) dt, \quad (31)$$

such that

$$G(p, \xi) = \eta(\dot{x}(p, \xi), x(p, \xi), p, \xi) + \int_0^\xi g(\dot{x}(p, t), x(p, t), p, t) dt \leq 0, \quad (32)$$

where $x(p, t)$ is given by the solution of the dynamic system:

$$\begin{aligned} \dot{x}(p, t) &= A(t)x(p, t) + B(t)p + q(t), \\ x(p, 0) &= Ep + k, \end{aligned}$$

P is a compact, convex and nonempty subset of \mathbb{R}^n ; and $\Xi = [t^L, t^U]$, $0 \leq t^L < t^U$.

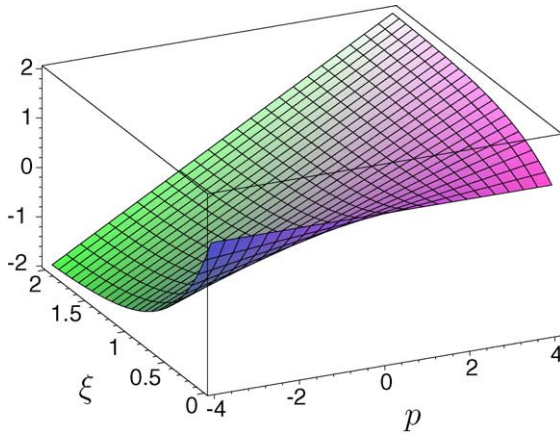


Fig. 9. Objective function surface plot for Example 6.

A common model transformation technique is often employed to transform this free terminal time problem into a fixed end time problem (Teo, Goh, & Wong, 1991), where ξ is treated as a parameter, and time is scaled by introducing a normalizing time variable, $\tau = t/\xi$. In that case, the integrals are converted to ones between 0 and 1 with respect to τ . The problem with adopting this approach is that bilinear/nonlinear terms are introduced into every equation of the embedded dynamic system. This would require methods of constructing convex relaxations for nonlinear systems, which are still under development (Singer & Barton, 2003a).

An alternative way of solving the problem is to note that for fixed ξ , Problem 2 reverts to Problem 1, which can be solved. We can then discretize the set \mathcal{E} , obtain the solution for the fixed end time problem at the mesh points, and choose the best feasible solution. This discretization technique has been employed in Canon, Cullum, and Polak (1970) for the solution of linear optimal control problems with linear cost objectives in the discrete time domain. However, in order to get ε tolerance in the variable ξ , we will need a very fine partition of the continuous time domain $[t^L, t^U]$, making it necessary to solve the fixed end time problem a large number of times, which might not be practical. Hence, a better method is needed.

To illustrate that the problem is inherently nonconvex, consider the following example with a simple end point objective.

Example 6. Consider the following problem

$$\min_{p, \xi} x(p, \xi),$$

where $x(p, \xi)$ is given by the solution to the following linear system,

$$\begin{aligned} \dot{x}(p, t) &= -2x(p, t) + p, \\ x(p, 0) &= 1, \\ p &\in P = [-4, 4], \quad \xi \in \mathcal{E} = [0, 2]. \end{aligned}$$

Fig. 9 shows that the objective function is not convex over

the set $P \times \mathcal{E}$. Since we have a LTV ODE system, in general, we would expect the problem to be nonconvex on \mathcal{E} even if we have p fixed. In order to use a B&B algorithm to obtain a global solution to Problem 2, we need a method to construct rigorous lower bounds for the objective function $F(p, \xi)$ on partitions of the search space $P \times \mathcal{E}$. We are currently exploring the use of a primal-relaxed dual decomposition approach (Wolsey, 1981; Floudas & Visweswaran, 1993; Liu & Floudas, 1996) to generate these rigorous lower bounds.

The convexity theory presented in the previous section allows a relaxation $U(p, \xi)$ to be constructed for $F(p, \xi)$ such that it is convex on P for all fixed $\xi \in \mathcal{E}$. In other words, $U(p, \xi)$ is *partially convex* on P . The idea is then to construct a relaxation $V(p, \xi)$ of $U(p, \xi)$ such that $V(p, \xi)$ is partially convex on both \mathcal{E} and P . We suspect that this task, although non-trivial, is less formidable than constructing a convex relaxation for $F(p, \xi)$ that is jointly convex on $P \times \mathcal{E}$. We are exploring whether existing methods for constructing convex envelopes for functions of a single variable (McCormick, 1976) can be utilized to achieve this task. Once $V(p, \xi)$ can be constructed, the primal-relaxed dual algorithms described above can be harnessed to obtain the required rigorous lower bounds.

6. Conclusions

The development of deterministic global optimization algorithms for nonconvex, nonsmooth dynamic optimization problems with nonlinear hybrid systems embedded has been motivated by the increasing need to devise robust and efficient methods for the automated design of optimal process operations such as start-up and shut-down procedures, as well as formal verification problems in the design of logic-based controllers which take into account the continuous dynamics of the underlying process.

This paper describes recent progress toward the development of suitable algorithms. A method to construct convex relaxations for general, nonlinear Bolza-type functionals subject to an embedded linear time-varying hybrid system with fixed transitions is presented. The theoretical basis for the above method lies in the development of a convexity theory (Singer & Barton, 2003b), that allows existing methods for constructing symbolic convex relaxations on Euclidean spaces to be harnessed for the above purpose.

A branch and bound algorithm, utilizing these convex relaxations to obtain rigorous lower bounds on partitions of the parameter space, has been developed to solve the optimization problem to guaranteed global optimality. In addition, a novel reformulation has been proposed for problems where the temporal sequence of model switches and jumps in the linear time-varying hybrid system is allowed to vary. By introducing binary decision variables which represent all possible sequences of modes, and retaining the linearity of the underlying dynamic system with the insertion of

additional continuous parameters, the convexity theory can be utilized to construct a lower bounding convex MINLP. This enables the development of an outer approximation algorithm to solve this nonconvex MINLP formulation to guaranteed global optimality.

The techniques described above will serve as the basis for the development of suitable algorithms for the optimization of general nonlinear hybrid systems. More research has to be conducted to investigate the computational efficiency of the proposed methods, on a variety of problems. In addition, there remain a lot of exciting and challenging obstacles to overcome. We have described some preliminary work on handling hybrid systems with varying transition times. Another important area under active research is the extension of the convexity theory to problems with nonlinear dynamic systems embedded. Although the direct construction of convex relaxations subject to an arbitrary nonlinear dynamic system appears difficult without the introduction of strongly restrictive assumptions, one can consider extending the convexity theory for linear systems to develop *bounding* linear systems for the nonlinear system of interest (Singer & Barton, 2003a).

Other future work that remains to be done includes the application of the presented algorithms to large-scale problems. Of particular interest is the development of algorithms for the formal verification of logic-based controllers. The formulation of a safety verification problem often results in a nonconvex MINLP. Because of the potential size of such problems, the outer approximation algorithm has to deal with a large number of binary decision variables. However, a distinctive feature of nonconvex outer approximation lies in the fact that the solution of the primal problems can be decoupled from the rest of the iterations and done in parallel. We are exploring the development of massively parallel implementations which have the potential to improve efficiency dramatically.

Acknowledgements

This work was supported by the DoD Multidisciplinary University Research Initiative (MURI) program administered by the Army Research Office under Grant DAAD19-01-1-0566. This material is based upon work supported by the National Science Foundation under Grant No. CCR-0208956.

References

- Adjiman, C. S., Androulakis, I. P., & Floudas, C. A. (2000). Global optimization of mixed-integer nonlinear problems. *AIChE Journal*, 46(9), 1769–1797.
- Adjiman, C. S., Dallwig, S., Floudas, C. A., & Neumaier, A. (1998). A global optimization method, α BB, for general twice-differentiable constrained NLPs. I. Theoretical advances. *Computers and Chemical Engineering*, 22(9), 1137–1158.
- Alur, R., Courcoubetis, C., Halbwachs, N., Henzinger, T. A., Ho, P.-H., Nicollin, X., Olivero, A., Sifakis, J., & Yovine, S. (1995). The algorithmic analysis of hybrid systems. *Theoretical Computer Science*, 138, 3–34.
- Avraam, M. P., Shah, N., & Pantelides, C. C. (1998). Modelling and optimisation of general hybrid systems in the continuous time domain. *Computers and Chemical Engineering*, 22(Suppl.), S221–S228.
- Bagajewicz, M. J., & Manousiouthakis, V. (1991). On the generalized Benders decomposition. *Computers and Chemical Engineering*, 15(10), 691–700.
- Barton, P. I., Allgor, R. J., Feehery, W. F., & Galan, S. (1998). Dynamic optimization in a discontinuous world. *Industrial Engineering and Chemistry Research*, 37(3), 966–981.
- Barton, P. I., Banga, J. R., & Galán, S. (2000). Optimization of hybrid discrete/continuous dynamic systems. *Computers and Chemical Engineering*, 24(9–10), 2171–2182.
- Barton, P. I., & Lee, C. K. (2002). Modeling, simulation, sensitivity analysis and optimization of hybrid systems. *ACM Transactions on Modeling and Computer Simulation*, 12(4), 256–289.
- Barton, P. I., & Pantelides, C. C. (1994). Modeling of combined discrete/continuous processes. *AIChE Journal*, 40, 966–979.
- Bemporad, A., Borrelli, F., & Morari, M. (2000). Optimal controllers for hybrid systems: Stability and piecewise linear explicit form. In *Proceedings of the 39th IEEE conference on decision and control* (vol. 2, pp. 1810–1815).
- Canon, M. D., Cullum, C. D., & Polak, E. (1970). *Theory of optimal control and mathematical programming*. New York: McGraw-Hill.
- Clabaugh, J. A., Tolsma, J. E., & Barton, P. I. (1999). ABACUSS II: Advanced modeling environment and embedded simulator. <http://yoric.mit.edu/abacuss2/abacuss2.html>.
- Coddington, E. A., & Levinson, N. (1955). *Theory of ordinary differential equations*. New York: McGraw-Hill.
- Cuzzola, F. A., & Morari, M. (2001). A generalized approach for analysis and control of discrete-time piecewise affine and hybrid systems. In M. D. D. Benedetto, & A. Sangiovanni-Vincentelli (Eds.), *Hybrid systems: computation and control* (vol. 2034, pp. 189–203). *Lecture Notes in Computer Science*. Berlin: Springer-Verlag.
- Duran, M. A., & Grossmann, I. E. (1986). An outer-approximation algorithm for a class of mixed-integer nonlinear programs. *Mathematical Programming*, 36, 307–339.
- Falk, J. E., & Soland, R. M. (1969). An algorithm for separable nonconvex programming problems. *Management Science*, 15(9), 550–569.
- Feehery, W. F., Tolsma, J. E., & Barton, P. I. (1997). Efficient sensitivity analysis of large-scale differential-algebraic systems. *Applied Numerical Mathematics*, 25(1), 41–54.
- Fletcher, R., & Leyffer, S. (1994). Solving mixed integer nonlinear programs by outer approximation. *Mathematical Programming*, 66, 327–349.
- Floudas, C. A. (1995). *Nonlinear and mixed-integer optimization: Fundamentals and applications*. Oxford: Oxford University Press.
- Floudas, C. A., & Visweswaran, V. (1993). Primal-relaxed dual global optimization approach. *Journal of Optimization Theory and Applications*, 78(2), 187–225.
- Galán, S., & Barton, P. I. (1998). Dynamic optimization of hybrid systems. *Computers and Chemical Engineering*, 22(Suppl.), S183–S190.
- Galán, S., Feehery, W. F., & Barton, P. I. (1999). Parametric sensitivity functions for hybrid discrete/continuous systems. *Applied Numerical Mathematics*, 31(1), 17–48.
- Glover, F. (1975). Improved linear integer programming formulations of nonlinear integer problems. *Management Science*, 22(4), 455–460.
- Kesavan, P., Allgor, R. J., Gatzke, E. P., & Barton, P. I. (2001). Outer approximation algorithms for separable nonconvex mixed-integer nonlinear programs. *Mathematical Programming*, submitted for publication. Available from <http://yoric.mit.edu/publications.html>.
- Kesavan, P., & Barton, P. I. (2000). Decomposition algorithms for nonconvex mixed-integer nonlinear programs. *AIChE Symposium Series*, 96(323), 458–461.

- Kocis, G. R., & Grossmann, I. E. (1989). A modelling and decomposition strategy for the MINLP optimization of process flowsheets. *Computers and Chemical Engineering*, 13(7), 797–819.
- Lee, C. K., Singer, A. B., & Barton, P. I. (2003). Global optimization of linear hybrid systems with explicit transitions. *Systems Control Letters*, in press.
- Liu, W. B., & Floudas, C. A. (1996). Generalized primal-relaxed dual approach for global optimization. *Journal of Optimization Theory and Applications*, 90(2), 417–434.
- McCormick, G. P. (1976). Computability of global solutions to factorable nonconvex programs. Part I. Convex underestimating problems. *Mathematical Programming*, 10, 147–175.
- Ryoo, H. S., & Sahinidis, N. V. (1996). A branch-and-reduce approach to global optimization. *Journal of Global Optimization*, 8(2), 107–139.
- Sahinidis, N. V., & Grossmann, I. E. (1991). Convergence properties of generalized Benders decomposition. *Computers and Chemical Engineering*, 15(7), 481–491.
- Shakernia, O., Pappas, G. J., & Sastry, S. (2000). Semidecidable controller synthesis for classes of linear hybrid systems. In *Proceedings of the 39th IEEE conference on decision control* (vol. 2, pp. 1834–1839).
- Singer, A. B., & Barton, P. I. (2003a). Global optimization with nonlinear ordinary differential equations. Technical report. Department of Chemical Engineering, MIT.
- Singer, A. B., & Barton, P. I. (2003b). Global solution of linear dynamic embedded optimization problems. *Journal of Optimization Theory and Applications*, in press.
- Teo, K., Goh, G., & Wong, K. (1991). A unified computational approach to optimal control problems. In *Pitman monographs and surveys in pure and applied mathematics*. New York: Wiley.
- Tolsma, J. E., & Barton, P. I. (1999). DAEPACK: A symbolic and numeric library for open modeling. <http://yoric.mit.edu/daepack/daepack.html>.
- Tolsma, J. E., & Barton, P. I. (2000). DAEPACK: An open modeling environment for legacy models. *Industrial Engineering and Chemical Research*, 39(6), 1826–1839.
- Tolsma, J. E., & Barton, P. I. (2002). Hidden discontinuities and parametric sensitivity calculations. *SIAM Journal on Scientific Computing*, 23(6), 1862–1875.
- Tolsma, J. E., Clabaugh, J. A., & Barton, P. I. (2002). Symbolic incorporation of external procedures into process modeling environments. *Industrial Engineering and Chemistry Research*, 41(16), 3867–3876.
- Trontis, A., & Spathopoulos, M. P. (2001). Target control for hybrid systems with linear continuous dynamics. In *Proceedings of the 40th IEEE conference on decision and control* (vol. 2, pp. 1229–1234).
- Wolsey, L. A. (1981). Decomposition algorithms for general mathematical programs. *Mathematical Programming Study*, 14, 244–257.
- Xu, X., & Antsaklis, P. J. (2001). An approach for solving general switched linear quadratic optimal control problems. In *Proceedings of the 40th IEEE conference on decision and control* (pp. 2478–2483).