Convex Underestimators For Dynamic Optimization Problems

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1 Summary of Proposed Research

The objective of the proposed research is to develop deterministic global optimization algorithms for nonconvex dynamic optimization. Problems considered under this formulation include, but are not limited to, classical variational calculus problems, optimal control problems, and mixed-integer dynamic optimization problems. We propose to develop rigorously proven algorithms guaranteeing theoretical convergence to the global minimum of such problems.

Many modern algorithms for deterministic global optimization in algebraic spaces rely on the notion of convex underestimators for generating rigorous lower bounds on the minimum of nonconvex functions. Convex underestimators are extraordinarily useful in a branch and bound framework because they possess the property that any minimum is guaranteed to be global. Several well known procedures exist for constructing convex underestimators when the functional form of an optimization problem in Euclidean space is known explicitly and can be manipulated symbolically. Unfortunately, none of these methods are directly applicable to optimization problems involving dynamic systems. Here, we propose a novel optimization technique in which the functional forms of the integrand and embedded differential equations are utilized to develop a new convexity theory enabling the generation of convex underestimators for nonconvex dynamic programs. A remarkable consequence of this approach is that the aforementioned known symbolic convex underestimators in algebraic spaces can be directly harnessed to construct convex underestimators for dynamic optimization problems.

The proposed research can be divided into two fundamental paradigms: the composite function approach and the variational approach. The composite function approach relies on the ability to transform a dynamic optimization problem into an algebraic optimization problem via the composition of the solution to an embedded dynamic system with a convex relaxation of the objective function. The variational approach derives convex underestimators for dynamic systems on linear spaces of functions and then seeks to solve these optimization problems via an augmented form of the Euler-Lagrange equations as derived via the classical calculus of variations. While both approaches clearly depend on different optimality conditions to guarantee local minimums, they share in common the branch and bound framework to converge to a global minimum. Furthermore, both approaches rely upon the generation, by standard techniques, of convex underestimators for integrands in order to derive relaxations of the nonconvex integral objective functions. Thus, both the composite function approach and the variational approach can be viewed as separate applications of a unified convexity theory for dynamic systems.

This research will yield fundamental contributions to dynamic optimization via the development of a convexity theory for dynamic embedded optimization problems and via the development of methods for the construction of convex underestimators for dynamic optimization problems. This theory will lead to a series of practical deterministic global optimization algorithms for the solution of these problems. Furthermore, the underlying theory governing the solution of these problems will guarantee global optimality. Moreover, this rigorous guarantee of global optimality for dynamic programs will have a profound influence on many industrial applications. For example, in the area of process operations, there is hope for solving problems such as formal safety verification, the synthesis of integrated batch processes, and the design of major process transients such as start-up and shut-down procedures. However, the scope of this research will not be limited merely to the chemical industries. It is believed that because these solution methods depend only on the mathematical structure of the dynamic program at hand, the developed techniques will be readily extendable to dynamic optimization problems encountered in almost all branches of the pure and applied sciences.

2 Introduction

Strong economic incentives exist for conducting process operations in the most efficient manner possible, particularly in the commodities sectors. With globalization of the world economy, these incentives will become even greater in the future. Moreover, an increasingly demand driven and competitive global economy is motivating many chemical and biological products to be manufactured in campaign continuous processes. These are flexible continuous processes that produce a variety of different but related products or grades of product. Each individual product is made during a short, demand driven campaign, and then a changeover occurs to a new product or grade; this cycle continues repeatedly. One example includes polymer processes where many different molecular weight grades are produced in a single plant. Another example is in fertilizer processes where many different N/K/P mixes are demanded by the market on a fluctuating basis. Campaign continuous processes may spend up to 50% of their total operating time in transitions between steady-states; thus, the performance of the process during these transients becomes as crucial as the steady-state performance. Therefore, consideration of operability and transient issues simultaneously with steady-state issues must be thoroughly addressed in order to achieve the most economic overall process design.

Another particularly important aspect of the study of dynamic systems is the relevance to environmental concerns. Most of the environmental impact of any continuous process is typically created during major transient, including off specification product, high energy consumption, waste products from suboptimal reactor operating conditions, etc. This derives from the fact that steady-state design has become such a refined art that processes producing large quantities of waste at steady-state have become economically unviable. Process safety is another area in which process transients play a crucial role. A much wider variety of hazardous situations can develop in a plant that experiences frequent transients and constant changeovers; thus, much more careful and thorough attention must be paid to mitigating these hazards.

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 processes, semi-continuous processes, and periodic process that operate at a cyclic steady-state. The design of inherently transient systems is in essence an exercise in optimal process operation. The batch mode of operation is the preferred method of manufacturing in the synthetic pharmacuetical, biotechnology, specialty polymers, electronic materials, and specialty agrochemicals industries. Moreover, much speculation presently exists that product design will emerge as the new paradigm of chemical engineering, and the related new chemical products will all be manufactured via batch processes. All of these considerations motivate research on design procedures for optimizing the performance of inherently transient manufacturing systems.

This proposal focuses on problems in process operations for which a detailed, typically nonlinear, differential equation model is employed to describe the behavior of the physical system. Often, one is interested in determining input profiles or parameters for a dynamic model for the purpose of optimizing the operation of a system over some period of time according to a specified performance metric. Such problems are referred to as dynamic optimization problems or open-loop optimal control problems. Examples include determination of optimal operating profiles for batch unit operations [59]; determination of optimal plantwide recipes for batch processes [20]; fitting of chemical reaction kinetics parameters to data [16]; determination of optimal changeover policies [29]; the determination of catalyst blend profiles for PFRs [47]; optimal drug scheduling for cancer chemotherapy [51]; process safety analysis [1]; optimization of chemical vapor deposition processes [58]; in principle, model predictive control with a continuous time model; etc.

One of the primary distinctions between optimizing a dynamic system and optimizing an algebraic system is that the optimization variables in a dynamic system lie in an infinite dimensional space while the optimization variables in an algebraic system lie in a finite dimensional space. For this reason, the methods employed for solving algebraic systems cannot be immediately extended to solving dynamic systems. The techniques utilized for solving dynamic systems fall under two broad frameworks: variational methods and discretization methods. The sequel addresses these two methods separately expounding upon the virtues and deficiencies of each.

The first technique, the variational approach, encompasses the classical methods of the calculus of variations and many of the modern methods of optimal control. These methods approach the problem in the infinite dimensional space and attempt to determine stationary functions via the solution of the Euler-Lagrange equations. The variational approach for solving dynamic optimization problems is extremely attractive because by solving the optimization problem in the infinite dimensional space, the problem can be solved in its original form without any mathematical transformations. Hence, the solution is guaranteed to be a rigorous solution to the original problem. Despite this benefit, the variational approach has several large drawbacks. Inherently, the Euler-Lagrange equations are difficult to solve numerically because they amount to a two point boundary value problems. Complicating this issue is the addition of Lagrangian inequality constraints on the state variables, an omnipresent artifact of practical optimal control problems. Many efforts have been made to address the solution of variational calculus and optimal control problems subject to bounded states beginning with the work of Valentine [71]. Among many other authors, determining necessary conditions for variational problems with inequality constrained state variables has been addressed by Dreyfus [23], Berkovitz [15], Chang [19], Speyer and Bryson [67], and Jacobson and Lele [40, 41]. Additionally, as noted, most of the work concerning variational problems with inequality constrained state variables has been in determining necessary conditions yielding stationary functions. However, any global optimization scheme requires that optimality conditions be both necessary and sufficient because the set of solutions satisfying only necessary conditions is actually a superset of the set containing all minimizing functions. In fact, not only does satisfying a necessary condition not yield the global minimum, the satisfaction of this condition does not guarantee even that a local minimum has been found. Unfortunately, the necessary and sufficient conditions are known only to match identically for the special case of unconstrained convex problems. Recently, Singer *et al.* [66] have proven that for convex variational problems subject to convex state inequality constraints, the necessary and sufficient conditions guaranteeing a minimum differ from each other only slightly. Future work addressing the variational approach will focus on closing this gap in the optimality conditions for the purpose of globally solving nonconvex dynamic optimization problems via a branch and bound algorithm based on convex relaxation.

In addition to the variational approach for solving dynamic optimization problems, there is another approach based upon discretization. While discretization has the disadvantage that it is only an approximation of the infinite dimensional problem, it possesses the tremendous advantage that it transforms the original infinite dimensional problem into a problem lying at least partially in a finite space; therefore, the problem can often be solved by standard nonlinear programming methods. Discretization can be subdivided into two broad classifications known as simultaneous and sequential. The simultaneous method is a complete discretization of both state and control variables often achieved via collocation [70, 56]. While completely transforming a dynamic system into a system of algebraic equations, simultaneous discretization has the unfortunate side effect of generating a multitude of additional variables yielding large, unwieldy nonlinear programs (NLPs) that are impractical to solve. Sequential discretization is usually achieved via control parameterization [63, 68] in which the control variable profiles are approximated by a collection of basis functions in terms of a finite set of real parameters. These parameters then become the decision variables in a dynamic embedded NLP. Function evaluations are provided to this NLP via numerical solution of a fully determined initial value problem (IVP), which is given by fixing the control profiles. This method has the advantages of yielding a relatively small NLP and exploiting the robustness and efficiency of modern IVP and sensitivity solvers [49, 28].

It has been known for a number of years that dynamic optimization problems encountered in chemical engineering applications exhibit multiple local minima almost pathologically [12, 48, 47]. This property, which can be attributed to nonconvexity of the functions participating in most chemical engineering models, implies that standard local optimization methods will often yield suboptimal solutions to problems. Suboptimality can have direct economic, safety, and environmental impacts if a suboptimal operating policy is implemented on a real process. The classical approach to nonconvex variational problems is to reformulate them so that they are convex and then apply the relevant necessary and sufficient Euler-Lagrange conditions [69]. However, only a very few small problems are accessible to such analysis. This deficiency has motivated researchers to develop global optimization algorithms for nonconvex dynamic optimization problems. Of particular interest are deterministic global optimization algorithms, or those methods rigorously proving the finite convergence of the algorithm to global optimality. The usage of these algorithms therefore guarantees the optimal operating policy has been found for the considered formulation.

A great deal of research has been devoted to the application of stochastic optimization methods to overcome convergence only to local minima. In chemical engineering, this body of research has been dominated by Banga and co-workers (e.g., [12, 18]) and Luus and co-workers (e.g., [48, 47]). While these methods often perform better than those mentioned above, they are typically very computationally expensive, and they typically have difficulty with highly constrained problems because they tend not to converge to solutions at which multiple constraints are active. Most importantly, however, even the best stochastic search method cannot guarantee locating the global solution in a finite number of iterations.

Galperin and Zheng [34] have developed a method for globally optimizing optimal control problems via a measure theory approach. Their contribution to dynamic optimization is based upon their previous work [33] in which they propose a global algorithm for solving nonlinear observation and identification problems. This method requires determining the Lebesgue measure of level sets of the objective function. While this technique theoretically guarantees determination of a global minimum, implementation for large problems is impractical due to the sampling required for generating level sets.

As previously discussed, one of the most important industrial applications of dynamic systems is to model the changing of operating conditions of a chemical process. Often, the chemicals produced during the changeover are unsuitable for market. Therefore, a very important dynamic optimization problem consists of determining the control procedure that minimizes the time required to switch from one operating condition to another. Canon *et al.* [17] have examined this problem and have outlined a solution technique for problems obeying a special structure. For final time minimization of a linear time-invariant system with piecewise constant controls subject to endpoint constraints, they have shown that via a time discretization approach, the problem can be reformulated as a sequence of linear programs. Because linear programs are inherently convex, their method achieves a global solution for the reformulated problem.

Many modern, general methods for deterministic global optimization in Euclidean spaces rely on the notion of a convex underestimator for a nonconvex function [52]. As the name implies, a convex underestimator is a convex function that underestimates a nonconvex function on the set of interest. The highest possible convex underestimator is termed the convex envelope of the nonconvex function [27]. Because convex underestimating problems can be solved to guaranteed global optimality, they are employed to generate rigorous lower bounds on nonconvex problems. For this reason, convex underestimators are ideally suited as the relaxations required by a deterministic global branch-and-bound algorithm for solving nonconvex NLPs [52, 27, 39]. Floudas and co-workers have demonstrated that a convex underestimator can be constructed for any twice continuously differentiable nonconvex function via a shift of the diagonal elements of the Hessian matrix of the nonconvex function [50]. The shift parameter, α, is utilized in conjunction with a branch-and-bound algorithm for the global solution of NLPs; this NLP solution technique has been termed αBB. In later work, Floudas *et al.* demonstrated a method by which rigorous values for α may be computed via interval analysis [4, 3], provided the functional form of the algebraic optimization problem is known explicitly as an elementary function and can be manipulated symbolically.

Building upon the αBB framework, Esposito and Floudas [26, 25] describe what is probably the first practical algorithm for the deterministic global optimization of dynamic systems. Subject to mild assumptions, they have shown that an NLP with a dynamic embedded system (potentially derived from the control parameterization of a dynamic optimization) is twice continuously differentiable; hence, similarly to αBB, a shift parameter for the Hessian can be found to yield a convex underestimator for any nonconvexities. This shift parameter, denoted β, is used in conjunction with a branch-and-bound algorithm to solve a dynamic embedded NLP; this technique has been termed βBB. As previously discussed, the rigorous calculation of a Hessian shift parameter requires the explicit functional form of the function to be underestimated. However, in a dynamic embedded problem, the functional dependence of the objective function and constraints on the control parameters is rarely known explicitly. Rather, the functional dependence is implied computationally by the numerical integration of the dynamic embedded system. Hence, except in analytically tractable problems, the interval analysis methods for generating rigorous β parameters are not applicable. To circumvent this problem, several heuristic methods have been proposed to compute β. Unfortunately, all of the proposed methods rely either on arbitrary selection of β or on sampling to determine estimates of the true Hessian matrix. Not only is this method of calculating β not rigorous, in fact, these methods cannot even provide guarantees that the derived underestimator is convex over the entire region of interest. Furthermore, in order to generate a reasonable value for β, the Hessian matrix requires a relatively large number of sampled points. Because the size of the sampling space grows exponentially with the number of decision variables, practical implementation of βBB would become intractable rather quickly.

In recent years, there has been growing interest in problems in process design and operations that can be formulated as dynamic optimization problems coupled with integer decisions; these problems are known as mixed-integer dynamic optimization (MIDO) problems [6, 7]. Binary or integer decision variables are often introduced in an optimization formulation to represent the inclusion or exclusion of elements in design, discontinuities in the model, and temporal sequencing decisions. If the underlying model is dynamic, such a formulation yields a MIDO problem. Examples thusfar reported in the literature include the synthesis of integrated batch processes [6, 7], the interaction of design and control and operations [53, 54, 64], kinetic model reduction [57, 8], and the design of batch distillation columns [65]. Similarly, problems in safety verification have been formulated as a mixed-integer optimization problem with a linear, discrete time model [22]; use of a more realistic nonlinear, continuous time model would directly yield a MIDO formulation. One should note that the use of a deterministic global optimization scheme is absolutely vital here, for formal safety verification requires a rigorous proof that the formulated safety property is satisfied by the model.

In addition to the recent interest in MIDO problems, there has also been growing interest in the optimization of dynamic systems containing discontinuities (events); these problems are termed hybrid discrete/continuous systems. As an example, these formulations can be used to design major process transients such as start-up and shut-down procedures [31, 14]. The most interesting class of problems are those in which the sequence of discontinuities along the optimal trajectory can vary with parameters in the decision space, and the optimal sequence of events is sought; such optimization problems have been shown to be nonsmooth [31, 32]. This suggests a MIDO formulation for hybrid discrete/continuous dynamic optimization in which binary variables are introduced to represent the different sequences of events that can occur [14]. Recently, it has been proposed to address the optimal design of campaign continuous processes via a combination of MIDO and hybrid dynamic optimization formulations [13].

Standard algorithms for general mixed-integer nonlinear optimization in Euclidean spaces assume that the participating functions are convex [36, 24, 30]. It is well known that if such algorithms are applied to problems in which the participating functions are nonconvex, the algorithm converges to arbitrary suboptimal solutions [45, 61, 11]. Convergence to such arbitrarily suboptimal solutions is far worse than convergence to a local minimum because the algorithms add constraints during the solution process that arbitrarily exclude portions of the search space. These observations extend identically to MIDO problems [6, 7]; however, this has not stopped several authors from applying these unsuitable algorithms to MIDO problems indiscriminately [53, 54, 64, 65], although one wonders about the utility of the answers found. Deterministic global optimization is really the only valid method to solve both mixed-integer optimization and MIDO problems. In recent years, a number of general deterministic global optimization algorithms have emerged for the solution of mixed-integer nonlinear programs and integer nonlinear programs in which the participating functions are nonconvex [61, 2, 42, 43, 44]. Although these algorithms are completely rigorous, they all rely on explicit knowledge of the functional form of the optimization problem in a Euclidean space. Hence, none of these algorithms are immediately applicable to dynamic embedded optimization problems.

The purpose of the proposed research is to develop deterministic global optimization algorithms for nonconvex dynamic embedded optimization, MIDO, nonconvex variational, and nonconvex optimal control problems. The proposed methods are based on novel extensions of convexity theory to dynamic optimization problems for use in the generation of convex relaxations. These convex underestimators will then be utilized in a conventional branch-and-bound framework to generate a deterministic algorithm for solving dynamic optimization to global optimality. The ultimate goal of the project is to use the derived theory to develop practical computer implementations of these algorithms to solve large scale dynamic optimization problems. This goal has only recently become feasible. Because our novel convexity theory requires the generation of standard convex underestimators for algebraic functions on Euclidean spaces, any algorithm would ideally automate this process of determining elementary convex underestimators. Recently, Smith [21] has developed an algorithm for decomposing complex elementary functions into simpler functions for which the convex underestimators are known. Moreover, Adjiman *et al.* have shown that the determination of the α for the αBB algorithm can be performed automatically [3]. Building on the work of Smith *et al.* and Adjiman *et al.*, Gatzke and co-workers have developed a code that enables convex underestimators for elementary functions to be determined automatically from FORTRAN source code [35]. It is anticipated that these automatic convexification techniques will prove indispensible in the generation of any fully automated deterministic global optimization algorithm for dynamic optimization problems.

3 Global Optimization with Linear Dynamic Embedded Systems

3.1 Problem Statement

In the following section, a novel deterministic method for globally solving dynamic optimization problems with linear dynamic systems embedded is developed. Additionally, in this section, much of the convexity theory required throughout the proposal will also be developed. We begin by stating the problem in its general form.

Problem 3.1.1. Let Y be a nonempty compact convex subset of $\mathbb{R}^n$, $X \subseteq \mathbb{R}^m$ such that $\mathbf{x}(t,\mathbf{y}) \in X$ $\forall\ (t,\mathbf{y}) \in [t_0,t_f]\times Y$, $X' \subseteq \mathbb{R}^m$ such that $\mathbf{x}'(t,\mathbf{y}) \in X'$ $\forall\ (t,\mathbf{y}) \in [t_0,t_f]\times Y$. Consider the following problem:

$$\min_{\mathbf{y}} F(\mathbf{y}) = \phi(\mathbf{x}(t_f,\mathbf{y}),\mathbf{x}'(t_f,\mathbf{y}),\mathbf{y}) + \int_{t_0}^{t_f} f(t,\mathbf{x}(t,\mathbf{y}),\mathbf{x}'(t,\mathbf{y}),\mathbf{y})\ dt$$

subject to

$$\begin{gathered}\mathbf{x}' = \mathbf{A}(t)\mathbf{x} + \mathbf{B}(t)\mathbf{y} + \mathbf{p}(t)\\ \mathbf{E_0}\mathbf{x}(t_0) + \mathbf{E_f}\mathbf{x}(t_f) = \mathbf{C}\mathbf{y} + \mathbf{d}\\ \mathbf{g}(\mathbf{y}) \le \mathbf{0}\end{gathered}$$

where $\mathbf{y} \in Y$; f is a continuous mapping $f : [t_0,t_f] \times X \times X' \times Y \to \mathbb{R}$; ϕ is a continuous mapping $\phi : X \times X' \times Y \to \mathbb{R}$; $\mathbf{g}$ is a convex mapping $\mathbf{g} : Y \to \mathbb{R}^d$; the functions $\mathbf{A}(t)$, $\mathbf{B}(t)$, and $\mathbf{p}(t)$ are continuous on $[t_0,t_f]$; and there are exactly m boundary equations. Additionally, for the set $G = \{\mathbf{y} \mid \mathbf{g}(\mathbf{y}) \le 0\}$, we require that $Y \cap G \neq \emptyset$.

Remark. While the problem formulation allows for a general boundary condition, a more familiar initial value formulation is achieved if $\mathbf{E_0} = \mathbf{I}$ and $\mathbf{E_f} = \mathbf{0}$, where $\mathbf{I}$ is the identity matrix and $\mathbf{0}$ is the zero matrix. Additionally, the sets Y, X, and X' are used throughout the paper. Unless otherwise specified, the definition of these sets is unchanged from that in Problem 3.1.1 above.

3.2 Existence of a Minimum to Problem 3.1.1

Existence of a minimum for Problem 3.1.1 is addressed sequentially. First, the existence of a solution to the embedded dynamic system is discussed. Once this existence is demonstrated, a brief discussion of the solution to the dynamic system is presented. This naturally leads to a proof of the continuity of $F(\mathbf{y})$ on Y, which immediately implies the existence of a minimum to Problem 3.1.1.

According to Theorem 6.1 [10], a solution to the embedded linear boundary value problem exists and is unique provided the matrix $\mathbf{Q} = \mathbf{E_0} + \mathbf{E_f}\mathbf{\Phi}(t_f,t_0)$ is nonsingular, where $\mathbf{\Phi}(t_f,t_0)$ is the transition matrix. We are interested only in those problems for which a solution to the dynamic embedded system exists; therefore, $\mathbf{Q}$ is assumed to be nonsingular throughout. Having established existence, we turn our attention to the functional form of the solution. From linear systems theory [46], the following provides a general solution to the differential equation:

$$\mathbf{x}(t,\mathbf{y}) = \mathbf{\Phi}(t,t_0)\mathbf{x}(t_0,\mathbf{y}) + \int_{t_0}^{t} \mathbf{\Phi}(t,\tau)\mathbf{B}(\tau)\mathbf{y}\ d\tau + \int_{t_0}^{t} \mathbf{\Phi}(t,\tau)\mathbf{p}(\tau)\ d\tau, \tag{1}$$

where $\mathbf{\Phi}(t,t_0)$ is the transition matrix, which is the solution of the matrix differential equation

$$\frac{d}{dt}\mathbf{\Phi}(t,t_0) = \mathbf{A}(t)\mathbf{\Phi}(t,t_0), \quad \forall\ t,$$

where $\mathbf{\Phi}(t_0,t_0) = \mathbf{I}$. Solving for the boundary condition and substituting the initial condition into Equation

1 results in

$$\mathbf{x}(t,\mathbf{y}) = \left\{ \mathbf{\Phi}(t,t_0)(\mathbf{E_0} + \mathbf{E_f}\mathbf{\Phi}(t_f,t_0))^{-1} \left[\mathbf{C} - \mathbf{E_f} \int_{t_0}^{t_f} \mathbf{\Phi}(t_f,\tau)\mathbf{B}(\tau)\ d\tau \right] + \int_{t_0}^{t} \mathbf{\Phi}(t,\tau)\mathbf{B}(\tau)\ d\tau \right\} \mathbf{y} + \mathbf{\Phi}(t,t_0)(\mathbf{E_0} + \mathbf{E_f}\mathbf{\Phi}(t_f,t_0))^{-1} \left[\mathbf{d} - \mathbf{E_f} \int_{t_0}^{t_f} \mathbf{\Phi}(t_f,\tau)\mathbf{p}(\tau)\ d\tau \right] + \int_{t_0}^{t} \mathbf{\Phi}(t,\tau)\mathbf{p}(\tau)\ d\tau. \quad (2)$$

The importance of the above equation is that the solution to the differential equations, $\mathbf{x}(t,\mathbf{y})$, is merely an affine function of $\mathbf{y}$ possessing the following structural form:

$$\mathbf{x}(t,\mathbf{y}) = \mathbf{M}(t)\mathbf{y} + \mathbf{n}(t), \quad (3)$$

where $\mathbf{M}$ and $\mathbf{n}$ reduce to constant valued matrices for fixed time.

We now prove the existence of a minimum to Problem 3.1.1. In order to accomplish this task, the continuity of $F(\mathbf{y})$ must be established. Proposition 3.2.1 below satisfies this requirement. As a corollary to this proposition, the existence of a minimum to Problem 3.1.1 is established.

Proposition 3.2.1. *Consider the following functional:*

$$F(\mathbf{y}) = \int_{t_0}^{t_f} f(t,\mathbf{x}(t,\mathbf{y}),\mathbf{x}'(t,\mathbf{y}),\mathbf{y})\ dt$$

subject to

$$\begin{aligned} \mathbf{x}' &= \mathbf{A}(t)\mathbf{x} + \mathbf{B}(t)\mathbf{y} + \mathbf{p}(t) \\ \mathbf{E_0}\mathbf{x}(t_0) + \mathbf{E_f}\mathbf{x}(t_f) &= \mathbf{C}\mathbf{y} + \mathbf{d}. \end{aligned}$$

where $\mathbf{y} \in Y$; $\mathbf{x}(t,\mathbf{y}) \in X$; $\mathbf{x}'(t,\mathbf{y}) \in X'$; f is a continuous mapping $f : [t_0,t_f] \times X \times X' \times Y \to \mathbb{R}$; the functions $\mathbf{A}(t)$, $\mathbf{B}(t)$, and $\mathbf{p}(t)$ are continuous on $[t_0,t_f]$; and there are exactly m boundary equations. If the above conditions are satisfied, then $F(\mathbf{y})$ is continuous on Y.

Proof. As previously demonstrated, Equation 2 is the solution to the above system of differential equations. Clearly, this equation is continuous on $[t_0,t_f] \times Y$, a compact space. We show that $[t_0,t_f] \times Y$ is indeed compact. Suppose $\{T_\alpha\}$ is any open covering of $[t_0,t_f]$ and that $\{G_\alpha\}$ is any open covering of Y. Then by the definition of compactness, there exist finite subcoverings $\{T_{\alpha_1},\ldots,T_{\alpha_n}\}$ of $[t_0,t_f]$ and $\{G_{\alpha_1},\ldots,G_{\alpha_n}\}$ of Y. Therefore, $\{T_\alpha\} \times \{G_\alpha\}$ is an open covering of $[t_0,t_f] \times Y$ and $\{T_{\alpha_1},\ldots,T_{\alpha_n}\} \times \{G_{\alpha_1},\ldots,G_{\alpha_n}\}$ provides a finite subcovering of $[t_0,t_f] \times Y$. This methodology is trivially extended to higher order Cartesian products. Now, by Theorem 4.14 [60], $\mathbf{x}([t_0,t_f] \times Y)$ and $\mathbf{x}'([t_0,t_f] \times Y)$ are compact. The following approximation is valid for all $\mathbf{y},\mathbf{y_0} \in Y$:

$$\begin{aligned} |F(\mathbf{y}) - F(\mathbf{y_0})| &= \left| \int_{t_0}^{t_f} f(t,\mathbf{x}(t,\mathbf{y}),\mathbf{x}'(t,\mathbf{y}),\mathbf{y}) - f(t,\mathbf{x}(t,\mathbf{y_0}),\mathbf{x}'(t,\mathbf{y_0}),\mathbf{y_0})\ dt \right| \\ &\le \int_{t_0}^{t_f} |f(t,\mathbf{x}(t,\mathbf{y}),\mathbf{x}'(t,\mathbf{y}),\mathbf{y}) - f(t,\mathbf{x}(t,\mathbf{y_0}),\mathbf{x}'(t,\mathbf{y_0}),\mathbf{y_0})|\ dt. \end{aligned}$$

Because f is continuous on a compact space, by Theorem 4.19 [60], f is uniformly continuous on this compact space. By definition, given $\frac{\varepsilon}{t_f - t_0} > 0$, there exists a $\delta' > 0$ such that

$$|f(t,\mathbf{x}(t,\mathbf{y}),\mathbf{x}'(t,\mathbf{y}),\mathbf{y}) - f(t,\mathbf{x}(t,\mathbf{y_0}),\mathbf{x}'(t,\mathbf{y_0}),\mathbf{y_0})| < \frac{\varepsilon}{t_f - t_0},$$

$$\text{for } |(t,\mathbf{x}(t,\mathbf{y}),\mathbf{x}'(t,\mathbf{y}),\mathbf{y}) - (t,\mathbf{x}(t,\mathbf{y_0}),\mathbf{x}'(t,\mathbf{y_0}),\mathbf{y_0})| < \delta' \quad \forall\ \mathbf{y},\mathbf{y_0} \in Y.$$

By uniform continuity of $\mathbf{x}(t, \mathbf{y})$ on $[t_0, t_f] \times Y$ and $\mathbf{x}'(t, \mathbf{y})$ on $[t_0, t_f] \times Y$, we can replace $|(t, \mathbf{x}(t, \mathbf{y}), \mathbf{x}'(t, \mathbf{y}), \mathbf{y}) - (t, \mathbf{x}(t, \mathbf{y_0}), \mathbf{x}'(t, \mathbf{y_0}), \mathbf{y_0})| < \delta'$ simply with $|\mathbf{y} - \mathbf{y_0}| < \delta$ for some $\delta > 0$. Using the estimate for the integral above, we now have

$$\begin{aligned}
|F(\mathbf{y}) - F(\mathbf{y_0})| &\leq \int_{t_0}^{t_f} |f(t, \mathbf{x}(t, \mathbf{y}), \mathbf{x}'(t, \mathbf{y}), \mathbf{y}) - f(t, \mathbf{x}(t, \mathbf{y_0}), \mathbf{x}'(t, \mathbf{y_0}), \mathbf{y_0})| \, dt \\
&\leq \int_{t_0}^{t_f} \frac{\varepsilon}{t_f - t_0} \, dt = \frac{\varepsilon}{t_f - t_0}(t_f - t_0) = \varepsilon \\
&\quad \text{for } |\mathbf{y} - \mathbf{y_0}| < \delta \quad \forall \, \mathbf{y}, \mathbf{y_0} \in Y.
\end{aligned}$$

Therefore, by definition, $F(\mathbf{y})$ is continuous.

□

Corollary 3.2.2. *There exists a minimum to Problem 3.1.1*

Proof. The objective function $F(\mathbf{y})$ as defined in Problem 3.1.1 is trivially continuous by Theorem 4.9 [60] and the above proposition. That is, $F(\mathbf{y})$ is the sum of the continuous functions $\phi(\mathbf{x}(t_f, \mathbf{y}), \mathbf{x}'(t_f, \mathbf{y}), \mathbf{y})$ and $\int_{t_0}^{t_f} f(t, \mathbf{x}(t, \mathbf{y}), \mathbf{x}'(t, \mathbf{y}), \mathbf{y}) \, dt$. By definition, F is a mapping from the nonempty compact space $Y \cap G$ into $\mathbb{R}$. Therefore, by Theorem 4.16 [60], the existence of a minimum to Problem 3.1.1 is guaranteed.

□

At this point, the existence of a minimum to Problem 3.1.1 as been established by demonstrating the existence and uniqueness of a solution to the embedded dynamic system and asserting Weierstrass' Theorem concerning the existence of a minimum of a continuous function on a nonempty compact set. Our attention is now turned to an algorithmic method for determining the point $\mathbf{y}$ at which this minimum value of the objective function occurs. The idea behind solving Problem 3.1.1 is to apply standard algebraic convex underestimator techniques to construct a branch and bound algorithm. Clearly, the objective is a function only of a vector from a Euclidean space. Thus, standard branch and bound techniques are applicable. However, it is not immediately evident how to treat convexity of the dynamic embedded system. Therefore, the following portion of this exposition focuses on the theoretical framework requisite for generating convex underestimators for Problem 3.1.1.

3.3 Convexity and Convex Underestimators

For the purposes of this discussion, the functions and variables are assumed to be either real or real vectored. Additionally, we will always assume that any integrand is a Riemann integrable function. We begin by defining algebraic convexity.

Definition 3.3.1. Let $f : S \to \mathbb{R}$, where S is a nonempty convex set in $\mathbb{R}^n$. The function f is said to be convex on S if

$$f(\lambda \mathbf{x} + (1 - \lambda)\mathbf{x_0}) \leq \lambda f(\mathbf{x}) + (1 - \lambda) f(\mathbf{x_0})$$

for each $\mathbf{x}$, $\mathbf{x_0} \in S$ and for each $\lambda \in (0, 1)$.

Having established our working definition for convexity, we are now prepared to derive a convex underestimator for Problem 3.1.1. Due to complexity, the derivation is performed sequentially. The first lemma below illustrates that the composition of a convex function on a set D' and an affine function on a set D remains convex on D. Immediately following the first lemma is another lemma that extends the standard monotonicity result of the Riemann integral to a parameter embedded integral. These facts are tantamount to deriving a convex underestimator for the objective function in Problem 3.1.1.

Lemma 3.3.2. *Let $I \subset \mathbb{R}^m$, $J \subset \mathbb{R}^n$, $g : I \to \mathbb{R}$ be a function convex on I, and $\mathbf{h} : J \to \mathbb{R}^m$ be an affine function of the form $\mathbf{h}(\mathbf{y}) = \mathbf{A}\mathbf{y} + \mathbf{b}$, where range$(\mathbf{h}) \subset I$. Then, the composite function $f : \mathbb{R}^n \to \mathbb{R}$ is defined as $f(\mathbf{y}) = g[\mathbf{h}(\mathbf{y})]$ and is a convex function on J.*

Proof. Given $\lambda \in (0,1)$, by the definition of convexity, we have

$$g(\lambda \mathbf{x} + (1-\lambda)\mathbf{x}_0) \leq \lambda g(\mathbf{x}) + (1-\lambda) g(\mathbf{x}_0) \quad \forall\ \mathbf{x}, \mathbf{x}_0 \in I.$$

However, by hypothesis, range($\mathbf{h}$) $\subset I$. Therefore, we have

$$g[\lambda \mathbf{h}(\mathbf{y}) + (1-\lambda)\mathbf{h}(\mathbf{y}_0)] \leq \lambda g[\mathbf{h}(\mathbf{y}) + (1-\lambda) g(\mathbf{h}(\mathbf{y}_0)] \quad \forall\ \mathbf{h}, \mathbf{h}_0 \in I.$$

We now perform the following algebraic operations:

$$\begin{aligned} g[\lambda \mathbf{h}(\mathbf{y}) + (1-\lambda)\mathbf{h}(\mathbf{y}_0)] &= g[\lambda(\mathbf{A}\mathbf{y} + \mathbf{b}) + (1-\lambda)(\mathbf{A}\mathbf{y_0} + \mathbf{b})] \\ &= g[\lambda \mathbf{A}\mathbf{y} + \lambda \mathbf{b} + \mathbf{A}\mathbf{y_0} - \lambda \mathbf{A}\mathbf{y_0} - \lambda \mathbf{b} + \mathbf{b}] \\ &= g[\mathbf{A}(\lambda \mathbf{y} + (1-\lambda)\mathbf{y}_0) + \mathbf{b}] \\ &= g[\mathbf{h}(\lambda \mathbf{y} + (1-\lambda)\mathbf{y}_0)] \quad \forall\ \mathbf{y}, \mathbf{y}_0 \in J, \end{aligned}$$

where the change of sets is evident from the definition of the mapping $\mathbf{h}$. Therefore,

$$g[\mathbf{h}(\lambda \mathbf{y} + (1-\lambda)\mathbf{y}_0)] \leq \lambda g[\mathbf{h}(\mathbf{y})] + (1-\lambda) g[\mathbf{h}(\mathbf{y}_0)] \quad \forall\ \mathbf{y}, \mathbf{y}_0 \in J,$$

which by definition shows that $g[\mathbf{h}(\mathbf{y})]$ is convex on J.

□

Lemma 3.3.3. *Let $y \in Y$, $t \in [t_0, t_f]$, and $f_1, f_2 : [t_0, t_f] \times Y \to \mathbb{R}$ such that f_1, f_2 are integrable. Denote $\mathbf{y}$ fixed by $\underline{\mathbf{y}}$. If*

$$f_1(t, \underline{\mathbf{y}}) \leq f_2(t, \underline{\mathbf{y}}) \qquad \forall\ (t, \underline{\mathbf{y}}) \in [t_0, t_f] \times Y$$

then

$$F_1(\mathbf{y}) = \int_{t_0}^{t_f} f_1(t, \mathbf{y})\ dt \leq \int_{t_0}^{t_f} f_2(t, \mathbf{y})\ dt = F_2(\mathbf{y}) \qquad \forall\ \mathbf{y} \in Y.$$

Proof. Choose any fixed $\underline{\mathbf{y}} \in Y$. By hypothesis,

$$f_1(t, \underline{\mathbf{y}}) \leq f_2(t, \underline{\mathbf{y}}) \qquad \forall\ (t, \underline{\mathbf{y}}) \in [t_0, t_f] \times Y.$$

Because $\underline{\mathbf{y}}$ is fixed, f_1 and f_2 are only functions of t on $[t_0, t_f]$. Therefore, we apply Theorem 6.12(b) [60] directly to yield.

$$\int_{t_0}^{t_f} f_1(t, \underline{\mathbf{y}})\ dt \leq \int_{t_0}^{t_f} f_2(t, \underline{\mathbf{y}})\ dt.$$

Because the above inequality holds for any $\underline{\mathbf{y}} \in Y$, it holds for all $\mathbf{y} \in Y$.

□

The following is the fundamental theorem for generating a convex underestimator for Problem 3.1.1. It illustrates that convexity of the integrand implies convexity of the integral. The theorem makes use of the notion of partial convexity as defined by Troutman [69]. As a reminder to the reader, partial convexity requires convexity in all variables after holding time fixed (denoted by $\underline{t}$). Additionally, before the presentation of the fundamental theorem, two new sets must be defined. These sets enable the theorem to be applied to time varying regions. The purpose of this seemingly insignificant addition will be made abundantly clear in the discussion of bounds tightening.

Definition 3.3.4. We define the following sets

$$\mathcal{X}(\underline{t}) = \{\mathbf{x}(\underline{t}, \mathbf{y}) \mid \mathbf{y} \in Y,\ \underline{t} \text{ fixed } \in [t_0, t_f]\}$$

$$\mathcal{X}'(\underline{t}) = \{\mathbf{x}'(\underline{t}, \mathbf{y}) \mid \mathbf{y} \in Y,\ \underline{t} \text{ fixed } \in [t_0, t_f]\}$$

$$\mathcal{X} = \bigcup_{\underline{t} \in [t_0, t_f]} \mathcal{X}(\underline{t})$$

$$\mathcal{X}' = \bigcup_{\underline{t} \in [t_0, t_f]} \mathcal{X}'(\underline{t}).$$

It is clear that $\mathcal{X} \subseteq X$ and $\mathcal{X}' \subseteq X'$.

Theorem 3.3.5. *Consider the following function:*

$$F(\mathbf{y}) = \int_{t_0}^{t_f} f(t, \mathbf{x}(t,\mathbf{y}), \mathbf{x}'(t,\mathbf{y}), \mathbf{y})\ dt$$

subject to

$$\mathbf{x}' = \mathbf{A}(t)\mathbf{x} + \mathbf{B}(t)\mathbf{y} + \mathbf{p}(t)$$
$$\mathbf{E_0}\mathbf{x}(t_0) + \mathbf{E_f}\mathbf{x}(t_f) = \mathbf{C}\mathbf{y} + \mathbf{d}.$$

where $\mathbf{y} \in Y$*;* $\mathbf{x}(t,\mathbf{y}) \in X$*;* $\mathbf{x}'(t,\mathbf{y}) \in X'$*;* f *is a mapping* $f : [t_0, t_f] \times X \times X' \times Y \to \mathbb{R}$*; the functions* $\mathbf{A}(t)$*,* $\mathbf{B}(t)$*, and* $\mathbf{p}(t)$ *are continuous on* $[t_0, t_f]$*; and there are exactly* m *boundary equations. If* $f(\underline{t}, \mathbf{x}, \mathbf{x}', \mathbf{y})$ *is convex on* $\mathcal{X}(\underline{t}) \times \mathcal{X}'(\underline{t}) \times Y\ \forall\ \underline{t} \in [t_0, t_f]$*, then* $F(\mathbf{y})$ *is convex on* Y*.*

Proof. For fixed t, by Equation 3, we have that $\mathbf{x}(t,\mathbf{y})$ is an affine function of $\mathbf{y}$. Furthermore, by inspection, one observes that $\mathbf{x}'$ is also an affine function of $\mathbf{y}$. By hypothesis, the integrand $f(\underline{t}, \mathbf{x}, \mathbf{x}', \mathbf{y})$ is convex on $\mathcal{X}(\underline{t}) \times \mathcal{X}'(\underline{t}) \times Y\ \forall\ \underline{t} \in [t_0, t_f]$. Therefore, we assert Lemma 3.3.2 yielding f convex on $[t_0, t_f] \times Y$ for each fixed t. Given $\lambda \in (0, 1)$, by the definition of convexity (on $[t_0, t_f] \times Y$ for each fixed t), we have

$$\begin{aligned} &f[t, \mathbf{x}(t, \lambda\mathbf{y} + (1-\lambda)\mathbf{y_0}), \mathbf{x}'(t, \lambda\mathbf{y} + (1-\lambda)\mathbf{y_0}), \lambda\mathbf{y} + (1-\lambda)\mathbf{y_0}] \leq \\ &\qquad \lambda f(t, \mathbf{x}(t,\mathbf{y}), \mathbf{x}'(t,\mathbf{y}), \mathbf{y}) + (1-\lambda) f(t, \mathbf{x}(t,\mathbf{y_0}), \mathbf{x}'(t,\mathbf{y_0}), \mathbf{y_0}) \qquad \forall\ (t,\mathbf{y}), (t,\mathbf{y_0}) \in [t_0, t_f] \times Y. \end{aligned}$$

From Lemma 3.3.3, the above equation implies

$$\begin{aligned} &\int_{t_0}^{t_f} f[t, \mathbf{x}(t, \lambda\mathbf{y} + (1-\lambda)\mathbf{y_0}), \mathbf{x}'(t, \lambda\mathbf{y} + (1-\lambda)\mathbf{y_0}), \lambda\mathbf{y} + (1-\lambda)\mathbf{y_0}]\ dt \leq \\ &\qquad \int_{t_0}^{t_f} \lambda f(t, \mathbf{x}(t,\mathbf{y}), \mathbf{x}'(t,\mathbf{y}), \mathbf{y})\ dt + \int_{t_0}^{t_f} (1-\lambda) f(t, \mathbf{x}(t,\mathbf{y_0}), \mathbf{x}'(t,\mathbf{y_0}), \mathbf{y_0})\ dt \qquad \forall\ \mathbf{y}, \mathbf{y_0} \in Y. \end{aligned}$$

which upon inspection is simply

$$F(\lambda\mathbf{y} + (1-\lambda)\mathbf{y_0}) \leq \lambda F(\mathbf{y}) + (1-\lambda) F(\mathbf{y_0}) \qquad \forall\ \mathbf{y}, \mathbf{y_0} \in Y.$$

Thus, by definition, $F(\mathbf{y})$ is convex on Y.

□

Corollary 3.3.6. *Consider the function* $F(\mathbf{y})$ *and constraints as described in the theorem above with the relaxation that* $f(t, \mathbf{x}, \mathbf{x}', \mathbf{y})$ *is nonconvex. If*

$$u(t, \mathbf{x}(t,\mathbf{y}), \mathbf{x}'(t,\mathbf{y}), \mathbf{y}) \leq f(t, \mathbf{x}(t,\mathbf{y}), \mathbf{x}'(t,\mathbf{y}), \mathbf{y}) \qquad \forall\ (t,\mathbf{y}) \in [t_0, t_f] \times Y$$

and if u *is convex on* $\mathcal{X}(\underline{t}) \times \mathcal{X}'(\underline{t}) \times Y\ \forall\ \underline{t} \in [t_0, t_f]$*, then* $U(\mathbf{y}) \leq F(\mathbf{y})\ \forall\ y \in Y$ *and* $U(\mathbf{y})$ *is convex on* Y*, where*

$$U(\mathbf{y}) = \int_{t_0}^{t_f} u(t, \mathbf{x}(t,\mathbf{y}), \mathbf{x}'(t,\mathbf{y}), \mathbf{y})\ dt.$$

Proof. The proof is immediately evident from Theorem 3.3.5 above and Lemma 3.3.3.

□

Remark. The above corollary is the fundamental result that enables one to derive a convex underestimator for Problem 3.1.1. Clearly, the corollary states that a convex underestimator for the integrand (on $\mathcal{X}(\underline{t}) \times \mathcal{X}'(\underline{t}) \times Y\ \forall\ \underline{t} \in [t_0, t_f]$) generates a convex underestimator for the integral (on Y). While the corollary does not require the continuity of $u(t, \mathbf{x}(t,\mathbf{y}), \mathbf{x}'(t,\mathbf{y}), \mathbf{y})$ to prove that $U(\mathbf{y})$ is a convex underestimator, continuity of $u(t, \mathbf{x}(t,\mathbf{y}), \mathbf{x}'(t,\mathbf{y}), \mathbf{y})$ is necessary to establish the existence of a minimum to the underestimating problem. Fortunately, this generally poses no difficulty as the standard methods used to derive convex underestimators for the integrand provide continuous functions. The addition of ϕ in the problem formulation provides no further complication. Because ϕ is defined as a continuous function for a fixed time, a convex underestimator is found for ϕ via Lemma 3.3.2 and standard methods. The sum of convex functions remains convex. Thus, the sum of a convex underestimator for ϕ and a convex underestimator for the integral is a convex underestimator for the objective function.

3.4 Bounds Tightening

One of the convergence criteria for any branch-and-bound algorithm is that the bounding operation is consistent (finitely consistent for finite termination) [38]. For algorithmic convergence, this statement implies that at every step, any unfathomed partition element can be further refined, and any decreasing sequence of successively refined partition elements satisfies the requirement that at the limit of the sequence, the lower bound equals the upper bound. From this statement, one infers that convergence is assisted by employing the highest possible lower bounding functions. As previously discussed, the lower bounding functions utilized in our algorithm are convex underestimators. By definition, the highest convex underestimator for a function is its convex envelope.

Obviously, using the convex envelope of a function for its convex underestimator would yield the best convergence results. Often, however, computing the convex envelope of a function is a prohibitively expensive task. Therefore, alternate techniques are employed for constructing convex underestimators, which may or may not yield convex envelopes. Several current methods exist for the generation of convex underestimators for functions; the methods employed in our algorithm are attributed to McCormick [52] and Adjiman [4]. While we restrict ourselves to the discussion of these two convex relaxation techniques, one should note that any method for deriving a convex underestimator that does not require the addition of new infinite dimensional variables to the objective function is applicable. The reason we require this restriction is that the addition of new infinite dimensional variables transforms the search space from a finite dimensional space to an infinite dimensional space hence requiring a variational optimization technique. We note, however, that terms (even integrals) containing only elements from Y may still be underestimated via a technique requiring the addition of new variables. A short example below illustrates the difficulty of employing a convex relaxation method that introduces new infinite dimensional variables to the objective function.

Example 3.4.1. Consider the following dynamic optimization problem with a linear dynamic embedded system:

$$\min_{\mathbf{y}} F(\mathbf{y}) = \int_{t_0}^{t_f} x_1 \cdot x_2 \ dt$$

subject to constraints of the same form as those of Problem 3.1.1. Al-Khayyal and Falk [5] give the convex envelope of a bilinear term on any rectangle in $\mathbb{R}^2$. In order to increase the smoothness of the convex underestimating problem, this result is often applied by introducing a new variable w and inequalities to the formulation. This yields the following convex relaxation:

$$U(\mathbf{y}, w) = \int_{t_0}^{t_f} w \ dt$$

subject to the original constraints and the new constraints

$$\begin{gathered} w \geq x_1^L(t) \cdot x_2 + x_2^L(t) \cdot x_1 - x_1^L(t) \cdot x_2^L(t) \\ w \geq x_1^U(t) \cdot x_2 + x_2^U(t) \cdot x_1 - x_1^U(t) \cdot x_2^U(t) \\ w \in C[t_0, t_f], \end{gathered}$$

where $C[t_0, t_f]$ represents the space of continuous functions on the interval $[t_0, t_f]$. Without introducing the new variable w, the embedded ODEs and boundary conditions allow the elimination of $\mathbf{x} \in (C^1[t_0, t_f])^m$ from the objective function enabling us to consider only an optimization problem on $Y \cap G$. Unfortunately, the newly added Lagrangian inequalities on w do not permit the elimination of w from the convex relaxation. Hence, the optimization problem must be considered on the space $(Y \cap G) \times C[t_0, t_f]$ subject to the Lagrangian inequality constraints. Problems of this nature are addressed by the variational approach in section 5.

One common feature of the aforementioned convex relaxation methods is the requirement that the domains of the functions are bounded. In fact, both the quality and the domain of applicability of the underestimator is directly dependent upon these requisite bounds. The optimization parameter in Problem 3.1.1 is the variable $\mathbf{y}$, which is an element of the bounded space Y, a nonempty compact convex subset of $\mathbb{R}^n$. Obviously, in the branch and bound framework, the refined partitions are generated by branching and possibly reducing the feasible solution space Y. Therefore, the bounds for $\mathbf{y}$ are fixed by the branch and bound algorithm. However, the bounds for $\mathbf{x}(t,\mathbf{y})$ are not specified, but rather implied by the solution of the embedded system. Clearly, from Corollary 3.3.6, the highest derived lower bounding convex underestimator for the integrand $f(t,\mathbf{x}(t,\mathbf{y}),\mathbf{x}'(t,\mathbf{y}),\mathbf{y})$ is sought. In this case, highest refers not necessarily to the convex envelope, but rather the highest convex underestimator that can be derived from the methods of McCormick and Adjiman in conjunction with Corollary 3.3.6. We now make a formal definition of highest derived convex underestimator and tightest bounds.

Definition 3.4.2. Define the set $\bar{X}$, whose elements are from a function space, to be the set of all bounds on $\mathbf{x}(t,\mathbf{y})$ such that no solutions to the embedded differential equations for the specified boundary conditions are excluded $\forall\ (t,\mathbf{y}) \in [t_0,t_f] \times Y$. Suppose that $u(t,\mathbf{x}(t,\mathbf{y}),\mathbf{x}'(t,\mathbf{y}))$ is a convex underestimator for some function $f(t,\mathbf{x}(t,\mathbf{y}),\mathbf{x}'(t,\mathbf{y}))$ such that $u(t,\mathbf{x}(t,\mathbf{y}),\mathbf{x}'(t,\mathbf{y}))$ is derived from the bounds $(\mathbf{x^L},\mathbf{x^U}) \in \bar{X}$. $u(t,\mathbf{x}(t,\mathbf{y}),\mathbf{x}'(t,\mathbf{y}))$ is the highest derived convex underestimator if for any other convex underestimator $u^*(t,\mathbf{x}(t,\mathbf{y}),\mathbf{x}'(t,\mathbf{y}))$ derived by the same method but with any bounds $(\mathbf{x^{L}}^*,\mathbf{x^{U}}^*) \in \bar{X}$, we have that

$$u(\underline{t},\mathbf{x}(\underline{t},\mathbf{y}),\mathbf{x}'(\underline{t},\mathbf{y})) \geq u^*(\underline{t},\mathbf{x}(\underline{t},\mathbf{y}),\mathbf{x}'(\underline{t},\mathbf{y})) \quad \forall\ (\underline{t},\mathbf{y}) \in [t_0,t_f] \times Y.$$

In this case, we call $(\mathbf{x^L},\mathbf{x^U})$ the tightest bounds (for this method).

Using Definition 3.4.2 above, we state the following proposition, which directly implies a method for determining the tightest bounds via interval analysis. The proposition is merely a restatement of the properties of the convex underestimators derived by McCormick and Adjiman. The proof of the following proposition as it relates to McCormick's work is found in McCormick [52]. The proof of the following proposition as it relates to Adjiman's underestimators is found in the previous work of Androulakis *et al.* [9] and Maranas and Floudas [50].

Proposition 3.4.3. *For the convex underestimator methods of McCormick and Adjiman, suppose the convex underestimator* $u^*(t,\mathbf{x}(t,\mathbf{y}),\mathbf{x}'(t,\mathbf{y}))$ *is derived from the bounds* $(\mathbf{x^L}^*,\mathbf{x^U}^*)$. *If the interval* $[\mathbf{x^L}^*(\underline{t}),\mathbf{x^U}^*(\underline{t})]$ *were reduced to the interval* $[\mathbf{x^L}(\underline{t}),\mathbf{x^U}(\underline{t})]$ *such that* $x_i^L(\underline{t}) \geq x_i^{L^*}(\underline{t})$ *and* $x_i^U(\underline{t}) \leq x_i^{U^*}(\underline{t})\ \forall\ \underline{t} \in [t_0,t_f]$, *then the convex underestimator derived on* $(\mathbf{x^L},\mathbf{x^U})$ *is a higher derived convex underestimator than the convex underestimator derived on* $(\mathbf{x^L}^*,\mathbf{x^U}^*)$.

From Proposition 3.4.3 above, one directly infers that the tightest bounds for a method are found pointwise by

$$[x_i^L(\underline{t}),x_i^U(\underline{t})] = \arg\min\{|x_i^U(\underline{t}) - x_i^L(\underline{t})|\ :\ [\mathbf{x^L}(\underline{t}),\ \mathbf{x^U}(\underline{t})] \in \bar{X}(\underline{t})\} \quad \forall\ \underline{t} \in [t_0,t_f], 1 \leq i \leq m. \tag{4}$$

Additionally, any convex underestimator obeying the property of Proposition 3.4.3 has the same tightest bounds independent of the method employed to construct the convex underestimator itself. This follows immediately from Definition 3.4.2 and Equation 4. Because all of the convex relaxation techniques leading to convergent branch-and-bound algorithms obey Proposition 3.4.3, Equation 4 could alternatively be used as the definition for tightest bounds.

We now return to the problem of calculating the tightest bounds for the solution of the embedded dynamic system. As stated previously, the bounds for $\mathbf{x}(t,\mathbf{y})$ are implied by the bounds on $\mathbf{y}$, for clearly the bounds on $\mathbf{x}(t,\mathbf{y})$ should not be chosen smaller than the solution envelope to the embedded dynamic system. That is, we require $(\mathbf{x^L},\mathbf{x^U}) \in \bar{X}$. The following theorem illustrates a method for calculating the tightest bounds for $\mathbf{x}(t,\mathbf{y})$. Letters in square brackets will be used to denote intervals. A bold variable in square brackets represents either a vector or matrix of intervals.

Theorem 3.4.4. *Consider the following set of differential equations and boundary conditions:*

$$\mathbf{x}' = \mathbf{A}(t)\mathbf{x} + \mathbf{B}(t)\mathbf{y} + \mathbf{p}(t)$$
$$\mathbf{E_0}\mathbf{x}(t_0) + \mathbf{E_f}\mathbf{x}(t_f) = \mathbf{C}\mathbf{y} + \mathbf{d},$$

If $\mathbf{y} \in Y = [\mathbf{y}^L,\mathbf{y}^U]$, *then the tightest bounds for the solution to the differential equations are given pointwise in time as the natural interval extension (to* Y*) of Equation 2.*

Proof. The functional form of the solution to the differential equation is given by Equation 3. For any fixed $\underline{t} \in [t_0, t_f]$, we write

$$\mathbf{x}(\underline{t}, \mathbf{y}) = \mathbf{M}(\underline{t})\mathbf{y} + \mathbf{n}(\underline{t}), \tag{5}$$

where $\mathbf{M}(\underline{t})$ and $\mathbf{n}(\underline{t})$ are constants for each fixed t. We now take the interval extension of Equation 5 to yield

$$[\mathbf{x}](\underline{t}, [\mathbf{y}]) = \mathbf{M}(\underline{t})[\mathbf{y}] + \mathbf{n}(\underline{t}), \tag{6}$$

where $[\mathbf{y}]$ is the interval $[\mathbf{y}^L, \mathbf{y}^U]$. We note that since Equation 5 is a rational function, Equation 6 is a natural interval extension (i.e., Equation 6 is identically Equation 5 with the variables replaced by intervals and the algebraic operations replaced by interval arithmetic operations). Thus, because Equation 6 above is a rational interval function and a natural interval extension of $\mathbf{x}(\underline{t}, \mathbf{y})$, by Corollary 3.1 [55], we have that

$$\overline{\mathbf{x}}(\underline{t}, [\mathbf{y}]) \subseteq [\mathbf{x}](\underline{t}, [\mathbf{y}]), \tag{7}$$

where $\overline{\mathbf{x}}(\underline{t}, [\mathbf{y}])$ represents the range of the function $\mathbf{x}(\underline{t}, \mathbf{y})$ over the interval $[\mathbf{y}]$. Furthermore, because $[\mathbf{x}](\underline{t}, [\mathbf{y}])$ is a natural interval extension of a rational function in which each variable occurs only once and to the first power, we have that Equation 7 holds with equality. Because t was fixed arbitrarily for any $t \in [t_0, t_f]$, Equation 7 holds pointwise with equality for all $t \in [t_0, t_f]$.

□

Corollary 3.4.5. *For the differential equations defined in Theorem 3.4.4, the tightest bounds for* $\mathbf{x}'(t, \mathbf{y})$ *are given pointwise in time by the following interval equation:*

$$[\mathbf{x}'](\underline{t}, [\mathbf{y}]) = (\mathbf{A}(\underline{t})\mathbf{M}(\underline{t}) + \mathbf{B}(\underline{t}))[\mathbf{y}] + \mathbf{A}(\underline{t})\mathbf{n}(\underline{t}) + \mathbf{p}(\underline{t}).$$

Proof. The functional form of the solution to the differential equation is given by Equation 3. For any fixed $\underline{t} \in [t_0, t_f]$, we substitute Equation 3 into the differential equations to yield

$$\mathbf{x}' = \mathbf{A}(\underline{t})(\mathbf{M}(\underline{t})\mathbf{y} + \mathbf{n}(\underline{t})) + \mathbf{B}(\underline{t})\mathbf{y} + \mathbf{p}(\underline{t}).$$

The above equation **must** be factored to yield

$$\mathbf{x}'(\underline{t}, \mathbf{y}) = (\mathbf{A}(\underline{t})\mathbf{M}(\underline{t}) + \mathbf{B}(\underline{t}))\mathbf{y} + \mathbf{A}(\underline{t})\mathbf{n}(\underline{t}) + \mathbf{p}(\underline{t}).$$

We now take the interval extension of the above equation to yield

$$[\mathbf{x}'](\underline{t}, [\mathbf{y}]) = (\mathbf{A}(\underline{t})\mathbf{M}(\underline{t}) + \mathbf{B}(\underline{t}))[\mathbf{y}] + \mathbf{A}(\underline{t})\mathbf{n}(\underline{t}) + \mathbf{p}(\underline{t}). \tag{8}$$

By an identical argument as in the proof of Theorem 3.4.4, we now have that Equation 8 is a natural interval extension of a rational function in which each variable occurs only once and to the first power. Thus,

$$\overline{\mathbf{x}'}(\underline{t}, [\mathbf{y}]) = [\mathbf{x}'](\underline{t}, [\mathbf{y}]).$$

Because t was fixed arbitrarily for any $\underline{t} \in [t_0, t_f]$, the above equation holds pointwise for all $t \in [t_0, t_f]$.

□

Remark. It is worth commenting on what is meant by the bounds being given by the pointwise natural interval extension to a function. Take for example Equation 6. At each fixed t, for $[\mathbf{y}] = [\mathbf{y}^L, \mathbf{y}^U]$ we have $[\mathbf{x}](\underline{t}, [\mathbf{y}]) = [\mathbf{x}^L(\underline{t}), \mathbf{x}^U(\underline{t})]$. The lower bound is then constructed pointwise by $\mathbf{x}(t) = \mathbf{x}^L(\underline{t})$ for each $\underline{t} \in [t_0, t_f]$ and the upper bound is then constructed pointwise by $\mathbf{x}(t) = \mathbf{x}^U(\underline{t})$ for each $\underline{t} \in [t_0, t_f]$.

Having elucidated a method for calculating the tightest bounds, a final brief corollary is added to demonstrate that these tightest bounds are continuous.

Corollary 3.4.6. *The tightest bounds* $\mathbf{x^L}(t)$ *and* $\mathbf{x^U}(t)$ *as determined from Theorem 3.4.4 are continuous on* $[t_0, t_f]$.

Proof. The proof follows immediately from Equation 3, the above theorem, and interval arithmetic.

□

Remark. By a similar argument, the tightest bounds on $\mathbf{x}'(t, \mathbf{y})$ are also continuous.

A small example is now presented to illustrate the application of Theorem 3.4.4 for calculating the tightest bounds for a linear dynamic embedded system.

Example 3.4.7. Consider the following system of linear differential equations:

$$\begin{gathered} x_1' = x_2 \\ x_2' = -x_1 \\ x_1(0) = 0,\ x_2(0) = y \\ y \in [-1, 1] \end{gathered}$$

The above system may be solved analytically with the following solution:

$$x_1(t, y) = y \sin(t) \quad \text{and} \quad x_2(t, y) = y \cos(t). \tag{9}$$

For any fixed $\underline{t} \in [t_0, t_f]$, we have the natural interval extensions of Equation 9:

$$[x_1] = [-1, 1] \sin(\underline{t}) \quad \text{and} \quad [x_2] = [-1, 1] \cos(\underline{t}).$$

Because the solution for x_1 and x_2 are very similar, we will restrict the remainder of this example to the discussion only of the tightest bounds for x_1. The tightest bounds are now found pointwise by the following formula:

$$x_1^L(t) = \min\{-1 \sin(\underline{t}), 1 \sin(\underline{t})\} \quad \text{and} \quad x_1^U(t) = \max\{-1 \sin(\underline{t}), 1 \sin(\underline{t})\} \quad \forall\ \underline{t} \in [t_0, t_f].$$

A plot of the tightest bounds for x_1 is found below. One very interesting point concerning the graph is that the upper and lower bounds for x_1 intersect at $t = n\pi,\ n \in \mathbb{N}$. Clearly, this implies that regardless of the value for the parameter y, the solution to the differential equation is fixed at $x = 0$. For this example, the solution to the differential equations was obtained analytically. However, for typical problems, the analytic solution to the embedded ODE system will not be known. Therefore, the tightest bounds must be obtained numerically from Equation 2. Two obstacles exists in obtaining the tightest bounds numerically. First, the numerical integration step is potentially very difficult and computationally expensive. Second, due to numerical error in the integration, steps must be taken to ensure that the bounds exclude all of $\bar{X}$ except the tightest bounds.

The following proposition links the idea of the highest derived underestimator for an algebraic function to the highest derived underestimator for an integral.

Proposition 3.4.8. *Consider the problem formulation of Corollary 3.3.6. If $u(t, \mathbf{x}(t, \mathbf{y}), \mathbf{x}'(t, \mathbf{y}))$ provides the highest convex underestimator with tightest bounds $[\mathbf{x^L}(t), \mathbf{x^U}(t)]$ for $f(t, \mathbf{x}(t, \mathbf{y}), \mathbf{x}'(t, \mathbf{y}))$, then $U(\mathbf{y})$ is the highest convex underestimator for $F(\mathbf{y})$ with the same tightest bounds.*

Proof. The proposition is immediately evident from Definition 3.4.2 and Lemma 3.3.3. □

Remark. It should also be clear that if one method yields a higher derived convex underestimator for the integrand than another method, the underestimator for the integral of the former is higher than the underestimator for the integral of the latter in accordance with the construction of Corollary 3.3.6. By this analysis, the convex envelope (in conjunction with the tightest bounds) for the integrand yields the highest possible convex underestimator for the integral that can be constructed via the method of Corollary 3.3.6.

At this point, a concrete example is presented to help solidify the theory presented above.

Example 3.4.9. Consider the following nonconvex integral:

$$\min_{\mathrm{y}} F(y) = \int_0^1 -x^2 \, dt$$

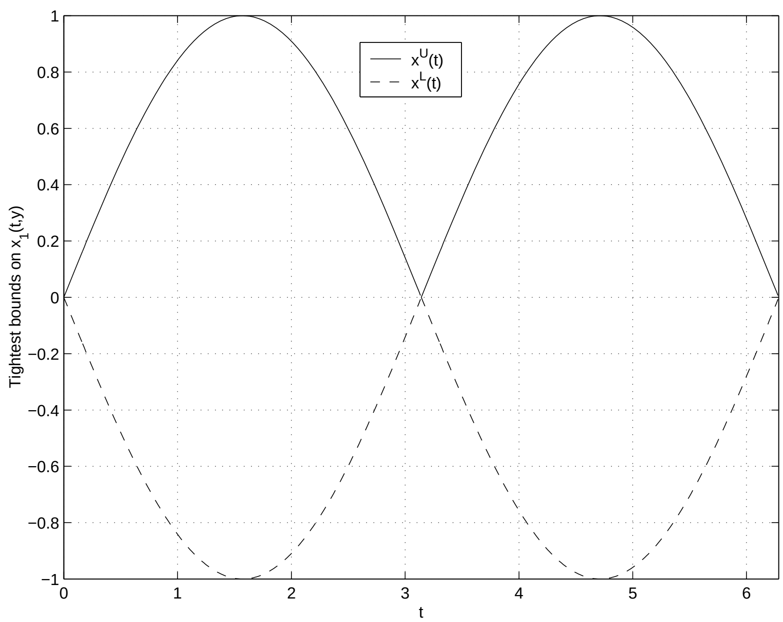

Figure 1: The tightest bounds for x_1.

subject to

$$\begin{gathered} x' = -2x + y \\ x(0) = 1 \\ y \in Y = [0,1] \\ x \in X = [0,1] \quad \forall\, t \in [0,1]. \end{gathered}$$

In order to construct a convex underestimator, we consider the integrand as a function on X. Since the integrand is a univariate concave function, its convex envelope on X is the secant connecting the two end points of X. Utilizing Corollary 3.3.6 yields the following convex underestimator for $F(y)$:

$$U(y) = \int_0^1 \frac{-(x^U)^2 + (x^L)^2}{x^U - x^L}(x - x^L) - (x^L)^2 \; dt.$$

Using the upper and lower bounds given in the problem statement, we have the following as our convex underestimator for $F(y)$:

$$U_{ps}(y) = \int_0^1 -x \; dt.$$

While $U_{ps}(y)$ yields a rigorous convex underestimator for $F(y)$, the underestimator is a rather weak one. Employing Theorem 3.4.4, we know that the tightest possible bounds are given by $x^L(t) = x(t,0)$ and $x^U(t) = x(t,1)$. Because the embedded differential equation is analytically solvable, we have that

$$x^L(t) = e^{-2t}$$

$$x^U(t) = \frac{e^{-2t} + 1}{2}.$$

Using these tightest possible time varying bounds on x (by inspection, we see that $[x^L(t), x^U(t)] \subseteq [0,1] \; \forall\, t \in [0,1]$), we construct the following convex underestimator for $F(y)$:

$$U_{tb}(y) = \int_0^1 \frac{-3xe^{-4t} + e^{-6t} + 2xe^{-2t} + x - e^{-2t}}{2e^{-2t} - 2} \; dt.$$

The nonconvex integrand and its two underestimators are illustrated below in Figure 2. It is important to note that while analytical solutions to the embedded differential equation and integrals were known and utilized for the construction of this example, neither is actually necessary for the construction of convex underestimators. Rather, to find the tightest bounds, the system may be numerically integrated to yield the matrix $\mathbf{M}(\underline{t})$ and the vector $\mathbf{n}(\underline{t})$ (see Equation 3) for each fixed $\underline{t}$ as chosen adaptively by the integrator. Additionally, $F(\mathbf{y})$ or $U(\mathbf{y})$ must be determined numerically pointwise in $\mathbf{y}$ in conjunction with the branch-and-bound algorithm.

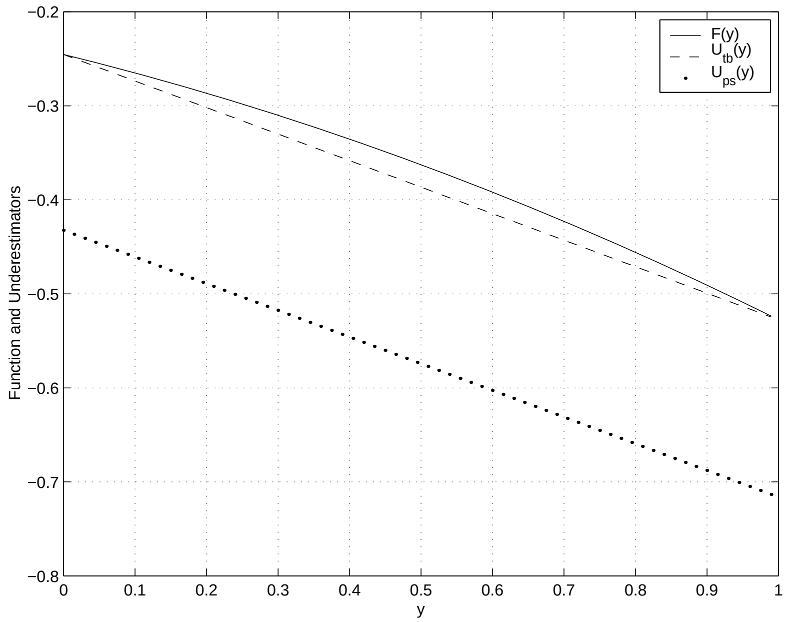

Figure 2: $F(y)$ and its convex underestimators $U_{ps}(y)$ and $U_{tb}(y)$.

3.5 Future Work in Linear Dynamic Embedded Systems

While much of the underlying convexity theory has already been developed, there still remains a wide body of unexplored research in global optimization with linear dynamic embedded systems. One area of primary concern is the implementation of a global optimization algorithm for Problem 3.1.1. From the above material, it should be obvious that standard branch-and-bound [27, 39] and branch-and-reduce [61, 62] methods for nonconvex NLPs can be applied to the optimization of dynamic optimizations with linear dynamic systems embedded. While the convergence properties of McCormick's underestimators and the αBB underestimators have been proven in algebraic spaces [52, 50], this property has yet to be proven for the dynamic case. Additionally, while it can be shown trivially that the convex envelope for the integrand yields the best possible convex underestimator in accordance with Corollary 3.3.6, we are currently unsure if the convex envelope for the integrand implies the convex envelope of the integral. Clearly, this would be a powerful result as it would imply that obtaining the convex envelope for the integrand and subsequently utilizing Corollary 3.3.6 to generate a convex underestimator would theoretically yield the tightest possible underestimators for the integral and hence the fastest possible convergence for the branch-and-bound algorithm. Obviously, much work remains in the details and testing of an algorithmic procedure to implement the already developed theory.

As presented, the composite function approach establishes a method for solving problems in which the parameters $\mathbf{y}$ are continuous variables. This makes the method ideal for solving control parameterization representations of optimal control problems with linear dynamic systems embedded. Moreover, the formulation of Problem 3.1.1 is ideally suited to be extended to handling $\mathbf{y}$ in an integer space. A number of general algorithms have emerged in recent years for the solution of MINLPs and INLPs in which the participating functions are nonconvex [61, 2, 42, 43, 44]. All of these methods rely on convex underestimators constructed on sets formed from the continuous relaxations of the integer variables. Hence, the theoretical framework above can be utilized to solve specific classes of MIDO problems.

In addition to the above challenges remaining, there are several other research areas yet to be explored. First, in its current formulation, Problem 3.1.1 can only handle a system of ordinary differential equations. We believe, however, that it can be shown that a system of linear differential algebraic equations always has a solution affine in $\mathbf{y}$. Hence, Lemma 3.3.2 will be applicable to DAE systems, which will broaden the range of problems directly solvable with the above developed theory. Second, we will explore methods encompassing problems in which the final time is allowed to vary. Inherently, this adds nonlinearity to the problem; thus, either we will seek a reformulation method to solve the problem directly in its linear form, or we will seek to solve the problem via the methods to be developed in Section 4. Finally, we will examine the influence of both equality and inequality path constraints on the system. Equality path constraints obviously will be handled by the techniques developed for solving DAEs. Inequality path constraints, on the other hand, will require a more sophisticated solution technique employing either the introduction of isoperimetric constraints on the integral violation of the path constraints or the enforcement of path constraints at a finite number of points in time.

4 Global Optimization with Nonlinear Dynamic Embedded Systems

This task will harness the composite function approach of the previous section to develop a global solution method for optimization problems with a nonlinear dynamic system embedded. For the sake of brevity, we will only examine the case of a simple formulation with a single state variable, but the extension to more general cases is evident. The problem is stated below in its general form.

Problem 4.0.1. Let Y be a nonempty compact convex subset of $\mathbb{R}^n$, $X \subseteq \mathbb{R}$ such that $x(t,\mathbf{y}) \in X\ \forall\ (t,\mathbf{y}) \in [t_o, t_f] \times Y$. Consider the following problem:

$$\min_{\mathbf{y}} F(\mathbf{y}) = \int_{t_0}^{t_f} f[x(t,\mathbf{y})]\ dt$$

subject to

$$\begin{gathered} x' = h(t,x,\mathbf{y}) \\ x(t_0) = \mathbf{q^T y} \\ \mathbf{g}(\mathbf{y}) \leq \mathbf{0} \\ y \in Y \end{gathered}$$

where f is a nonconvex continuous mapping $f : X \to \mathbb{R}$, h is a Lipschitz continuous mapping $h : [t_0, t_f] \times X \times Y \to \mathbb{R}$, and g is a convex mapping $g : Y \to \mathbb{R}^d$. Additionally, for the set $G = \{\mathbf{y} \mid \mathbf{g}(\mathbf{y}) \leq \mathbf{0}\}$, we require that $Y \cap G \neq \emptyset$.

In order to construct a convex underestimator, convexity of the integrand is only required for fixed t. McCormick [52] proposed the following method for constructing convex underestimators. Consider the composite function $f[x(\mathbf{y})]$, where f is a continuous function of a single variable, and $x(\mathbf{y})$ is a continuous function of n variables. Suppose that the convex envelope e of f is known on some interval $[a,b]$ of interest; this additionally implies that its minimum on this interval may be computed. Suppose also that a convex function c and a concave function C are known such that

$$c(\mathbf{y}) \leq x(\mathbf{y}) \leq C(\mathbf{y}) \quad \forall\ \mathbf{y} \in Y.$$

Then, a convex underestimating function for $f[x(\mathbf{y})]$ on $\mathbf{y} \in Y \cap \{\mathbf{y} \mid a \leq x(\mathbf{y}) \leq b\}$ is given by

$$e(\text{mid}[c(\mathbf{y}), C(\mathbf{y}), z_{min}]),$$

where $z_{min} \in [a,b]$ is a point at which f attains its minimum on $[a,b]$ and $\text{mid}(z_1, z_2, z_3)$ is the function that selects the middle value of its three scalar arguments. McCormick [52] also introduced the notion of a factorable programming representation, which employs the above result recursively in order to apply it to a very broad class of functions.

We propose to apply McCormick's result to the construction of convex underestimators for nonlinear dynamic embedded problems such as Problem 4.0.1. We will assume that the convex envelope of the integrand f on any scalar interval can be constructed. Consider the solution to the embedded initial value problem $x(t, \mathbf{y})$. Suppose for each fixed t we have a pair of dynamic systems whose solutions $c(t, \mathbf{y})$ and $C(t, \mathbf{y})$ satisfy the following:

$$c(t,\mathbf{y}) \leq x(t,\mathbf{y}) \leq C(t,\mathbf{y}) \quad \forall\ (\underline{t}, \mathbf{y}) \in [t_0, t_f] \times Y. \tag{10}$$

Then, if $c(t, \mathbf{y})$ is partially convex and $C(t, \mathbf{y})$ is partially concave, we can use these functions to construct the desired convex underestimator for the integrand via McCormick's method. Suppose an analytical solution for $x(t, \mathbf{y})$ is obtainable. Then, $c(t, \mathbf{y})$ and $C(t, \mathbf{y})$ could be constructed by inspection. However, for realistic problems, the analytical solution to the nonlinear dynamic embedded system will rarely be known. Therefore, we seek an alternative solution.

Suppose that $c(t, \mathbf{y})$ and $C(t, \mathbf{y})$ are the solutions to linear dynamic systems. We have already established that such solutions are affine with respect to $\mathbf{y}$. By definition, affine functions are both convex and concave; hence, $c(t, \mathbf{y})$ and $C(t, \mathbf{y})$ would trivially satisfy the requirements of convexity and concavity respectively. Suppose that we have the following linear system subject to the same initial condition as x':

$$c' = A(t)c + \mathbf{B}(t)\mathbf{y} + p(t)$$

such that

$$A(t)c(t,\mathbf{y}) + \mathbf{B}(t)\mathbf{y} + p(t) \leq h(t, x(t,\mathbf{y}), \mathbf{y}) \quad \forall\ (\underline{t}, \mathbf{y}) \in [t_0, t_f] \times Y.$$

Clearly, the following must be valid (although this is not to be confused with a solution technique for solving the ODE):

$$x(t,\mathbf{y}) = \int_{t_0}^{t} h(t, x(t,\mathbf{y}), \mathbf{y})\ dt + \mathbf{q}^{\mathbf{T}}\mathbf{y}$$

$$c(t,\mathbf{y}) = \int_{t_0}^{t} A(t)c + \mathbf{B}(t)\mathbf{y} + p(t)\ dt + \mathbf{q}^{\mathbf{T}}\mathbf{y}.$$

By Lemma 3.3.3, the left hand part of Equation 10 is satisfied. Analogously, an overestimating linear dynamic system $C'(t, \mathbf{y})$ could be found yielding a valid inequality for the right hand side of Equation 10. We therefore propose to seek methods for rigorously calculating the functions $\mathbf{c}(t, \mathbf{y})$ and $\mathbf{C}(t, \mathbf{y})$ for multivariate state equations. This can be accomplished either by generating linear differential systems whose solutions obey the properties of Equation 10 or by utilizing interval extensions to ODEs to bound the solution space of $\mathbf{x}(t, \mathbf{y})$ and determine $\mathbf{c}(t, \mathbf{y})$ and $\mathbf{C}(t, \mathbf{y})$ based on these bounds. Additionally, we will consider complications similar to those in the linear embedded dynamic programs such as extensions to DAEs, state inequality bounds, etc.

5 Variational Approach

Until now, we have only considered solving discretizations of variational calculus and optimal control problems via control parameterizaton. However, often times, one may wish to solve the dynamic program in the original infinite dimensional space. Because variational problems are solved in an infinite dimensional space, the approach is very different from those previously considered. Despite these differences, the two different approaches are amalgamated to form a cohesive whole by the notions of convexity and convex underestimators. We will therefore begin our analysis by examining how convexity extends into an infinite dimensional space. Again, for brevity, we only consider a univariate variational problem; extensions to multivariate cases are feasible, but not trivial. Additionally, in this section, we assume that all functions have continuous partial derivatives with respect to their arguments. This enables us to employ the following working definition of convexity.

Definition 5.0.2. The real valued function f will be convex on $D \subset \mathbb{R}^d$ if it has continuous partial derivatives on D and satisfies the inequality

$$f(\mathbf{x}) \geq f(\mathbf{x}_0) + \nabla f(\mathbf{x}_0) \cdot (\mathbf{x} - \mathbf{x}_0), \qquad \forall\, \mathbf{x}, \mathbf{x}_0 \in D$$

In variational problems, the objective is actually a functional that maps elements of an infinite dimensional function space to real values. Of particular interest are integral functionals on linear spaces of functions. Integral functionals are functionals that map a linear space of functions to a real value via a definite integral. We define convexity on a linear space of functions $\mathcal{X}$ in the following manner ($\delta J(x; v)$ is the Gâteaux variation of J at x in the direction v).

Definition 5.0.3. A functional J on a set $\mathcal{D} \subset \mathcal{X}$ is said to be [strictly] convex on $\mathcal{D}$ provided that when x and $x + v \in \mathcal{D}$ then $\delta J(x; v)$ is defined and $J(x + v) - J(x) \geq \delta J(x; v)$ [with equality if and only if v=$\mathcal{O}$, where $\mathcal{O}$ is the unique vector such that $c\mathcal{O} = 0x = \mathcal{O},\ \forall x \in \mathcal{X},\ c \in \mathbb{R}$].

Convexity is an important notion in optimization algorithms in a finite algebraic space because convexity implies that any stationary point found is a global minimum (the unique global minimum for strict convexity). As expected, an analogous result exists for the minimization of convex functionals, as stated in the following proposition.

Proposition 5.0.4. *If J is [strictly] convex on $\mathcal{D} \subset \mathcal{X}$ then each $x_0 \in \mathcal{D}$ for which $\delta J(x_0; v) = 0$, $\forall\, x_0 + v \in \mathcal{D}$ minimizes J on $\mathcal{D}$ [uniquely].*

Proof. By the definition of convexity, we have $J(x + v) - J(x) \geq \delta J(x; v)$. By hypothesis $x_0 \in \mathcal{D}$ makes $\delta J(x_0; v) = 0$. Hence, we have

$$J(x_0 + v) - J(x_0) \geq \delta J(x_0; v) = 0$$

[with equality *iff* $v = \mathcal{O}$]. But clearly, all admissible $x \in \mathcal{D}$ can be written as $x_0 + v$ since by hypothesis the above inequality holds $\forall\, x_0 + v$. Thus, $x = x_0 + v$ and

$$J(x) \geq J(x_0)$$

[with equality *iff* $x = x_0$], which by definition implies x_0 minimizes J on $\mathcal{D}$ [uniquely].

□

Note that the above Proposition illustrates the fundamental principle that minimization of convex functionals occurs for the function that makes the Gâteaux variation equal to zero.

Utilizing the above theoretical developments, we are in a position to now create convex underestimators for variational problems. At the heart of this analysis is the following fundamental theorem, which links convexity and underestimation of real functions to convexity and underestimation of integral functionals. One should note the similarity between this theorem and Theorem 3.3.5 and Corollary 3.3.6.

Theorem 5.0.5. *Let the functionals*

$$F(x) = \int_a^b f(t, x(t), x'(t))\, dt \qquad \textit{and} \qquad U(x) = \int_a^b u(t, x(t), x'(t))\, dt$$

be defined on the set

$$\mathcal{D} = \{x \in C^1[a, b]; (x(t), x'(t)) \in D \subset \mathbb{R}^2\}.$$

If $u(\underline{t}, x, x')$ is partially convex on $[a, b] \times D$ and

$$u(\underline{t}, x, x') \leq f(\underline{t}, x, x'), \qquad \forall \textit{ fixed } t \in [a, b] \textit{ and } x(t), x'(t) \in D$$

then $U(x)$ is convex on $\mathcal{D}$ and $U(x) \leq F(x)$. That is, if $u(t, x, x')$ is a convex underestimator for $f(t, x, x')$ on $[a, b] \times D$, then $U(x)$ is a convex underestimator for $F(x)$ on $\mathcal{D}$.

Proof. When $x,\ x+v \in \mathcal{D}$, then by partial convexity, we have that at each $t \in (a,b)$, the convexity of u yields

$$u(t, x+v, x'+v') - u(t,x,x') \geq u_x(t,x,x')v + u_{x'}(t,x,x')v'.$$

The above equation is integrated to yield

$$\int_a^b u(t, x(t)+v(t), x'(t)+v'(t)) - u(t, x(t), x'(t))\, dt \geq \int_a^b u_x(t,x(t),x'(t))v(t) + u_{x'}(t,x(t),x'(t))v'(t)\, dt \quad \forall\ x \in \mathcal{D}.$$

However, this is equivalent to

$$U(x+v) - U(x) \geq \delta U(x; v),$$

which by Definition 5.0.3 shows that $U(x)$ is convex. It remains to show that $U(x) \leq F(x)$, but this is evident from the comparison theorem for integrals [60] because by assumption, we have that $u(\underline{t}, x, x') \leq f(\underline{t}, x, x')$, $\forall$ fixed $t \in [a,b]$, and $x(t),\ x'(t) \in D$.

□

Remark. This theorem enables any known method for convex underestimation of real functions to be harnessed in the convex underestimation of integral functionals. We note that because we are already optimizing in an infinite dimensional space, we are not limited to methods that do not introduce new variables.

The standard method of determining a stationary function for a variational problem is to solve the Euler-Lagrange equations (e.g. [69]). In the classical derivation of the Euler-Lagrange equations, the state variable is unbounded. However, as we have previously seen, deriving convex underestimators in algebraic spaces often requires bounds on the state variables; therefore, the standard Euler-Lagrange equations are inadequate for our task. Beginning with the work of Valentine [71] early in the last century, many authors have attempted to derive new necessary conditions for determining stationary functions for variational problems. We restate the fact that in order to construct a rigorous procedure for determining a global minimum to an optimization problem, the optimality conditions must be both necessary and sufficient. Merely satisfying a necessary condition does not even imply local minimality. However, to the best of the author's knowledge, prior to this work, no one has produced a generally suitable sufficiency condition for variational problems with bounded state variables. We present the proof of sufficiency below in two steps. First, a lemma is proven demonstrating that the minimization of a Lagrangian augmented function yields the minimum to the original state bounded problem. The theorem that follows presents the sufficiency condition for optimizing a variational problem with a bounded state variable.

Lemma 5.0.6. *Suppose $f = f(t, \hat{x}(t), \hat{x}'(t))$ and $g = g(t, \hat{x}(t), \hat{x}'(t))$ are continuous on $[a,b] \times \mathbb{R}^2$ and there exists a function $\hat{\lambda}(t) \in \hat{C}[a,b]$, for which x_0 minimizes $\tilde{F}(\hat{x}) = \int_a^b \tilde{f}(t, \hat{x}(t), \hat{x}'(t))\, dt$ on $\hat{\mathcal{D}} \subseteq \hat{C}^1[a,b]$ where $\tilde{f} \stackrel{\text{def}}{=} f + \hat{\lambda} g$. Then x_0 minimizes $F(\hat{x}) = \int_a^b f(t, \hat{x}(t), \hat{x}'(t))\, dt$ on $\hat{\mathcal{D}}$ under the following constraints:*

1. $g(t, \hat{x}(t), \hat{x}'(t)) \leq 0, \quad t \in (a,b)$
2. $\hat{\lambda}(t) \geq 0, \quad t \in (a,b)$
3. $\hat{\lambda}(t) g(t, \hat{x}_0(t), \hat{x}_0'(t)) \equiv 0$

Proof. If $\hat{x} \in \hat{\mathcal{D}}$, the following will be true by the definition of a minimum:

$$\begin{aligned}
\tilde{F}(\hat{x}) &\geq \tilde{F}(\hat{x}_0) \\
F(\hat{x}) + \int_a^b \hat{\lambda}(t) g(t, \hat{x}(t), \hat{x}'(t))\, dt &\geq F(\hat{x}_0) + \int_a^b \hat{\lambda}(t) g(t, \hat{x}_0(t), \hat{x}_0'(t))\, dt \\
F(\hat{x}) - F(\hat{x}_0) &\geq \int_a^b (\hat{\lambda}(t) g(t, \hat{x}_0(t), \hat{x}_0'(t)) - \hat{\lambda}(t) g(t, \hat{x}(t), \hat{x}'(t)))\, dt
\end{aligned}$$

By the constraint 3,

$$F(\hat{x}) - F(\hat{x}_0) \geq -\int_a^b (\hat{\lambda}(t)g(t, \hat{x}(t), \hat{x}'(t)))\, dt.$$

Due to the nonnegativity of $\hat{\lambda}(t)$, constraint 1 may be multiplied by $\hat{\lambda}(t)$ without altering the sign of the inequality

$$\hat{\lambda}(t)g(t, \hat{x}(t), \hat{x}'(t)) \leq 0 \ .$$

It immediately follows that

$$F(\hat{x}) \geq F(\hat{x}_0).$$

□

Remark. Although the product $\hat{\lambda}(t)g(t, \hat{x}(t), \hat{x}'(t))$ may only be piecewise continuous, this poses no difficulty to integration provided there exist only finitely many points of discontinuity (cf. Rudin [60]).

The following Theorem states the sufficiency condition for minimizing a bounded convex functional.

Theorem 5.0.7. *For a domain D of $\mathbb{R}^2$ suppose that $f(\underline{t}, x(t), x'(t)) \in C^1([a, b] \times D)$ is convex, and we wish to minimize*

$$F(\hat{x}) = \int_a^b f(t, \hat{x}(t), \hat{x}'(t))\, dt$$

on

$$\hat{\mathcal{D}} = \{\hat{x}(t) \in \hat{C}^1[a, b] : \hat{x}(a) = a_1, \hat{x}(b) = b_1\},$$

subject to the inequality constraint

$$g(t, \hat{x}(t)) \leq 0, \qquad t \in (a, b),$$

where $g(\underline{t}, \hat{x})$ is also convex on $[a, b] \times \mathbb{R}$. For any $\hat{x}_0 \in \mathcal{D}$ satisfying the inequality, the following conditions are sufficient to guarantee a minimum: There exists a $\lambda(t) \in \hat{C}[a, b]$ such that $\lambda(t) \geq 0$ and $\lambda(t)g(\underline{t}, x_0(t)) \equiv 0$. Additionally, for all intervals excluding corner points the following equation must be satisfied:

$$\frac{d}{dt} f_{x'}(t, \hat{x}_0(t), \hat{x}_0'(t)) - f_x(t, \hat{x}_0(t), \hat{x}_0'(t) = \lambda(t) g_x(\underline{t}, \hat{x}_0(t)).$$

At any corner point c, the following condition must hold:

$$f_{x'}(c-, \hat{x}_0(c-), \hat{x}_0'(c-)) = f_{x'}(c+, \hat{x}_0(c+), \hat{x}_0'(c+)).$$

Proof. First, construct the functional

$$\tilde{F}(\hat{x}) = \int_a^b f(t, \hat{x}(t), \hat{x}'(t) + \lambda(t) g(\underline{t}, \hat{x}(t))\, dt \quad \text{on } \hat{\mathcal{D}}.$$

Lemma 5.0.6 above establishes that a minimizing solution to $\tilde{F}(\hat{x})$ will also be a minimizing solution for $F(\hat{x})$ under the given inequality constraint and hypothesis. Therefore, it will be sufficient to demonstrate that $\hat{x}_0(t)$ minimizes $\tilde{F}(\hat{x})$. By hypothesis, we have $\hat{x} \in \hat{C}^1[a, b]$, and we also have the following condition of stationarity at non-corner points:

$$\frac{d}{dt} f_{x'}(t, \hat{x}(t), \hat{x}'(t) - f_x(t, \hat{x}(t), \hat{x}'(t) = \lambda(t) g_x(t, \hat{x}(t)).$$

Moreover, by assumption, we also have

$$\tilde{f}(\underline{t}, \hat{x}_0(t), \hat{x}_0'(t) = f(\underline{t}, \hat{x}_0(t), \hat{x}_0'(t) + \lambda(\underline{t}) g(\underline{t}, \hat{x}),$$

which is convex at non-corner points. Additionally by hypothesis, $\hat{x}_0$ satisfies the stated corner condition at any corner point. Therefore, by Theorem 7.12 [69], $\hat{x}_0$ provides a minimum for $\tilde{F}$ and hence F.

□

Remark. It should be noted that the differential equation defining optimality is the first Euler-Lagrange equation for the modified function $\tilde{F}(\hat{x})$. Additionally, while the above theorem is proven only for one constraint, it should be obvious that the same theorem can trivially be extended to multiple constraints provided the constraints are nonintersecting. This follows because the minimum $\hat{x}_0(t)$ cannot exist at multiple distinct points simultaneously. Thus, when $\hat{x}_0(t)$ lies on one constraint, the multiplier for any other constraint is simply 0.

Hestenes [37] presents a very similar necessary condition that differs only slightly from our sufficiency condition in the Weierstrass-Erdmann corner condition. One of the primary focuses of the research in this area will be to close this small gap between necessity and sufficiency, yielding an optimality condition appropriate for global optimization.

To this point, we have presented a method for the generation of convex underestimators for variational problems and a theorem yielding sufficiency for minimality of these convex underestimating problems. However, several large difficulties remain before a global optimization algorithm for nonconvex variational problems can be implemented. First and foremost is the reliable numerical solution of the Euler-Lagrange equations, which take the form of two-point boundary value problems. We propose to perform a thorough evaluation of existing techniques for solving two-point boundary value problems and then either implement one of these methods or derive a method of our own. Second, we propose to utilize convex underestimators in a branch-and-bound framework to solve variational problems to global minimality. However, unlike in the composite function approach, the branching would be required to be performed on an infinite dimensional space. This poses a large difficulty because due to the nature of an infinite dimensional space, there is not an obvious method for dividing the space into usable subregions. Finally, we propose to address other smaller details such as extending the problem scope to address multiple states, isoperimetric constraints, optimal control problems, etc.

6 Conclusions

The objective of the proposed research is to generate practically implementable algorithms for globally optimizing dynamic programs. Dynamic optimization problems compose an extremely important class of problems in the chemical industries as well as industries relevant to other engineering disciplines. A few examples of such applications were listed: optimization of batch processes, process changeovers, process safety verification, etc. In addition to this list, the proposed optimization techniques will be able to solve mixed-integer dynamic optimization problems such as kinetic model reductions.

The strategy for optimizing dynamic programs has been categorized into two fundamental paradigms: the composite function approach and the variational approach. The composite function approach utilizes the composition of two functions to reduce the optimization problem from an infinite dimensional function space to a finite dimensional algebraic space. The composite function approach is further divided into two methods that exploit the structure of the dynamic system embedded to facilitate the solution of the problem; these two structures are linear dynamic systems embedded and nonlinear dynamic systems embedded. Currently, a large body of work has already been developed for optimizing dynamic problems with linear dynamic systems embedded. A convexity theory has been developed that employs readily available algebraic convex relaxation techniques to generate convex underestimators for the dynamic optimization problems. This enables these problems to be solved within a conventional branch-and-bound or branch-and-reduce framework. The task of optimizing problems subject to nonlinear dynamic systems embedded is not as well developed as the linear case. However, it is believed that McCormick's underestimation techniques in conjunction with the theory for linear dynamic systems embedded will eventually lead to a concrete algorithm for the global optimization of dynamic programs with nonlinear dynamic systems embedded. Both subclasses of the composite function approach are ideally suited for solving optimal control problems via control parameterization. It is therefore believed that the completion of this research will have a profound impact on solving many important dynamic optimization problems.

The other broad framework, the variational approach, is also designed to solve dynamic optimizations to global optimality; however, unlike the composite function approach, the variational approach attacks the optimization problem in the original infinite dimensional space. While the variational approach is very attractive because it does not require the discretization of the original problem, solving optimization problems in an infinite dimensional space poses many serious difficulties. Among all of the difficulties, three stand out as being of particular interest. First, the solution of variational problems consists primarily of solving the Euler-Lagrange equations, which unfortunately take the form of difficult to solve two-point boundary value problems. The second dilemma is in finding a necessary and sufficient condition for state space constrained variational problems. Although we have already derived a sufficiency condition based upon convexity results, there still exists a narrow gap between our sufficiency condition and the previously known necessary condition. Finally, we have proposed that the methodology for solving the variational problems will consist of a branch-and-bound framework. However, it is currently unclear how to branch in an infinite dimensional functional space.

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