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Method for Automatic Costate Calculation

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A method for the automatic calculation of costates using only the results obtained from direct optimization techniques is presented. The approach exploits the relation between the time-varying costates and certain sensitivities of the variational cost function, a relation that also exists between the Lagrangian multipliers obtained from a direct optimization approach and the sensitivities of the associated nonlinear-programming cost function. The complete theory for treating free, control-constrained, interior-point-constrained, and state-constrained optimal control problems is presented. As a numerical example, a state-constrained version of the brachistochrone problem is solved and the results are compared to the optimal solution obtained from Pontryagin's minimum principle. The agreement is found to be excellent.

Nomenclature

f	= right-hand side of state equations
g_e	= control equality constraints
g_i	= control inequality constraints
h_e	= state equality constraints
h_i	= state inequality constraints
J	= cost function
M	= interior-point constraints
m	= dimension of control vector $\boldsymbol{u}$
N	= total number of nodes minus 1 = total number of subintervals
n	= dimension of state vector $\boldsymbol{x}$
PWC	= set of piecewise continuous functions
t	= time
t_f	= final time
t_i	= nodes along the time axis
t_0	= initial time
$\boldsymbol{u}$	= control vector
$\boldsymbol{x}$	= state vector
$\boldsymbol{x}_f$	= final state
$\boldsymbol{x}_i$	= state vector at node t_i
$\boldsymbol{x}_0$	= initial state
$\lambda(t)$	= costate
λ_i	= Lagrangian multiplier associated with differential constraints along subinterval i
μ_i	= Lagrangian multiplier associated with state constraints at node i
σ_i	= Lagrangian multiplier associated with control constraints along subinterval i
Φ	= cost function
ψ_f	= boundary conditions at final time
ψ_0	= boundary conditions at initial time

I. Introduction

THE methods of solution for optimal control problems are divided into two major classes, namely, direct and indirect methods. Indirect methods are based on Pontryagin's minimum principle[1–5] and require the numerical solution of multipoint boundary value problems (MPBVPs).[6–8] The advantages of these methods lie in their fast convergence in the neighborhood of the optimal solution, even if the cost gradients are very shallow. Furthermore, the optimal solutions are obtained with extremely high precision, and subtle properties of the optimal solution can be identified clearly. On the other hand, indirect optimization techniques usually require excellent initial guesses before convergence can be achieved at all. This requirement is especially restrictive because these methods involve Lagrangian multipliers whose physical meaning is nonintuitive and provides little help for generating reasonable initial guesses on an ad hoc basis. Furthermore, the switching structure, that is, the sequence in which different control logics become active along the optimal solution, has to be guessed in advance.

Direct optimization techniques rely on restricting the infinite dimensional space of admissible candidate trajectories to a finite dimensional subspace of the original function space.[9] The optimal solution within this subspace then is determined by directly optimizing the cost criterion through nonlinear programming (NLP).[10] The convergence radius of such methods is usually much larger than that of indirect methods. Furthermore, initial guesses have to be provided only for physically intuitive quantities such as states and, possibly, controls. Finally, the switching structure of the optimal solution need not be guessed at all.

In an attempt to get the best of both worlds, the present paper introduces a method to approximately calculate the costates associated with optimal control problems, based only on the results obtained from a direct optimization approach. The starting point is the well-known relation between the time-varying costates and certain sensitivities of the variational cost function.[2,11] These sensitivities are represented approximately by the cost sensitivities of the direct optimization approach, for which expressions in terms of the Lagrangian multipliers obtained from the NLP approach are derived.

Numerically, the method requires only the calculation of a single near-optimal trajectory, which represents a significant improvement over the method presented previously.[11] However, the analytical results are tailored to a specific discretization scheme, namely, collocation with a simple trapezoidal integration rule. The expressions for costate estimates would have to be rederived if this discretization scheme were changed. For most schemes, this task should be straightforward as long as the near-optimal trajectory is calculated as the solution of a single NLP problem. Note, however, that concatenated or sequential approaches, such as the ones introduced elsewhere,[12,13] cannot be treated with an approach of the general nature presented here.

Other methods for automatic costate calculation are discussed elsewhere.[14–16] For example, the final costate values associated with the prescribed boundary conditions are integrated backward along the frozen solution obtained through direct optimization.[14] This approach requires the explicit implementation of the costate dynamics. In another example,[15] a best-match discretized costate function of time associated with the frozen trajectory obtained through direct optimization is obtained by minimizing a least-squares error comprising the transversality conditions and discretized costate dynamics. The linearity of the costate dynamics and the transversality conditions make this method noniterative. Elsewhere,[16] a

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relation between the discrete NLP multipliers and the time-varying Lagrangian multipliers is derived and exploited for automatic costate calculation.

The present paper is structured as follows: Sec. II defines a general optimal control problem and summarizes the associated variational optimality conditions. In Sec. III, the discretized problem formulation is introduced, and relations for certain cost sensitivities are derived in terms of the Kuhn–Tucker multipliers obtained from the NLP solution. In Sec. IV, the results of Sec. III are used to generate the desired costate estimates. Section V gives some remarks and relates the present paper to previously obtained results. In Sec. VI, a state-constrained version of the brachistochrone is treated as a numerical example, and the results are compared to the optimal solution obtained from Pontryagin's minimum principle. The agreement is found to be excellent.

II. Optimal Control Problem

In this section, we introduce a somewhat general optimal control problem, and in Sec. II.B, we present the associated necessary conditions for optimality. This defines the nomenclature for the various constant and time-varying multipliers used for the remainder of the paper.

Note that we do not consider interior-point constraints in the original problem formulation. However, such constraints arise naturally in our treatment of state inequality constraints.

A. Problem Formulation

Let us consider the following optimal control problem stated in Mayer form:

$$\min_{u\in(\mathrm{PWC}[t_0,t_f])^m,\ t_0\in R,\ t_f\in R} \phi[x(t_f),\ t_f] \tag{1}$$

subject to the conditions

$$\dot{x}(t) = f[x(t), u(t), t] \tag{2}$$

$$\psi_0[x(t_0), t_0] = 0 \tag{3}$$

$$\psi_f[x(t_f), t_f] = 0 \tag{4}$$

$$g_e[x(t), u(t), t] = 0 \tag{5}$$

$$g_i[x(t), u(t), t] \le 0 \tag{6}$$

$$h_e[x(t), t] = 0 \tag{7}$$

$$h_i[x(t), t] \le 0 \tag{8}$$

Here, $t \in R$, $x(t) \in R^n$, and $u(t) \in R^m$ are time, state vector, and control vector, respectively. The functions

$$\phi: R^{n+1} \to R, \qquad f: R^{n+m+1} \to R^n$$

$$\psi_0: R^{n+1} \to R^{k_0}, \qquad \psi_f: R^{n+1} \to R^{k_f}$$

$$k_0 \le n+1, \qquad k_f \le n$$

$$g_e: R^{n+m+1} \to R^{k_{ge}}, \qquad g_i: R^{n+m+1} \to R^{k_{gi}}$$

$$h_e: R^{n+1} \to R^{k_{he}}, \qquad h_i: R^{n+1} \to R^{k_{hi}}$$

are assumed to be sufficiently smooth with respect to their arguments of whatever order is required in this paper. The set of all piecewise continuous functions defined on the interval $[t_0, t_f]$ into R^m is denoted by $(\mathrm{PWC}[t_0, t_f])^m$. Conditions (2–8) represent the differential equations of the underlying dynamic system, the initial conditions, the final conditions, the control constraints, and the state constraints, respectively.

For the remainder of this paper, we assume that an optimal solution to problem (1–8) does exist and that $\partial\hat{g}/\partial u$ has full rank for all times $t \in [t_0, t_f]$ along the optimal solution. Here, $\hat{g}$ represents the vector of control constraints (including those arising from active state constraints) that are active at any given time t.

B. Necessary Conditions for Optimality

Let us assume that a solution to problem (1–8) exists, and, for simplicity, let us first consider the case where no state constraints (7) and (8) are active. Then, under certain normality and regularity conditions,[1–5] it can be shown that there are constant multiplier vectors $\nu_0 \in R^{k_0}$, $\nu_f \in R^{k_f}$ and a time-varying multiplier vector $\lambda(t) \in R^n$, which is nonzero for all times $t \in [t_0, t_f]$ such that

$$\dot{\lambda}^T = -\frac{\partial H}{\partial x} - \mu^T\frac{\partial \hat{g}}{\partial x} \tag{9}$$

$$\lambda(t_0)^T = -\nu_0^T\frac{\partial \psi_0}{\partial x(t_0)} \tag{10}$$

$$\lambda(t_f)^T = \frac{\partial \phi}{\partial x(t_f)} + \nu_f^T\frac{\partial \psi_f}{\partial x(t_f)} \tag{11}$$

$$H[x(t_0), \lambda(t_0), u(t_0), t_0] = \nu_0^T\frac{\partial \psi_0}{\partial t_0} \tag{12}$$

$$H[x(t_f), \lambda(t_f), u(t_f), t_f] = -\frac{\partial \phi}{\partial t_f} - \nu_f^T\frac{\partial \psi_f}{\partial t_f} \tag{13}$$

where

$$H(x, \lambda, u, t) = \lambda^T f(x, u, t) \tag{14}$$

denotes the Hamiltonian and $\hat{g}$ denotes the vector of active constraint functions. At each instant of time, the optimal control u^* satisfies the Pontryagin minimum principle, i.e.,

$$u^* = \arg\begin{cases}\min_u H(x, \lambda, u, t)\\ \text{subject to}\\ \hat{g}(x,\ u,\ t) = 0\end{cases} \tag{15}$$

The (time-varying) multiplier vector μ has the same dimension as $\hat{g}$ and is obtained from the Karush–Kuhn–Tucker (KKT) conditions applied to the optimization problem (15). As long as no state constraints (7), (8) are active, the Hamiltonian (14) is continuous throughout the time interval, including at times when control constraints become active or inactive.

To discuss the optimality conditions associated with state-constrained arcs, let us consider the case of a single, scalar state inequality constraint, $h(x, t) \le 0$, and let us assume that in the optimal solution to problem (1–8) this state inequality constraint becomes active in the following form:

$$h[x(t), t]\begin{cases} <0 & \text{for} \quad t \in [t_0, t_a)\\ =0 & \text{for} \quad t \in [t_a, t_b]\\ <0 & \text{for} \quad t \in (t_b, t_f]\end{cases} \tag{16}$$

The formal extension of the results below to vector-valued state constraints and to other switching structures then is straightforward.

In the variational approach to state-constrained optimal control problems, it is most customary to transform the active state constraint, say

$$h[x(t), t] = 0 \qquad \text{on} \qquad t \in [t_a, t_b] \tag{17}$$

into an equivalent combination of an interior-point constraint and a control constraint. Explicitly, Eq. (17) holds if and only if

$$M[x(t_a), t_a] \triangleq \begin{bmatrix} h(x,t)|_{t_a} \\ \left.\dfrac{\mathrm{d}h(x,t)}{\mathrm{d}t}\right|_{t_a} \\ \vdots \\ \left.\dfrac{\mathrm{d}^{q-1}h(x,t)}{\mathrm{d}t^{q-1}}\right|_{t_a}\end{bmatrix} = 0 \tag{18}$$

and

$$c[x(t), u(t), t] \triangleq \frac{\mathrm{d}^q h(x,t)}{\mathrm{d}t^q} = 0 \qquad \text{on} \qquad t \in [t_a, t_b] \tag{19}$$

Here, q is the smallest integer i for which a control u appears explicitly in $[\mathrm{d}^i h(x, t)]/\mathrm{d}t^i$ and is called the order of the state constraint.

Note that, along state-constrained arcs, the left-hand side of the control constraint (19) becomes a component of the constraint function $\hat{g}$ introduced in Eq. (9).

At the beginning of the state-constrained arc, the interior-point constraint (18) causes a discontinuous jump in the multipliers $\lambda(t)$ and in the Hamiltonian H, namely,

$$\lambda(t_a^+)^T = \lambda(t_a^-)^T - l^T \frac{\partial M[x(t_a), t_a]}{\partial x(t_a)} \tag{20}$$

$$H|_{t_a^+} = H|_{t_a^-} + l^T \frac{\partial M[x(t_a), t_a]}{\partial t_a} \tag{21}$$

Here, $l^T = [l_0, \ldots, l_{q-1}]$ is a q-dimensional vector of constant multipliers that compensates for the q degrees of freedom lost by enforcing conditions (18).

C. Relation Between Sensitivities and Lagrangian Multipliers

It is well known that the Lagrangian multipliers $\lambda(t)$, loosely speaking, represent the sensitivity of the optimal cost with respect to perturbations in the state vector x at time t (Ref. 2). A comprehensive study of these sensitivities is given elsewhere.[11] In the following, the main results are briefly summarized.

Let $J[x(t), t]$ denote the value of the optimal cost (1) obtained by solving problem (1–8) with the initial conditions (3) replaced by the condition that the state at some time t be $x(t)$. Then, along arcs where no state constraints are active, we have

$$\lambda(t)^T = \frac{\partial J[x(t), t]}{\partial x(t)} \tag{22}$$

Now, assume that a qth-order scalar state inequality constraint $h(x, t) \leq 0$ becomes active along the time interval $[t_a, t_b]$. Then, following Eqs. (16–21), the Lagrangian multipliers $\lambda(t)$ experience a discontinuous jump at t_a, with the height of the jump determined by the constant multiplier vector $l \in R^q$. The value of λ just before the jump, $\lambda(t_a^-)$, satisfies the sensitivity equation (22) because it belongs to an unconstrained part of the trajectory. The constant multiplier l satisfies

$$l^T = -\left.\frac{\partial J[x(t_a), t_a, b]}{\partial b}\right|_{b=0} \tag{23}$$

where b denotes the q vector $b = [b_0, \ldots, b_{q-1}]^T$ and $J[x(t_a), t_a, b]$ denotes the value of the optimal cost (1) obtained by solving problem (1–8) with the initial conditions (3) replaced by the condition that the state at time t_a be $x(t_a)$ and with the state constraint $h(x, t) = 0$ on $[t_a, t_b]$ replaced by

$$h(x, t) - \sum_{k=0}^{q-1} \frac{b_k}{k!}(t - t_a)^k = 0 \qquad \text{on} \qquad [t_a, t_b] \tag{24}$$

For times $t_i \subset (t_a, t_b)$ in the interior of the state-constrained arc, the right-hand side of Eq. (22) defines an artificial Lagrangian multiplier $\lambda(t_i^-)$ that would exist as a real multiplier only if t_i were the beginning of the constrained arc. The multiplier $\lambda(t_i)$ is related to $\lambda(t_i^-)$ through the jump condition (20), with t_a and $\lambda(t_i^+)$ replaced by t_i and $\lambda(t_i)$, respectively, and with the constant multiplier $l \in R^q$ defined by Eq. (23), also with t_a replaced by t_i. The constant multiplier vectors ν_0 and ν_f associated with the initial and final conditions (3) and (4), respectively, satisfy

$$\nu_0 = \left.\frac{\partial J(c_0, c_f)}{\partial c_0}\right|_{\substack{c_0=0\\c_f=0}} \tag{25}$$

$$\nu_f = \left.\frac{\partial J(c_0, c_f)}{\partial c_f}\right|_{\substack{c_0=0\\c_f=0}} \tag{26}$$

respectively. Here, $J(c_0, c_f)$ denotes the value of the optimal cost of problem (1–8) with the boundary conditions (3) and (4) replaced by

$$\begin{aligned} \psi_0[x(t_0), t_0] - c_0 &= 0 \\ \psi_f[x(t_0), t_0] - c_f &= 0 \end{aligned} \tag{27}$$

The relations (25) and (26) were not stated explicitly in our previous work[11] but can be derived easily with the methods presented there.

III. Direct Approach

Solving an optimal control problem on the basis of the necessary conditions summarized in Sec. II.B leads to an MPBVP. Numerically, this represents a nonlinear zero-finding problem. The main unknowns are the lengths of all time intervals involved, the initial values for the states that are not prescribed explicitly through the initial conditions (3), the initial values of the time-varying costates $\lambda(t)$, and the constant multipliers l, ν_0, ν_f introduced in Eqs. (9–21). Additionally, before a boundary value problem (BVP) can be set up, the analyst has to correctly guess the temporal sequence in which different control logics become active along the optimal solution (i.e., the optimal switching structure).

In an obvious way, direct approaches to trajectory optimization provide guesses for the optimal switching structure, including the length of each subarc, and guesses for the state histories. However, it is not clear, a priori, how estimates for the costates $\lambda(t)$ and the constant multipliers l, ν_0, ν_f can be obtained.

It is known that the multipliers in question represent sensitivities of the optimal cost with respect to perturbations in certain state initial values.[2,11] The equivalent sensitivities of the parameter optimal solution are captured in the KKT multipliers associated with the prescribed initial states, if only the initial states are prescribed explicitly.

In the following, we state the discretized form of the original optimal control problem (1–8). Then, we define two auxiliary problems with explicitly prescribed initial states. The important result is that the solution of the auxiliary problems, including all multipliers involved, can be determined analytically from the solution to the original discretized optimal control problem. Thus, cost sensitivities of the parameter optimal solution can be derived in terms of the KKT multipliers associated with the NLP solution to the original discretized optimal control problem.

A. Discretized Optimal Control Problem (Problem A)

One of the most successful discretization methods is the collocation approach in which both states and controls are discretized and the dynamic and state constraints (2), (5), (6), (7), and (8) are enforced only at isolated points. Using a trapezoidal rule to enforce the equations of motion at a single point between neighboring nodes, this scheme leads to the following NLP problem:

$$\min_{x_0,\ldots,x_N,\, u_1,\ldots,u_N,\, t_0,\, t_N \in R^{n(N+1)+mN+2}} \phi(x_N, t_N) \tag{28}$$

subject to the conditions

$$\dot{\bar{x}}_j - f(\bar{x}_j, u_j, \bar{t}_j) = 0, \qquad j = 1, \ldots, N \tag{29}$$

$$\psi_0(x_0, t_0) = 0 \tag{30}$$

$$\psi_f(x_N, t_N) = 0 \tag{31}$$

$$\left.\begin{aligned} g_e(\bar{x}_j, u_j, \bar{t}_j) &= 0, \\ g_i(\bar{x}_j, u_j, \bar{t}_j) &\leq 0, \end{aligned}\right\} \qquad j = 1, \ldots, N \tag{32}$$

$$\left.\begin{aligned} h_e(x_j, t_j) &= 0, \\ h_i(x_j, t_j) &\leq 0, \end{aligned}\right\} \qquad j = 0, \ldots, N \tag{33}$$

where

$$t_j = (t_N - t_0)\tau_j, \qquad j = 0, \ldots, N \tag{34}$$

$$\left.\begin{aligned} \bar{t}_j &= \frac{t_j + t_{j-1}}{2} \\ \bar{x}_j &= \frac{x_j + x_{j-1}}{2} \\ \dot{\bar{x}}_j &= \frac{x_j - x_{j-1}}{t_j - t_{j-1}} \end{aligned}\right\} \qquad j = 1, \ldots, N \tag{35}$$

N is a user-chosen integer, and $0 = \tau_0 < \tau_1 < \cdots < \tau_{N-1} < \tau_N = 1$ is a user-chosen subdivision of the unit time interval [0, 1]. Noting that any reasonable function can be approximated arbitrarily closely in norm even by step functions,[17] it can be expected that, under mild assumptions, the optimal solution t_0^*, t_N^*, x_i^*, $i = 0, \ldots, N$ of the discretized problem (28–35) converges to the optimal solution t_0^*, t_f^*, $x^*(t_i)$, $i = 0, \ldots, N$ of the continuous problem (1–8) as $N \to \infty$.

For the remainder of the paper, let problem (28–33) be denoted as problem A. Following the general formalism of the KKT conditions (A4, A5), we associate problem A with the Lagrangian function

$$L^A = \phi(x_N, t_N) + \pi_f^T \psi_f(x_N, t_N) + \sum_{j=1}^{N} \lambda_j^T [f(\bar{x}_j, u_j, \bar{t}_j) - \dot{\bar{x}}_j]$$

$$+ \sum_{j=1}^{N} \sigma_j^T g(\bar{x}_j, u_j, \bar{t}_j) + \sum_{j=0}^{N} \mu_j^T h(x_j, t_j) + \pi_0^T \psi_0(x_0, t_0) \quad (36)$$

In an obvious way, Eq. (36) identifies the cost function, the constraints, and the nomenclature used for the multipliers associated with the various constraints (29–33).

The main result is a method by which costate estimates for the continuous optimal control problem can be determined from the Lagrangian multipliers associated with the solution to the discretized optimal control problem. These costate estimates are obtained through some postprocessing of the Lagrangian multipliers appearing in Eq. (36). The basic underlying assumption is, loosely speaking, that the cost sensitivity of the original optimal control problem with respect to perturbations in the initial states can be well approximated by that of the discretized problem.

To develop the explicit postprocessing procedures, we need to introduce two auxiliary problems.

B. Auxiliary Problem B

To determine cost sensitivities with respect to changes in the initial states, we consider now a new problem, denoted by B_0, that differs from problem A in that the initial conditions (30) are replaced by conditions that explicitly prescribe the initial time and the initial states, namely,

$$t_0 = \left(t_0^A\right)^*, \qquad x_0 = \left(x_0^A\right)^* \quad (37)$$

Here, $(t_0^A)^*$, $(x_0^A)^*$ denote the values of the quantities t_0, x_0 associated with the optimal solution to problem A, respectively. Furthermore, to avoid redundancy or incompatibility with the conditions (37), we assume that no state constraints are present or active at node 0. More precisely, the latter assumption means that there are no state equality constraints in Eq. (33) and that all state inequality constraints in Eq. (33) are satisfied with strict inequality at node 0. To derive the results that will be obtained in the present section without this assumption, we will have to slightly modify our approach (see auxiliary problem C in Sec. III.C). Following the nomenclature introduced in Eq. (36), problem B_0 is represented by the Lagrangian function

$$L^{B_0} = \phi(x_N, t_N) + \pi_f^T \psi_f(x_N, t_N) + \sum_{j=1}^{N} \lambda_j^T [f(\bar{x}_j, u_j, \bar{t}_j) - \dot{\bar{x}}_j]$$

$$+ \sum_{j=1}^{N} \sigma_j^T g(\bar{x}_j, u_j, \bar{t}_j) + \sum_{j=1}^{N} \mu_j^T h(x_j, t_j)$$

$$+ \alpha_0\left[t_0 - \left(t_0^A\right)^*\right] + \beta_0^T\left[x_0 - \left(x_0^A\right)^*\right] \quad (38)$$

Obviously, by construction of the initial conditions (37), the optimal values of all independent variables x_i, $i = 0, \ldots, N$, u_i, $i = 1, \ldots, N$, t_0, and t_N are identical for problems A and B_0. To determine the values of the KKT multipliers associated with the optimal solution to problem B_0, we note that the functional form of the expressions

$$\frac{\partial L^{B_0}}{\partial x_i}, \quad i = 1, \ldots, N, \qquad \frac{\partial L^{B_0}}{\partial u_i}, \quad i = 1, \ldots, N, \qquad \frac{\partial L^{B_0}}{\partial t_N}$$

is identical to the functional form of the expressions

$$\frac{\partial L^A}{\partial x_i}, \qquad i = 1, \ldots, N, \qquad \frac{\partial L^A}{\partial u_i}, \qquad i = 1, \ldots, N, \qquad \frac{\partial L^A}{\partial t_N}$$

respectively. From here, it can be shown quickly that all first-order KKT conditions

$$\frac{\partial L^{B_0}}{\partial x_i} = 0, \qquad i = 1, \ldots, N$$

$$\frac{\partial L^{B_0}}{\partial u_i} = 0, \qquad i = 1, \ldots, N, \qquad \frac{\partial L^{B_0}}{\partial t_N} = 0$$

are satisfied if the expressions on the left-hand side are evaluated at $x_i = (x_i^A)^*$, $i = 0, \ldots, N$; $u_i = (u_i^A)^*$, $i = 1, \ldots, N$; $t_0 = (t_0^A)^*$, $t_N = (t_N^A)^*$; $\lambda_i = (\lambda_i^A)^*$, $i = 1, \ldots, N$; $\sigma_i = (\sigma_i^A)^*$, $i = 1, \ldots, N$; and $\mu_i = (\mu_i^A)^*$, $i = 1, \ldots, N$. The remaining first-order conditions, $\partial L^{B_0}/\partial t_0 = 0$ and $\partial L^{B_0}/\partial x_0 = 0$, then can be used to determine α_0 and β_0, respectively. For β_0, this yields explicitly

$$-\beta_0^T = \frac{\lambda_1^T}{2} \frac{\partial f}{\partial x}\bigg|_{\substack{x=\bar{x}_1 \\ u=u_1 \\ t=\bar{t}_1}} + \frac{\lambda_1^T}{t_1 - t_0} + \frac{\sigma_1^T}{2} \frac{\partial g}{\partial x}\bigg|_{\substack{x=\bar{x}_1 \\ u=u_1 \\ t=\bar{t}_1}} \quad (39)$$

In light of Eq. (A6), it is clear that the negative of the multiplier $-\beta_0$ represents the sensitivity of the optimal cost (28) associated with problem B_0 with respect to perturbations in the initial states x_0 prescribed in Eq. (37). Hence, β_0^T represents an approximation to the right-hand side of Eq. (22), evaluated at $t = t_0$. Note also that the right-hand side of Eq. (39) involves only quantities that are known once an optimal solution to problem A is obtained.

C. Auxiliary Problem C

In the preceding section, an expression was derived for the sensitivity of the optimal cost (28) with respect to perturbations in the state values prescribed at initial time. In this derivation, an important assumption was that none of the state constraints (33) are present or active at the starting node 0.

For the case where this assumption is violated, we now derive an expression for the cost sensitivity β_0 that is valid an arbitrarily small ϵ-time step before the initial time t_0, as long as no state constraints (33) are active at the node introduced preceding node 0. Let us denote this node by subscript $0 - \epsilon$. We arbitrarily introduce the control constraint

$$u - u_{\text{const}} = 0 \quad (40)$$

on the interval from node $0 - \epsilon$ to node 0. Here, u_{const} is a constant control vector independent of ϵ, chosen such that 1) all control constraints are satisfied at $t = t_0$, $x = x_0$, $u = u_{\text{const}}$, and 2) $(\mathrm{d}^{q_i} h_i/\mathrm{d}t^{q_i}) > 0$ at $t = t_0$, $x = x_0$, $u = u_{\text{const}}$ for all components i of the state constraint vector h that are active at $t = t_0$, $x = x_0$, with q_i denoting the order of the ith state constraint. The discretized equations of motion are enforced through a backward Euler step on the interval from node 0 to $0 - \epsilon$, and the initial conditions enforced at node $0 - \epsilon$ are

$$t_{0-\epsilon} = \left(t_0^A\right)^* - \epsilon$$
$$x_{0-\epsilon} = \left(x_0^A\right)^* - f(x_0, u_{\text{const}}, t_0) \cdot \epsilon \quad (41)$$

Note that for sufficiently small $\epsilon > 0$, condition 2 guarantees that the state constraint $h \leq 0$ is satisfied with strict inequality at node $0 - \epsilon$. The underlying assumption on the existence of a control u_{const} that satisfies points 1 and 2 at the beginning of or in the interior of a state-constrained arc is rather mild, because it is tantamount to the assumption that there is a control that would lead to a violation of the state constraint after node 0.

The so-obtained discretized optimal control problem is represented by the Lagrangian function

$$
\begin{aligned}
L^{C_0} &= \phi(x_N, t_N) + \pi_f^T \psi_f(x_N, t_N) + \sum_{j=1}^{N} \lambda_j^T [f(\bar{x}_j, u_j, \bar{t}_j) - \dot{\bar{x}}_j] \\
&+ \sum_{j=1}^{N} \sigma_j^T g(\bar{x}_j, u_j, \bar{t}_j) + \sum_{j=0}^{N} \mu_j^T h(x_j, t_j) \\
&+ \tilde{\lambda}_0^T \left[f(x_0, u_0, t_0) - \frac{x_0 - x_{0-\epsilon}}{\epsilon} \right] + \tilde{\sigma}_0^T (u_0 - u_{\text{const}}) \\
&+ \tilde{\alpha}_0 \left\{ t_{0-\epsilon} - \left[(t_0^A)^* - \epsilon \right] \right\} \\
&+ \tilde{\beta}_0^T \left\{ x_{0-\epsilon} - \left[(x_0^A)^* - \epsilon \cdot f(x_0, u_{\text{const}}, t_0) \right] \right\}
\end{aligned} \tag{43}
$$

Using arguments similar to the ones of the preceding section, it can be verified quickly that all first-order KKT conditions

$$
\frac{\partial L^{C_0}}{\partial x_i} = 0, \qquad i = 1, \ldots, N
$$

$$
\frac{\partial L^{C_0}}{\partial u_i} = 0, \qquad i = 1, \ldots, N, \qquad \frac{\partial L^{C_0}}{\partial t_N} = 0
$$

are satisfied if the expressions on the left-hand side are evaluated at $x_i = (x_i^A)^*$, $i = 0, \ldots, N$; $u_i = (u_i^A)^*$, $i = 1, \ldots, N$; $t_0 = (t_0^A)^*$; $t_N = (t_N^A)^*$; $\lambda_i = (\lambda_i^A)^*$, $i = 1, \ldots, N$; $\sigma_i = (\sigma_i^A)^*$, $i = 1, \ldots, N$; and $\mu_i = (\mu_i^A)^*$, $i = 0, \ldots, N$. The remaining first-order conditions,

$$
\frac{\partial L^{C_0}}{\partial x_0} = 0, \qquad \frac{\partial L^{C_0}}{\partial u_0} = 0, \qquad \frac{\partial L^{C_0}}{\partial t_{0-\epsilon}} = 0, \qquad \frac{\partial L^{C_0}}{\partial x_{0-\epsilon}} = 0
$$

can then be used to determine $\tilde{\lambda}_0$, $\tilde{\sigma}_0$, $\tilde{\alpha}_0$, and $\tilde{\beta}_0$. For $\tilde{\beta}_0$, we obtain explicitly (use $\partial L^{C_0}/\partial x_{0-\epsilon} = 0$ to show that $\tilde{\lambda}_0 = -\epsilon \tilde{\beta}_0$ and insert this result into $\partial L^{C_0}/\partial x_0 = 0$)

$$
\begin{aligned}
-\tilde{\beta}_0^T &= \left[\frac{\lambda_1^T}{2} \frac{\partial f}{\partial x} \bigg|_{\substack{x=\bar{x}_1 \\ u=u_1 \\ t=\bar{t}_1}} + \frac{\lambda_1^T}{t_1 - t_0} + \frac{\sigma_1^T}{2} \frac{\partial g}{\partial x} \bigg|_{\substack{x=\bar{x}_1 \\ u=u_1 \\ t=\bar{t}_1}} + \mu_0^T \frac{\partial h}{\partial x} \bigg|_{\substack{x=x_0 \\ t=t_0}} \right] \\
&\times \left[I - \epsilon \left(\frac{\partial f}{\partial x} \bigg|_{\substack{x=x_0 \\ u=u_{\text{const}} \\ t=t_0}} + \frac{\partial f}{\partial x} \bigg|_{\substack{x=x_0 \\ u=u_0 \\ t=t_0}} \right) \right]^{-1}
\end{aligned} \tag{44}
$$

I denotes the $n \times n$ identity matrix. As ϵ shrinks to zero, the limit of $-\tilde{\beta}_0$ is well defined. With the definition $-\beta_0^T = \lim_{\epsilon \to 0} -\tilde{\beta}_0^T$, we obtain

$$
\beta_0^T = \frac{\lambda_1^T}{2} \frac{\partial f}{\partial x} \bigg|_{\substack{x=\bar{x}_1 \\ u=u_1 \\ t=\bar{t}_1}} + \frac{\lambda_1^T}{t_1 - t_0} + \frac{\sigma_1^T}{2} \frac{\partial g}{\partial x} \bigg|_{\substack{x=\bar{x}_1 \\ u=u_1 \\ t=\bar{t}_1}} + \mu_0^T \frac{\partial h}{\partial x} \bigg|_{\substack{x=x_0 \\ t=t_0}} \tag{45}
$$

In light of Eq. (A6), it is clear that the negative of the multiplier β_0 represents the left-hand limit of the sensitivity of the optimal cost (28) associated with problem C_0 with respect to perturbations in the initial states x_0 at time t_0. Hence $-\beta_0^T$ represents an approximation to the left-hand limit of the right-hand side of Eq. (22), evaluated at $t = t_0$.

Note also that the right-hand side of Eq. (45) involves only quantities that are known once an optimal solution to problem A is obtained. Furthermore, Eq. (45) reduces to Eq. (39) if $\mu_0 = 0$, i.e., if no state constraints (33) are active at node 0 in the solution to problem A. It is also interesting that the same expression (45) would have been formally obtained in the preceding section, had we not imposed the restriction that none of the state constraints (33) must be active at node 0. However, we see no justification for taking this approach.

IV. Costate Estimates

Our goal is to present a method by which estimates for the constant multipliers l, ν_0, ν_f, and the time-varying multipliers $\lambda(t)$ associated with the continuous optimal control problem (1–8) can be constructed from the solution of the discretized optimal control problem (28–33). The general idea is to approximate the cost sensitivities appearing on the right-hand side of Eqs. (22), (23), (25), and (26) through the appropriate cost sensitivities associated with the discretized optimal control problem (28–33).

In the following, estimates for $\lambda(t_i)$, $i \geq 0$, are first developed under the assumption that no state constraints are active at time t_i, using Eq. (45). If a state constraint is active, then the so-obtained costate estimate, $\lambda(t_i^-)$, represents the value that $\lambda(t)$ would have possessed along an unconstrained arc, just before hitting the state constraint at time t_i. The correct multiplier value $\lambda(t_i^+)$ then is obtained by adding the jump given by Eq. (20).

A. Costate Estimate at Initial Time t_0

In light of Eq. (A6), it is clear that $-\tilde{\beta}_0$ defined in Eq. (44) represents the sensitivity of the optimal cost (28) associated with problem C_0 with respect to perturbations in the initial states prescribed at the beginning of an artificially introduced interval of length ϵ preceding t_0, along which no state constraints are active. Hence, in light of Eq. (22), the expression $-\beta_0$ defined in Eq. (45) represents an approximation to the left-hand limit of the time-varying Lagrangian multiplier $\lambda(t)$ at t_0. (Strictly speaking, it is necessary to define a new variational problem on the interval $[t_{0-\epsilon}, t_f]$ such that its finite dimensional discretization is represented by problem C_0. This step should be clear and it is omitted in this paper, for conciseness.) That is,

$$
\lambda(t_0^-)^T \doteq \frac{\lambda_1^T}{2} \frac{\partial f}{\partial x} \bigg|_{\substack{x=\bar{x}_1 \\ u=u_1 \\ t=\bar{t}_1}} + \frac{\lambda_1^T}{t_1 - t_0} + \frac{\sigma_1^T}{2} \frac{\partial g}{\partial x} \bigg|_{\substack{x=\bar{x}_1 \\ u=u_1 \\ t=\bar{t}_1}} + \mu_0^T \frac{\partial h}{\partial x} \bigg|_{\substack{x=x_0 \\ t=t_0}} \tag{46}
$$

If no state constraints are active at t_0, then $\lambda(t)$ is continuous at t_0, and the left-hand side of Eq. (46) can be replaced by $\lambda(t_0)^T$. Note that, in this case, $\mu_0 = 0$ and the right-hand sides of Eqs. (45) and (46) reduce to the right-hand side of Eq. (39).

In case at least one of the state constraints (7) or (8) is active at t_0, the expression (46) has to be interpreted as an estimate for the multiplier $\lambda(t_0)$ just before the state constraint is hit. The correct multiplier value along the state-constrained arc then can be formally obtained from Eq. (20) with t_a replaced by t_0, if only the constant multiplier vector l is known. A method to estimate l is discussed in Sec. IV.E.

B. Costate Estimate at Nodal Time t_i

The concepts presented in the preceding section to estimate $\lambda(t_0)$ can be extended easily to the calculation of $\lambda(t)$ at any of the nodal times $t = t_i$, $i = 1, \ldots, N-1$. The basic idea is to delete the i leading nodes $(0, \ldots, i-1)$ in problem A and to consider t_i as the new initial time. Then, in analogy to problems B_0 and C_0 defined in Secs. III.B and III.C, respectively, auxiliary problems B_i and C_i in the independent variables $x_i, \ldots, x_N$, $u_{i+1}, \ldots, u_N$, t_i, t_N, and $x_{i-\epsilon}$, $x_i, \ldots, x_N$, u_i, $u_{i+1}, \ldots, u_N$, $t_{i-\epsilon}$, t_N, respectively, are defined. The initial conditions and the Lagrangian functions associated with problems B_i/C_i are given by Eqs. (37) and (38)/(41) and (43) with 0 replaced by i and 1 replaced by $i+1$, everywhere. In complete analogy to the analysis presented in the preceding section, we then arrive at the costate estimate

$$
\begin{aligned}
\lambda(t_i^-)^T &\doteq \frac{\lambda_{i+1}^T}{2} \frac{\partial f}{\partial x} \bigg|_{\substack{x=\bar{x}_{i+1} \\ u=u_{i+1} \\ t=\bar{t}_{i+1}}} + \frac{\lambda_{i+1}^T}{t_{i+1} - t_i} + \frac{\sigma_{i+1}^T}{2} \frac{\partial g}{\partial x} \bigg|_{\substack{x=\bar{x}_{i+1} \\ u=u_{i+1} \\ t=\bar{t}_{i+1}}} \\
&+ \mu_i^T \frac{\partial h}{\partial x} \bigg|_{\substack{x=x_i \\ t=t_i}}, \qquad i = 0, \ldots, N-1
\end{aligned} \tag{47}
$$

If no state constraints are active at t_i, then $\lambda(t)$ is continuous at t_i, and the left-hand side of Eq. (47) can be replaced by $\lambda(t_i)^T$. If at least one of the constraints (7) or (8) is active at node i, then Eq. (47) has to be interpreted again as an estimate for $\lambda(t_i^-)$, i.e., the value of $\lambda(t)$

at the end of an infinitesimally short unconstrained arc preceding t_i. The correct multiplier value at t_i^+, the beginning of the state-constrained arc, then can be obtained formally from Eq. (20) with t_a replaced by t_i, if only the constant multiplier vector $\boldsymbol{l}$ is known. A method to estimate $\boldsymbol{l}$ is discussed in Sec. III.E. An implicit assumption made in the current section is that the truncated solution of the original discretized problem constitutes an optimal solution to the truncated discretized problem. That this assumption may not be satisfied has been shown in Ref. 18. It can be expected, however, that the violation of the principle of optimality for discretized optimal control problems and the resulting errors introduced into the costate approximation (47) are of very small magnitude. A precise quantitative investigation of this matter has not yet been conducted.

C. Costate Estimates at Final Time t_f

At the final node t_N the method for estimating $\boldsymbol{\lambda}(t_i^-)$ as discussed in the previous section breaks down. Note that the quantities $\boldsymbol{x}_{i+1}$, $\boldsymbol{u}_{i+1}$, t_{i+1}, $\boldsymbol{\lambda}_{i+1}$, $\boldsymbol{\sigma}_{i+1}$ appearing on the right-hand side of Eq. (47) do not exist for $i = N$. An alternative method for estimating $\boldsymbol{\lambda}(t_f)$ can be developed from Eq. (11) if only an estimate for the constant multiplier $\boldsymbol{\nu}_f \in \boldsymbol{R}^q$ is available. Then,

$$\boldsymbol{\lambda}(t_N)^T \doteq \left.\frac{\partial \phi}{\partial \boldsymbol{x}}\right|_{\substack{x=x_N\\ t=t_N}} + \boldsymbol{\nu}_{f,\text{estimate}}^T \left.\frac{\partial \boldsymbol{\psi}_f}{\partial \boldsymbol{x}}\right|_{\substack{x=x_N\\ t=t_N}} \tag{48}$$

An estimate, $\boldsymbol{\nu}_{f,\text{estimate}}$, for the constant multiplier vector $\boldsymbol{\nu}_f$ is presented in Sec. III.D. Note that Eq. (48) is valid irrespective of whether any state constraints are active at the final node t_N.

D. Estimates for the Multiplier Vectors ν_0 and ν_f

From Eqs. (25) and (26), we know that the constant multiplier vectors $\boldsymbol{\nu}_0$ and $\boldsymbol{\nu}_f$ represent the sensitivity of the optimal cost associated with the variational solution to perturbations in the right-hand side of the boundary conditions (3) and (4), respectively. Hence, in light of Eq. (A6), it is clear that the negatives of the multiplier vectors $\boldsymbol{\pi}_0$ and $\boldsymbol{\pi}_f$ associated with the optimal solution to the discretized problem A represent approximations for $\boldsymbol{\nu}_0$ and $\boldsymbol{\nu}_f$, respectively, i.e.,

$$\boldsymbol{\nu}_0 \doteq -\boldsymbol{\pi}_0 \tag{49}$$

$$\boldsymbol{\nu}_f \doteq -\boldsymbol{\pi}_f \tag{50}$$

E. Estimate for the Multiplier Vector l

In this section, we consider only the case of a single, scalar state inequality constraint $h(\boldsymbol{x}, t) \le 0$, and we assume that the optimal variational solution has the switching structure given by Eq. (16). Generalization of the results to vector-valued state constraints (equality and inequality) and to other switching structures is straightforward. For the optimal solution to the discretized optimal control problem A, we assume that

$$h[\boldsymbol{x}(t), t] \begin{cases} <0 & \text{at nodes} \quad 0, \ldots, i_{a-1} \\ =0 & \text{at nodes} \quad i_a, \ldots, i_b \\ <0 & \text{at nodes} \quad i_{b+1}, \ldots, N \end{cases} \tag{51}$$

with $0 \le i_a < i_b \le N$.

According to Eq. (23), the constant multiplier vector $\boldsymbol{l} \in \boldsymbol{R}^q$ appearing in Eqs. (20) and (21) represents the sensitivity of the optimal cost associated with the variational solution to problem (1–6) and (24) with respect to perturbations in the parameter vector $\boldsymbol{b}$ about its nominal value, $\boldsymbol{b} = 0 \in \boldsymbol{R}^q$. In the following, an estimate for $\boldsymbol{l}$ is developed by replacing the right-hand side of Eq. (23) through the appropriate sensitivity of the optimal cost associated with a discretized optimal control problem, namely, problem A with the constraints (33) replaced by

$$h(\boldsymbol{x}_j, t_j) - \sum_{k=0}^{q-1} \frac{b_k}{k!}\left(t_j - t_{i_a}\right)^k = 0 \quad \text{for} \quad [i_a \le j \le i_b] \tag{52}$$

problem A. Clearly, perturbations in the parameter vector $\boldsymbol{b}$ in Eq. (52) lead to a well-defined change in the value of $h(\boldsymbol{x}, t)$ at each individual node. In light of Eq. (A6), the sensitivity of the optimal cost with respect to perturbations in the prescribed value of $h(\boldsymbol{x}, t)$ at an individual node number i is given by the negative of the multiplier μ_i, $i = 0, \ldots, N$. Hence, the total sensitivity of the optimal cost with respect to the kth component of $\boldsymbol{b}$ in Eq. (52), $k = 1, \ldots, q-1$, is given by

$$\left.\frac{\partial J}{\partial b_k}\right|_{b=0} = \sum_{i_a \le j \le i_b} \left.\frac{\partial J}{\partial h(\boldsymbol{x}_j, t_j)} \frac{\partial h(\boldsymbol{x}_j, t_j)}{\partial b_j}\right|_{b=0} = \sum_{i_a \le j \le i_b} -\mu_j \frac{\left(t_j - t_{i_a}\right)}{k!} \tag{53}$$

By construction, the left-hand side of Eq. (53) represents an approximation to the kth component of the right-hand side of Eq. (23). Hence we obtain

$$l_k \doteq \sum_{i_a \le j \le i_b} -\mu_j \frac{\left(t_j - t_{i_a}\right)}{k!}, \qquad k = 0, \ldots, q-1 \tag{54}$$

F. Practical Application

Assume that an optimal control problem of the general form (1–8) is given, and assume that an optimal solution to the discretized optimal control problem (28–33) has been obtained. In the following, the nomenclature for the time-varying and constant multipliers involved in a variational solution is adopted from Sec. II.B. The nomenclature for the multipliers associated with the direct approach (28–35) is indicated in the Lagrangian function (36). For simplicity, we consider only a single, scalar state constraint $h(\boldsymbol{x}, t) \le 0$. Let this state constraint be of order q, and assume that 1) $h(\boldsymbol{x}, t) = 0$ at all nodes i with $i_a \le i \le i_b$; 2) if $i_a \ne 0$, then $h(\boldsymbol{x}, t) < 0$ at node i_{a-1}; and 3) if $i_b \ne N$, then $h(\boldsymbol{x}, t) < 0$ at node i_{b+1}.

At nodes i, $i < N$, where the state constraint (33) is not active, an estimate for the transpose of the time-varying Lagrangian multiplier $\boldsymbol{\lambda}(t_i)^T$ is given by the right-hand side of Eq. (47). At node i_a, an estimate for $\boldsymbol{\lambda}(t_a^-)^T$ is given by the right-hand side of Eq. (47) with i replaced by i_a. An estimate for $\boldsymbol{\lambda}(t_a^+)^T$ can be obtained by adding the multiplier jump (20), where the components of the constant multiplier vector $\boldsymbol{l}$ are determined from Eq. (54). At all following nodes, i, with $i_a < i \le i_b$, an estimate for $\boldsymbol{\lambda}(t_i)^T$ can be obtained by first calculating the artificial quantity $\boldsymbol{\lambda}(t_i^-)^T$ from Eq. (47) and then performing the multiplier jump

$$\boldsymbol{\lambda}(t_i)^T = \boldsymbol{\lambda}\left(t_i^-\right)^T - \boldsymbol{l}^T \frac{\partial \boldsymbol{M}[\boldsymbol{x}(t_i), t_i]}{\partial \boldsymbol{x}(t_i)} \tag{55}$$

where the components of $\boldsymbol{l}$ are determined from

$$l_j = \sum_{k=i}^{i_b} \frac{\mu_k}{j!}(t_k - t_i)^j, \qquad j = 0, \ldots, q-1 \tag{56}$$

At the final node t_N, a costate estimate is obtained from Eq. (48), irrespective of whether or not any state constraints are active at t_N.

V. Remarks and Extensions

A. Interior-Point Constraints

In the original problem formulation (1–8), interior-point constraints were not considered explicitly. Such constraints were introduced only later in Eq. (18) through the treatment of state inequality constraints, and the associated necessary conditions for optimality in the variational approach were stated.

Note that the treatment of state inequality constraints through the direct approach presented in Sec. III.A did not require the treatment of interior-point constraints, because the state inequality constraints were enforced directly at individual nodes, without transforming them into a combination of interior-point constraints and control constraints. In fact, the treatment of interior-point constraints with our direct optimization approach would have required the introduction of multiple phases, i.e., it would have been necessary to divide the original time interval $[t_0, t_f]$ into subarcs $[t_0, t_s]$ and $[t_s, t_f]$, where the additional parameter t_s denotes the location of the interior point. Obviously, the introduction of interior-point constraints would have complicated the presentation of the results obtained. Without proof, it is stated here, however, that the extension of the methods and results presented in this paper to the case of interior-point constraints is straightforward.

B. Relation to Previously Published Work

The basic idea of this paper is to make use of the physical interpretation of Lagrangian multipliers in terms of the sensitivities of the variational cost function with respect to perturbations in the initial states and to approximate the Lagrangian multipliers by the cost sensitivities associated with near-optimal solutions obtained through parameter optimization. The same idea has already been used[11]; however, the cost sensitivities associated with the parameter optimal solution were obtained through finite differences, whereas, in the present paper, the required sensitivities are expressed in terms of the KKT multipliers obtained from the NLP solution. As a consequence, the previous approach[11] requires much more CPU time, and the expected precision in the costate estimates should be lower. However, an important advantage of the finite difference approach[11] is that no new relations between KKT multipliers and cost sensitivities need to be derived if the discretization scheme is changed.

A seemingly very different costate estimation method was presented by von Stryck.[16] For ease of comparison, let us consider only the case where no state constraints (33) are present. Then, the discretization chosen by von Stryck[16] is identical to the one used in the present paper, even though the nomenclature is somewhat different. Restated in terms of the nomenclature used in the present paper, it was shown that the quantities $-\lambda_{i+1}/(t_{i+1}-t_i)$ satisfy a discretized version of the continuous Euler–Lagrange equations (9) (Ref. 16). From this observation, costate estimates at the midpoints, $\bar{t}_{i+1} = (t_{i+1}+t_i)/2$, between neighboring nodes t_{i+1} and t_i were derived, namely,

$$\lambda(\bar{t}_{i+1}) \doteq \frac{-\lambda_{i+1}}{t_{i+1}-t_i}, \qquad i = 0, \ldots, N-1 \tag{57}$$

The associated result of the present paper, Eq. (47), with $\lambda(t_i^-)$ replaced by $\lambda(t_i)$ and with μ_i set equal to zero to reflect the fact that no state constraints are present, can be written in the form

$$\begin{aligned}\lambda(t_i)^T &= -\frac{\lambda_{i+1}^T}{t_{i+1}-t_i} - \frac{\lambda_{i+1}^T}{2}\frac{\partial f}{\partial x}\bigg|_{\substack{x=\bar{x}_{i+1}\\ u=u_{i+1}\\ t=\bar{t}_{i+1}}} - \frac{\sigma_{i+1}^T}{2}\frac{\partial g}{\partial x}\bigg|_{\substack{x=\bar{x}_{i+1}\\ u=u_{i+1}\\ t=\bar{t}_{i+1}}}\\ &= \frac{-\lambda_{i+1}^T}{t_{i+1}-t_i} - \left[\frac{t_{i+1}-t_i}{2}\left(-\frac{-\lambda_{i+1}^T}{t_{i+1}-t_i}\frac{\partial f}{\partial x}\bigg|_{\substack{x=\bar{x}_{i+1}\\ u=u_{i+1}\\ t=\bar{t}_{i+1}}}\right.\right.\\ &\qquad \left.\left. - \frac{-\sigma_{i+1}^T}{t_{i+1}-t_i}\frac{\partial g}{\partial x}\bigg|_{\substack{x=\bar{x}_{i+1}\\ u=u_{i+1}\\ t=\bar{t}_{i+1}}}\right)\right]\end{aligned} \tag{58}$$

Note that the term in square brackets on the right-hand side of Eq. (58) represents an implicit-Euler integration step of the Euler–Lagrange equations (9) from time t_i to $\bar{t}_{i+1}$. This is the discretization within which the results (57) and (58) are consistent.

VI. Numerical Example

We consider the same numerical example as previously considered,[11] i.e., a state-constrained brachistochrone problem. In Meyer form, the problem can be stated as follows:

$$\min_{u\in \mathrm{PWC}[t_0, t_f]} t_f \tag{59}$$

subject to the equations of motion

$$\dot{x}(t) = v(y)\cos\theta(t), \qquad \dot{y}(t) = v(y)\sin\theta(t) \tag{60}$$

the boundary conditions

$$x(0) = 0, \qquad x(t_f) = 1, \qquad y(0) = 0, \qquad y(t_f) \text{ free} \tag{61}$$

and the state constraint

$$y(t) - x(t)\tan\gamma - h_0 \le 0 \tag{62}$$

Here, x and y are the state variables and θ is the only control. The quantity v denotes the velocity and is a shorthand notation for $v = \sqrt{(v_0^2 + 2gy)}$. The quantities v_0, g, γ, and h_0 are constant. For numerical calculations, we use

$$v_0 = 1, \qquad g = 1, \qquad \gamma = 20\,\text{deg}, \qquad h_0 = 0.05 \tag{63}$$

The state inequality constraint (62) is of first order, and the optimal switching structure for problem (59–63) is

$$\text{free—constrained—free} \tag{64}$$

A precise treatment of the variational optimality conditions is given elsewhere.[11] To generate a finite dimensional approximation to the variational solution in the style of problem A introduced in Sec. III.A, the time interval is divided into 100 equidistant subintervals by introducing the nodal times

$$t_i = (t_f - t_0)(i/100), \qquad i = 0, \ldots, N \tag{65}$$

In Figs. 1–6, the exact optimal time histories of the states x and y, the costates λ_x and λ_y, the constraint $c = y - x\tan\gamma - h_0$ and the multiplier μ, respectively, are represented as solid lines. Here, μ is the multiplier function associated with the control constraint

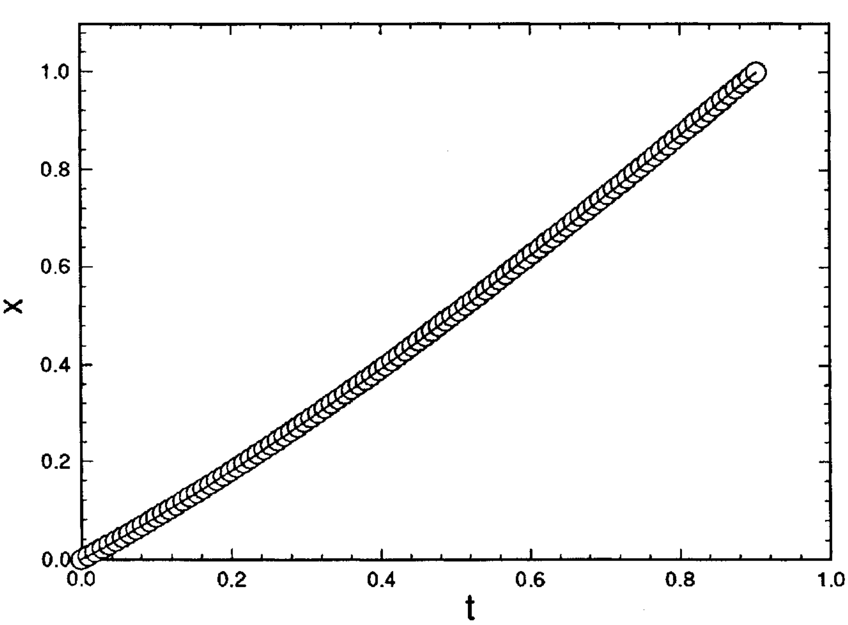

Fig. 1 State x vs time t: ——, shooting solution and ○, direct solution (101 nodes).

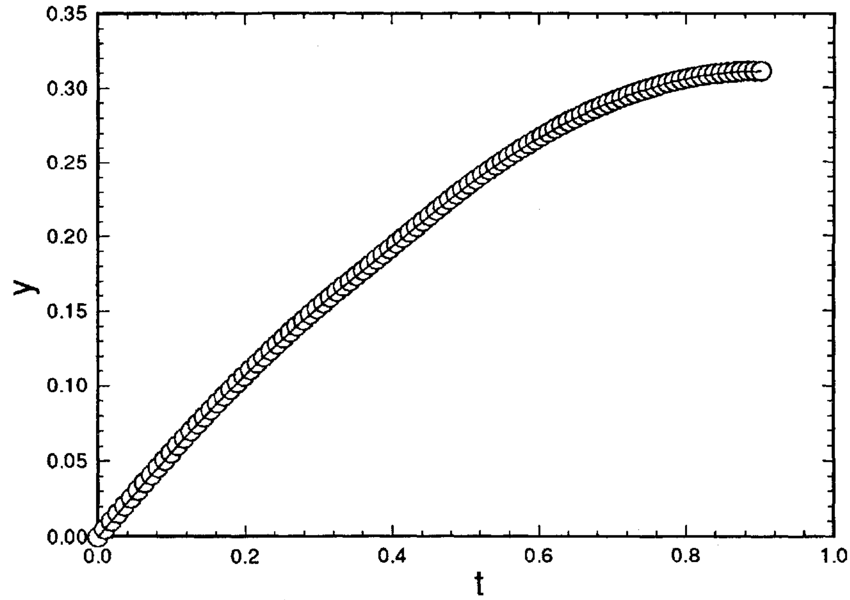

Fig. 2 State y vs time t: ——, shooting solution and ○, direct solution (101 nodes).

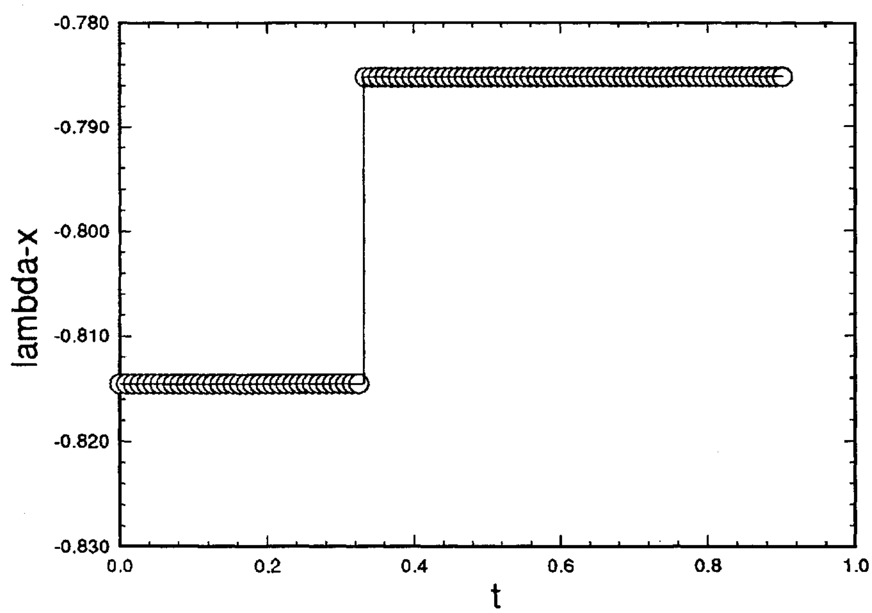

Fig. 3 Costate λ_x vs time t: ——, shooting solution and ○, calculated estimates.

obtained from the qth time derivative of the state constraint, q being the order of the state constraint. Superimposed as circles in Figs. 1, 2, and 6, respectively, are the results for the states x, y, and the constraint c, obtained with the discretization scheme of Sec. III.A. A total of $N = 100$ nodes were used, and all nodes were placed equidistantly. In Figs. 3 and 4, the circles represent the costate estimates λ_x and λ_y generated with the method summarized in Sec. IV.F. The agreement with the variational solution is excellent, even across the discontinuous jump of the multipliers at the beginning of the state constrained arc. As discussed in Sec. IV, the calculation of Lagrangian multiplier estimates along the state-constrained arc is a two-step procedure that requires an estimate for the height of multiplier jumps. This height l varies with the time t at which costate estimates need to be calculated. Along unconstrained arcs, all components of $l(t)$ are zero, and it can be shown analytically that the first component, $l_0(t)$, of the so-defined function $l(t)$ is identical to the multiplier function $\mu(t)$. In Fig. 6, the circles represent the approximate values for l_0 obtained from Eq. (56). Again, the agreement with the variational solution is excellent.

It is interesting to compare the results obtained here with the results obtained earlier.[11] In general, it is observed that the costate approximations obtained here are better. The noisiness of the costate estimates obtained earlier[11] can be attributed to the imprecisions resulting from the finite difference nature of the approach. However, in addition, a very consistent deviation of the costate estimates from the correct variationally obtained solution is observed along the state-constrained arc. This deviation represents an additional discretization error stemming from the fact that, along state-constrained arcs, cost sensitivities were calculated without introducing an additional node an ϵ-interval before the node of interest (compare auxiliary problems B and C of Sec. III herein). It is clear, however, that this additional discretization error shrinks to zero as the fineness of the discretization grid is increased.

In terms of CPU time, the present method is also much superior to the method presented earlier.[11] There, cost sensitivities were calculated through finite differences, which require calculation of many perturbed trajectories. Thus, the numerical procedure for calculating costate estimates typically takes long compared to calculating the reference trajectory. In comparison, the CPU time requirement

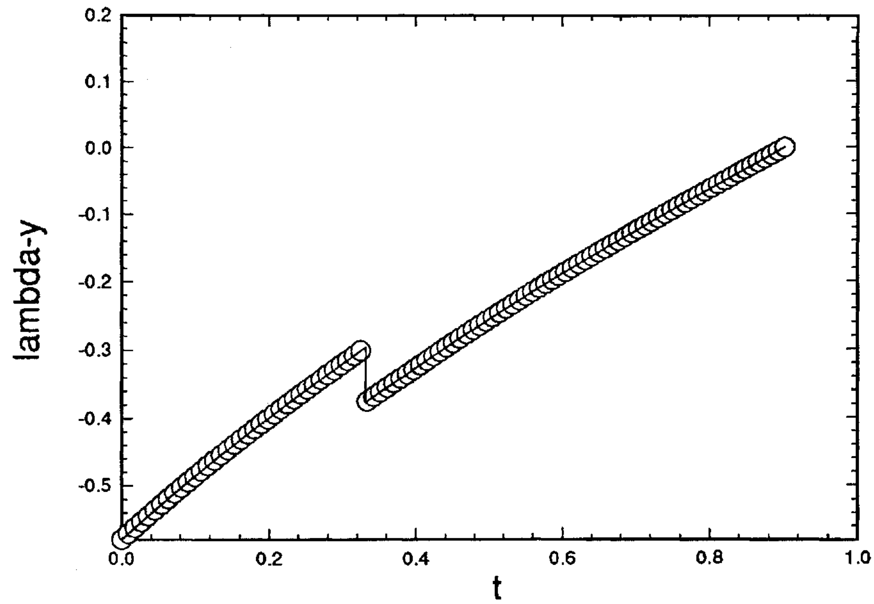

Fig. 4 Costate λ_y vs time t: ——, shooting solution and ○, calculated estimates.

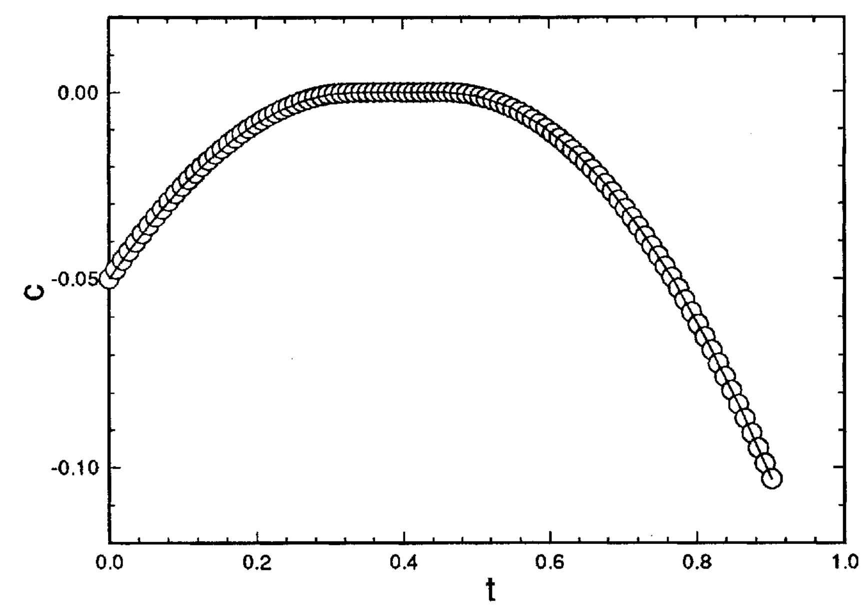

Fig. 5 Constraint c vs time t: ——, shooting solution and ○, direct solution (101 nodes).

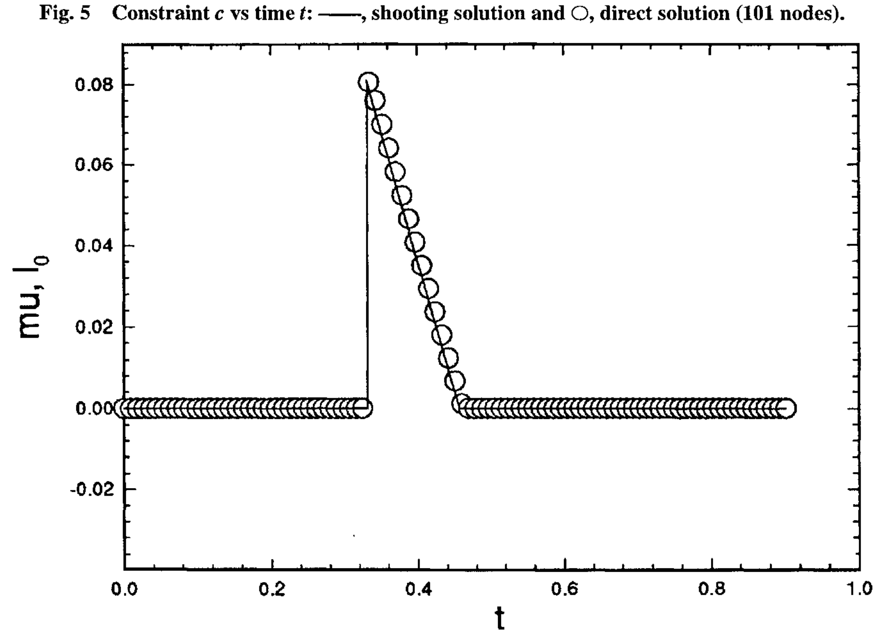

Fig. 6 Multiplier μ vs time t: ——, shooting solution μ and ○, calculated estimates for l_0.

for the method presented in this paper is negligible even compared to the effort involved in calculating a single trajectory.

However, a caution is in place for numerical implementation. The main results of this paper, Eqs. (46), (47), and (56), change dramatically if the problem discretization is changed. This should be expected intuitively, for example, if the trapezoidal integration step (29) is replaced by a third-order Simpson integration step. But even minute changes, such as multiplication of condition (29) with -1, would make it necessary to replace $\boldsymbol{\lambda}_{i+1}$ by $-\boldsymbol{\lambda}_{i+1}$ in Eq. (47). Further sign changes are required in Eqs. (46) and (47) and Eq. (56) if the NLP code used as optimization engine is a maximizer instead of a minimizer, or if the underlying augmented cost function (70) is defined by subtracting the cost terms instead of adding them.

VII. Conclusions

A method was introduced in this paper for the automatic calculation of costates using only results obtained from a collocation-type direct optimization approach. The class of problems addressed in this paper is fairly general and includes problems with state constraints of arbitrary finite order. As a starting point, the known relations between Lagrangian multipliers and certain cost sensitivities were used. Then, the cost sensitivities of the variational solution were approximated by the cost sensitivities of the discretized solution. As a result, costate estimates at the nodal points were obtained in terms of the Kuhn–Tucker multipliers associated with the NLP solution. The obtained results also were shown to be consistent with results obtained previously by other researchers. As a numerical example, a state-constrained version of the brachistochrone problem was solved and the results were compared to the variational solution. The agreement was excellent. The CPU time requirement for the costate estimation step is negligible. Even though the derivations in this paper are fairly general, the obtained results are highly customized to a specific discretization scheme to a certain format of the problem formulation.

Appendix: KKT Conditions

We consider a generic NLP problem of the form

$$\min_{y \in R^n} f(y) \tag{A1}$$

$$a_i(y) = b_i, \qquad i = 1, \ldots, m_e \tag{A2}$$

$$a_i(y) \le b_i, \qquad i = m_e + 1, \ldots, m_e + m_i \tag{A3}$$

where

$$f: \boldsymbol{R}^n \to \boldsymbol{R}, \qquad \boldsymbol{a}: \boldsymbol{R}^n \to \boldsymbol{R}^{m_e + m_i}, \qquad \text{and} \qquad \boldsymbol{b} \in \boldsymbol{R}^{m_e + m_i}$$

is an arbitrary but fixed vector of constants. Note that the discretized optimal control problem (28–35) is of this general form.

Under the assumption (normality) that the gradients of the active constraints $\hat{\boldsymbol{a}}$ are linearly independent, the solution to problem (A1–A3) satisfies the KKT conditions, namely,

$$\frac{\partial L(y, \alpha)}{\partial y} = 0 \tag{A4a}$$

$$a_i(y) = b_i, \qquad i = 1, \ldots, m_e \tag{A4b}$$

$$a_i(y) \le b_i, \qquad i = m_e + 1, \ldots, m_e + m_i \tag{A4c}$$

$$\alpha_i \begin{cases} = 0 & \text{if} \quad a_i(y) < b_i, \\ \ge 0 & \text{if} \quad a_i(y) = b_i, \end{cases} \qquad i = m_e + 1, \ldots, m_e + m_i \tag{A4d}$$

$$\Delta y^T \left[\frac{\partial^2 L(y, \alpha)}{\partial y^2} \right] \Delta y \ge 0$$

$$\text{for all } \Delta y \in \boldsymbol{R}^n \text{ satisfying } \frac{\partial \hat{a}}{\partial y} \Delta y = 0 \tag{A4e}$$

Here,

$$L(y, \alpha) = f(y + \alpha^T [a(y) - b] \tag{A5}$$

denotes the Lagrangian and the vector function $\hat{\boldsymbol{a}}$ consists of the left-hand sides of Eq. (A2) and the left-hand sides of the active components of Eq. (A3).

The Lagrangian multipliers α can be interpreted as sensitivities of the optimal cost value f^* with respect to changes in the constraints (A2) and (A3). More precisely, let $\boldsymbol{y}^*(\boldsymbol{b})$ denote the optimal solution of problem (A1–A3) as a function of the parameter vector $\boldsymbol{b}$. Then, with the help of Eq. (A4a), we find

$$\frac{\partial f[y^*(b)]}{\partial b} = \left.\frac{\partial f}{\partial y}\right|_{y*(b)} \frac{\partial y^*(b)}{\partial b} = -\alpha^T \left.\frac{\partial a}{\partial y}\right|_{y*(b)} \frac{\partial y^*(b)}{\partial b}$$

$$= -\alpha^T \frac{\partial a[y^*(b)]}{\partial b} = -\alpha^T \tag{A6}$$

Note that these relations can only be guaranteed if the normality condition stated at the beginning of the Appendix is satisfied. This normality condition may be violated either because of incompatibility or through (local) redundancy of certain constraint components. In case of incompatibility, no solution exists. In case of redundancy, the optimal solution may still exist, and if it exists, it is guaranteed to satisfy the KKT conditions (A4a–A4e). However, the multiplier vector α is no longer determined uniquely [there may even be solutions that violate the sign condition (A4d)], and the sensitivity equation (A6) is no longer applicable.

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