A Survey on Optimal Control Problems with Differential-Algebraic Equations

Matthias Gerdts

Abstract The paper provides an overview on necessary and, whenever available, on sufficient conditions of optimality for optimal control problems with differential-algebraic equations (DAEs) and on numerical approximation techniques. Local and global minimum principles of Pontryagin type are discussed for convex linear-quadratic optimal control problems and for non-convex problems. The main steps for the derivation of such conditions will be explained. The basic working principles of different approaches towards the numerical solution of DAE optimal control problems are illustrated for direct shooting methods, full discretization techniques, projected gradient methods, and Lagrange–Newton methods in a function space setting.

Keywords Differential-algebraic equations • Direct discretization method • Lagrange–Newton method • Necessary conditions • Projected gradient method • Optimal control • Sufficient conditions

Subject Classifications: 49-02, 49K15, 49M05, 49M15, 49M25, 49N10, 34A09, 65L80

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1 Introduction

Differential-algebraic equations (DAEs) are composite systems of ordinary differential equations and algebraic equations. Such systems are frequently used in mechanical engineering, process engineering, electrical engineering, and in other disciplines as well, to describe the motion of a time dependent process. In an industrial environment, DAEs are appealing because such systems can be set up automatically by software packages, whereas an equivalent formulation in terms of explicit ordinary differential equations (ODEs) is typically more difficult to achieve and depends on a proper choice of coordinates, e.g., minimal coordinates for mechanical multi-body systems. However, the formulation as a DAE, although simple from the modeling point of view, has implications in view of numerical treatment and solution properties in general. More specifically, the existence of a solution is not guaranteed in general and depends on the structure of the DAE and on external inputs, e.g., control inputs. Moreover, not all initial values are suitable and thus only so-called consistent initial conditions are permitted. A survey on solution theory for linear DAEs can be found in the recent survey paper [106]. A comprehensive structural analysis of linear and nonlinear DAEs can be found in the monographs [68] and [80]. Finally, DAEs differ in their stability properties from ODEs. While ODEs can be viewed as well-behaved systems (with respect to small perturbations and subject to a Lipschitz condition of the right hand-side), DAEs are inherently ill-posed. The degree of ill-posedness depends on the structure and can be measured by the so-called perturbation index, compare [59, Def. 1.1]. This inherent ill-posedness of higher index DAEs requires suitable numerical integration schemes, see [21, 58, 59], [68, Chap. 5], and index reduction techniques, see [68, Chap. 6], as well as stabilization techniques, see e.g., [42, 43].

In this paper we focus on DAEs, which can be controlled by some vector-valued control input $u : I \longrightarrow \mathbb{R}^{n_u}$, $n_u \in \mathbb{N}$, on some fixed compact time interval $I = [t_0, t_f]$ with initial time t_0 and final time $t_f > t_0$. In its most general form, the DAE is defined by the implicit ordinary differential equation

$$F(t, x(t), x'(t), u(t)) = 0, \tag{1.1}$$

where $x : I \longrightarrow \mathbb{R}^{n_x}$, $n_x \in \mathbb{N}$, denotes the state, x' its derivative w.r.t. time t, and $F : I \times \mathbb{R}^{n_x} \times \mathbb{R}^{n_x} \times \mathbb{R}^{n_u} \longrightarrow \mathbb{R}^{n_x}$ is a given function. Throughout it is assumed that F is sufficiently smooth, i.e., it possesses continuous partial derivatives up to a requested order. If the Jacobian $F'_{x'}$ is nonsingular in a solution x, then Eq. (1.1) can be solved for x' by the implicit function theorem and an explicit ODE is obtained. We are particularly interested in the case where $F'_{x'}$ is singular, in which case (1.1) contains ODEs as well as algebraic equations. Particular examples with singular Jacobian are semi-explicit DAEs of type

$$F(t,x,x',u) = \begin{pmatrix} M(t,x_d)x'_d - f(t,x_d,x_a,u) \\ g(t,x_d,x_a,u) \end{pmatrix}, \qquad x := (x_d,x_a)^\top, \tag{1.2}$$

with a nonsingular matrix M and the so-called differential state vector x_d and the algebraic state vector x_a. Such systems occur, e.g., in process engineering and mechanical multi-body systems, whereas electric circuits can be modeled by quasi linear DAEs of type

$$F(t,x,x',u) = Q(t,x)x' - f(t,x,u) \tag{1.3}$$

with a possibly singular matrix function Q. Linear DAEs of type

$$F(t,x,x',u) = E(t)x' - A(t)x - B(t)u - q(t) \tag{1.4}$$

with time dependent matrices E, A, B, and inhomogeneity q are of particular interest in controller design. This form is referred to as descriptor form.

Now the task is to find an optimal control u such that a given objective function is minimized subject to the DAE and further control and state constraints. To this end let $\varphi : \mathbb{R}^{n_x} \times \mathbb{R}^{n_x} \longrightarrow \mathbb{R}$, $f_o : I \times \mathbb{R}^{n_x} \times \mathbb{R}^{n_u} \longrightarrow \mathbb{R}$, $c : I \times \mathbb{R}^{n_x} \times \mathbb{R}^{n_u} \longrightarrow \mathbb{R}^{n_c}$, $n_c \in \mathbb{N}$, $\psi : \mathbb{R}^{n_x} \times \mathbb{R}^{n_x} \longrightarrow \mathbb{R}^{n_\psi}$, $n_\psi \in \mathbb{N}$, be given functions and $\mathscr{U} \subseteq \mathbb{R}^{n_u}$ a set. A general prototype optimal control problem reads as follows:

Problem 1.1 (OCP) Minimize

$$\varphi(x(t_0), x(t_f)) + \int_{t_0}^{t_f} f_0(t, x(t), u(t))dt$$

subject to the DAE (1.1), the control-state constraints

$$c(t, x(t), u(t)) \leq 0,$$

the boundary condition

$$\psi(x(t_0), x(t_f)) = 0,$$

and the set constraints

$$u(t) \in \mathscr{U}.$$

It is important to point out that OCP is merely a generic container for different types of DAE optimal control problems, but its formulation is yet too vague for a thorough analysis. Most importantly, the function spaces from which x and u shall be chosen have to be defined appropriately. Typically, in the nonlinear setting of OCP, u is supposed to be an essentially bounded function from the Banach space $L^\infty(I, \mathbb{R}^{n_u})$, or a square integrable function from the Hilbert space $L^2(I, \mathbb{R}^{n_u})$ for linear-quadratic problems. The choice of a proper space for the state x is more subtle since the components of x may have different smoothness properties depending on the structure of the DAE. In classic ODE optimal control theory the natural space for x would be the Banach space $W^{1,\infty}(I, \mathbb{R}^{n_x})$ of essentially bounded functions with essentially bounded first derivatives in the nonlinear case or the Hilbert space $W^{1,2}(I, \mathbb{R}^{n_x})$ of L^2-functions with L^2-derivative in the linear-quadratic case. In the presence of DAEs, however, the DAE might not possess a solution in these classic spaces. This immediately becomes clear for the semi-explicit DAE (1.2). Suppose that the algebraic constraint $0 = g(t, x_d, x_a, u)$ can be solved for x_a, i.e., $x_a = x_a(t, x_d, u)$. In this case the smoothness of x_a depends on the smoothness of the control input u. Thus, for an L^∞-input u one can only expect the algebraic variable x_a to be an L^∞-function rather than a $W^{1,\infty}$-function. One can easily imagine that the situation for general DAEs (1.1) is even more complicated. For this reason the discussion in the following sections is restricted to appropriate subclasses of (1.1) and of OCP whenever necessary.

Once appropriate spaces have been identified, the key issue in the analysis of OCP is necessary optimality conditions. To this end OCP and the special cases in Sects. 2 and 3 will be considered as nonlinear optimization problems in a Banach space setting of type NLP in Problem 1.2 below. Then, the necessary conditions in Theorems 1.3 and 1.4 will be applied to the optimal control problems in Sects. 2 and 3.

Let Z, V, W be Banach spaces equipped with norms $\|\cdot\|_Z$, $\|\cdot\|_V$, $\|\cdot\|_W$, respectively, and let $J : Z \longrightarrow \mathbb{R}$, $G : Z \longrightarrow W$, $H : Z \longrightarrow V$ be given mappings. Let $K \subseteq W$ be a non-empty closed convex cone with vertex at zero and $S \subseteq Z$ a non-empty set.

Problem 1.2 (NLP) Minimize $J(z)$ subject to the constraints

$$z \in S, \qquad G(z) \in K, \qquad H(z) = 0.$$

Herein, $z \in S$ is referred to as set constraint, $G(z) \in K$ as inequality (or cone) constraint, and $H(z) = 0$ as equality constraint. Note that the cone K induces a partial ordering on W according to the relation $x \leq_K y$ which holds if and only if $x - y \in K$. With this the cone constraint $G(z) \in K$ reads $G(z) \leq_K 0$.

First order necessary conditions of optimality are provided by the following theorem, compare [48, Theorem 2.3.24], which can be found in similar form in [83] and [75, Theorems 3.1,4.1]. Herein,

$$K^- := \{k^* \in W^* \mid k^*(k) \leq 0 \ \forall k \in K\}$$

denotes the negative dual cone of K and W^* denotes the dual space of W.

Theorem 1.3 (Fritz John Conditions) *Let Banach spaces* $(Z, \|\cdot\|_Z)$, $(V, \|\cdot\|_V)$, $(W, \|\cdot\|_W)$ *be given.*

(a) *Let* $S \subseteq Z$ *be a closed convex set with non-empty interior and* $K \subseteq W$ *a closed convex cone with vertex at zero and non-empty interior.*
(b) *Let* $J : Z \longrightarrow \mathbb{R}$ *and* $G : Z \longrightarrow W$ *be Fréchet-differentiable and let* $H : Z \longrightarrow V$ *be continuously Fréchet-differentiable.*
(c) *Let* $\hat{z}$ *be a local minimum of NLP.*
(d) *Let the image of* $H'(\hat{z})$ *be closed in* V.

Then there exist nontrivial multipliers $(\ell_0, \mu^*, \lambda^*) \in \mathbb{R} \times W^* \times V^*$, $(\ell_0, \mu^*, \lambda^*) \neq 0$, *such that*

$$\ell_0 \geq 0, \tag{1.5}$$

$$\mu^* \in K^-, \tag{1.6}$$

$$\mu^*(G(\hat{z})) = 0, \tag{1.7}$$

$$\ell_0 J'(\hat{z})(d) + \mu^*(G'(\hat{z})(d)) + \lambda^*(H'(\hat{z})(d)) \geq 0, \quad \textit{for all } d \in S - \{\hat{z}\}. \tag{1.8}$$

Every point $(z, \ell_0, \mu^*, \lambda^*) \in Z \times \mathbb{R} \times W^* \times V^*$ with $(\ell_0, \mu^*, \lambda^*) \neq 0$ and (1.5)–(1.8) is called Fritz John point of NLP. Every Fritz John point $(z, \ell_0, \mu^*, \lambda^*)$ with $\ell_0 \neq 0$ is called Karush-Kuhn-Tucker (KKT) point.

Assumption (d) is satisfied, if $H'(\hat{z})$ is surjective. It may happen that Theorem 1.3 only holds with $\ell_0 = 0$. In this case the Fritz John conditions (1.5)–(1.8) are not very useful since the objective function J does not appear. To exclude this degenerated situation, a constraint qualification is required.

Theorem 1.4 (KKT Conditions) *Let the assumptions of Theorem 1.3 be satisfied. Theorem 1.3 holds with* $\ell_0 = 1$ *if one of the following constraint qualifications is satisfied:*

(a) Linear independence constraint qualification (LICQ):
$\hat{z} \in int(S)$ *and the operator* $(G'(\hat{z}), H'(\hat{z}))$ *is surjective in* $W \times V$.
(b) Constraint qualification of Mangasarian-Fromowitz:
$H'(\hat{z})$ *is surjective and there exists some* $\hat{d} \in int(S - \{\hat{z}\})$ *with*

$$H'(\hat{z})(\hat{d}) = 0, \qquad G(\hat{z}) + G'(\hat{z})(\hat{d}) \in int(K).$$

For a proof see [48, Sect. 2.3.5], [75, Theorems 3.1,4.1].

The purpose of the paper is to provide an overview on different aspects in optimal control with DAEs and to summarize the literature in this field to the best of the author's knowledge. Naturally many aspects occur and not all of them can be covered in depth, compare the recent monograph [16]. The reader will find more detailed references for the different topics in the subsequent sections. An outline of the paper is as follows. Necessary and sufficient conditions for linear-quadratic DAE optimal control problems will be investigated in Sect. 2. In Sect. 3 we will focus on necessary conditions in terms of local (or weak) minimum principles and global (or strong) minimum principles for a class of nonlinear DAE optimal control problems. Herein, the local minimum principles are derived by application of Theorem 1.3. Direct discretization methods are discussed in Sect. 4, while Sect. 5 is devoted to two function space methods, the projected gradient method and the Lagrange–Newton method. Conclusions and suggestions for further research in the section "Conclusions and Future Directions" conclude the paper.

Notation

We use the convention that the dimension of a real-valued vector x is denoted by $n_x \in \mathbb{N}$, that is $x \in \mathbb{R}^{n_x}$.

In order to simplify notation, we use the abbreviation $f[t]$ for a function of type $f(t, z(t))$, which depends on time and on one or more time dependent functions.

The partial derivatives of a function $f : \mathbb{R}^{n_x} \times \mathbb{R}^{n_y} \longrightarrow \mathbb{R}^{n_f}$, $(x, y) \mapsto f(x, y)$, at (x, y) are denoted by $f'_x(x, y)$ and $f'_y(x, y)$.

The Lebesque space of all measurable vector valued functions $f : I \longrightarrow \mathbb{R}^n$, $I = [t_0, t_f]$, which are bounded in the L^p-norm $\|f\|_p := (\int_I \|f(t)\|^p \, dt)^{1/p}$, is denoted by $L^p(I, \mathbb{R}^n)$, $1 \le p < \infty$. $L^\infty(I, \mathbb{R}^n)$ with norm $\|\cdot\|_\infty$ denotes the space of essentially bounded functions on I. $C(I, \mathbb{R}^n)$ denotes the space of continuous vector valued functions $f : I \longrightarrow \mathbb{R}^n$, $BV(I, \mathbb{R}^n)$ the space of measurable vector valued functions of bounded variation on I, and $NBV(I, \mathbb{R}^n)$ the space of normalized measurable vector valued functions of bounded variation on I, i.e., measurable vector valued functions of bounded variation that are continuous from the right and zero at t_0.

For $1 \le p \le \infty$, $W^{1,p}(I, \mathbb{R}^n)$ denotes the Sobolev space of absolutely continuous vector valued functions f that are bounded w.r.t. the norm $\|f\|_{1,p} := \max\{\|f\|_p, \|f'\|_p\}$.

Throughout, X^* denotes the dual space of a Banach space X.

2 Optimality Conditions for Linear-Quadratic DAE Optimal Control Problems

Linear-quadratic optimal control problems play an important role in the design of feedback controllers for control problems, see, e.g., [77, 87]. Typically the linear dynamics are obtained by linearization of the nonlinear dynamics (1.1) at an equilibrium point or along a given reference trajectory. The task is to minimize a convex quadratic objective function with the aim to minimize the control effort and the deviation of the state from a reference solution, which is given w.l.o.g. by the zero function.

Linear-quadratic optimal control problems are commonly approached as follows:

(a) A boundary value problem (BVP) (“optimality system”) is formulated that consists of the original DAE with initial condition, of an adjoint DAE with terminal condition, and of a stationarity condition.
(b) It is typically straightforward to show with minimal assumptions that solvability of the BVP is actually sufficient for optimality.
(c) The solvability of the BVP is analyzed and conditions are formulated under which a solution of the BVP exists.

This approach differs to some extend from the standard approach in optimization, where necessary conditions are investigated first and afterwards it is shown that the necessary conditions in the convex case are sufficient as well. In the DAE context however, it may happen that the “optimality system” in (a) is not necessary for optimality since existence of a solution in (b) is not guaranteed automatically.

In order to motivate the adjoint DAE and to illustrate the difficulties in deriving necessary conditions we try to derive them by exploitation of Theorem 1.4. To this end we need to properly formulate the function spaces in which the optimal control problem lives. Instead of the descriptor form (1.4) of a linear DAE we follow [10] and consider linear DAEs with the special leading term formulation

$$A(t)(D(t)x(t))' + B(t)x(t) + P(t)u(t) = q(t) \tag{2.1}$$

with continuous matrix functions $A \in L^\infty(I, \mathbb{R}^{n_x \times m})$, $m \in \mathbb{N}$, $D \in L^\infty(I, \mathbb{R}^{m \times n_x})$, $B \in L^\infty(I, \mathbb{R}^{n_x \times n_x})$, $P \in L^\infty(I, \mathbb{R}^{n_x \times n_u})$, $q \in L^\infty(I, \mathbb{R}^{n_x})$, and $\ker A \oplus \operatorname{im} D = \mathbb{R}^m$. If D in (2.1) or E in (1.4) are smooth, both forms can be transformed into each other, compare [8, 10]. As we shall see, the leading term formulation reveals a nice symmetry in the original DAE and its adjoint DAE.

The leading term $A(Dx)'$ has the advantage that it indicates more appropriately from which space the state x and the control u should be chosen. For linear DAEs in descriptor form (1.4) transformations are necessary to reveal the spaces, compare Sect. 2.3.

To this end, the matrix D can be understood as a filter that filters out the differentiable components of x. A natural choice is to use the spaces

$$\begin{aligned} X &:= W_D^{1,2}(I,\mathbb{R}^{n_x}) := \{x \in L^2(I,\mathbb{R}^{n_x}) \mid Dx \in W^{1,2}(I,\mathbb{R}^m)\}, \\ U &:= L^2(I,\mathbb{R}^{n_u}), \end{aligned}$$

both being Hilbert spaces, compare Theorem 7.1 in Sect. 7.

For essentially bounded symmetric matrices $Q \in L^\infty(I,\mathbb{R}^{n_x \times n_x})$ and $R \in L^\infty(I,\mathbb{R}^{n_u \times n_u})$ and a given consistent vector $x_0 \in \mathbb{R}^{n_x}$ with x_0 in the range of $D(t_0)$ consider the following linear-quadratic optimal control problem.

Problem 2.1 (LQOCP) Minimize

$$\frac{1}{2}\int_I x(t)^\top Q(t)x(t) + u(t)^\top R(t)u(t)dt$$

with respect to $(x,u) \in X \times U$ subject to the constraints

$$\begin{aligned} A(t)(D(t)x(t))' + B(t)x(t) + P(t)u(t) &= q(t), \\ D(t_0)x(t_0) &= x_0. \end{aligned}$$

The following subsections are devoted to the analysis of necessary and sufficient conditions for LQOCP.

2.1 Necessary Conditions

Define the functional $J : X \times U \longrightarrow \mathbb{R}$ by

$$J(x,u) := \frac{1}{2}\int_I x(t)^\top Q(t)x(t) + u(t)^\top R(t)u(t)dt$$

and the linear operator $H : X \times U \longrightarrow L^2(I,\mathbb{R}^{n_x}) \times \mathbb{R}^m$ by

$$H(x,u) := \begin{pmatrix} A(\cdot)(D(\cdot)x(\cdot))' + B(\cdot)x(\cdot) + P(\cdot)u(\cdot) - q(\cdot) \\ D(t_0)x(t_0) - x_0 \end{pmatrix}.$$

J and H are continuously Fréchet-differentiable and LQOCP reads

$$\text{Minimize} \qquad J(x,u) \qquad \text{subject to} \qquad H(x,u) = 0\,,$$

i.e., LQOCP is of type NLP with $z = (x, u)$, $Z = X \times U$, $S = Z$, and we like to apply Theorem 1.4. To this end, let $\hat{z} = (\hat{x}, \hat{u})$ be a minimum of LQOCP and let Assumption 2.2 below hold.

Assumption 2.2 *$H'(\hat{x}, \hat{u})$ is surjective, that is, the initial value problem (IVP)*

$$\begin{aligned} A(t)(D(t)x(t))' + B(t)x(t) + P(t)u(t) &= r(t), \\ D(t_0)x(t_0) &= r_0 \end{aligned}$$

possesses a solution $(x, u) \in X \times U$ for any $(r, r_0) \in L^2(I, \mathbb{R}^{n_x}) \times \mathbb{R}^m$.

Under these assumptions, Theorem 1.4 yields the existence of a multiplier $(\lambda^*, \sigma) \in L^2(I, \mathbb{R}^{n_x})^* \times \mathbb{R}^m$ with

$$0 = L'_{(x,u)}(\hat{x}, \hat{u}, \lambda^*, \sigma)(x, u) \qquad \forall (x, u) \in X \times U, \tag{2.2}$$

where $L : X \times U \times L^2(I, \mathbb{R}^{n_x})^* \times \mathbb{R}^m \longrightarrow \mathbb{R}$,

$$L(x, u, \lambda^*, \sigma) := J(x, u) + \lambda^*(H(x, u)) + \sigma^\top (D(t_0)x(t_0) - x_0)$$

denotes the Lagrange function of LQOCP. Since $L^2(I, \mathbb{R}^{n_x})$ is a Hilbert space, the multiplier λ^* can be represented as $\lambda^*(h) = \langle \lambda, h \rangle_{L^2(I, \mathbb{R}^{n_x})}$ with some $\lambda \in L^2(I, \mathbb{R}^{n_x})$ by the theorem of Riesz. Hence,

$$\begin{aligned} L(x, u, \lambda^*, \sigma) = J(x, u) &+ \int_I \lambda(t)^\top \left(A(t)(D(t)x(t))' + B(t)x(t) + P(t)u(t) - q(t) \right) dt \\ &+ \sigma^\top (D(t_0)x(t_0) - x_0) \end{aligned}$$

and the variational equation (2.2) implies

$$\begin{aligned} 0 = \int_I & \hat{x}(t)^\top Q(t)x(t) + \lambda(t)^\top \left(A(t)(D(t)x(t))' + B(t)x(t) \right) dt \\ & + \sigma^\top D(t_0)x(t_0), \end{aligned} \tag{2.3}$$

$$0 = \int_{t_0}^{t_f} \left(R(t)^\top \hat{u}(t) + P(t)^\top \lambda(t) \right)^\top u(t) dt \tag{2.4}$$

for all $x \in X$ and all $u \in U$. The variational equation (2.4) implies the condition

$$0 = R(t)^\top \hat{u}(t) + P(t)^\top \lambda(t) \qquad \text{a.e. in } I. \tag{2.5}$$

For a further manipulation of the variational equation (2.3) we assume that $A(\cdot)^\top\lambda(\cdot)$ is in $W^{1,2}(I,\mathbb{R}^m)$ or equivalently, $\lambda \in W^{1,2}_{A^\top}(I,\mathbb{R}^{n_x}) := \{\lambda \in L^2(I,\mathbb{R}^{n_x}) \mid A^\top\lambda \in W^{1,2}(I,\mathbb{R}^m)\}$. Then partial integration yields for all $x \in X$,

$$0 = \left[\left(A(t)^\top\lambda(t)\right)^\top (D(t)x(t))\right]_{t_0}^{t_f} + \sigma^\top D(t_0)x(t_0) + \int_{t_0}^{t_f} \left(\hat{x}(t)^\top Q(t) + \lambda(t)^\top B(t) - \left((A(t)^\top\lambda(t))'\right)^\top D(t)\right) x(t)\, dt.$$

Application of a variation lemma, see [48, Lemma 3.1.9], yields the adjoint DAE

$$-D(t)^\top(A(t)^\top\lambda(t))' + Q(t)\hat{x}(t) + B(t)^\top\lambda(t) = 0 \qquad \text{a.e. in } I, \tag{2.6}$$

and the transversality conditions

$$D(t_0)^\top\left(A(t_0)^\top\lambda(t_0) - \sigma\right) = 0, \qquad D(t_f)^\top A(t_f)^\top\lambda(t_f) = 0. \tag{2.7}$$

We summarize the findings.

Theorem 2.3 (Necessary Conditions for LQOCP) *Let $(\hat{x},\hat{u})$ be a minimum of LQOCP and let Assumption 2.2 hold.*

Then there exists $\lambda \in L^2(I,\mathbb{R}^{n_x})$ and $\sigma \in \mathbb{R}^m$ such that (2.5) and (2.3) hold for every $x \in X$.

Moreover, if $\lambda \in W^{1,2}_{A^\top}(I,\mathbb{R}^{n_x})$, then (2.6) and (2.7) hold as well.

Theorem 2.3 is based on two crucial assumptions, namely Assumption 2.2 and the assumption $\lambda \in W^{1,2}_{A^\top}(I,\mathbb{R}^{n_x})$, which will not be satisfied for arbitrary data. A further analysis of the DAE (2.1) and the adjoint DAE (2.6) becomes necessary.

For index-1 tractable problems, the surjectivity assumption in Assumption 2.2 follows with [10, Theorem 3.2] with $D(t_0)$ being surjective, but for index-2 tractable problems surjectivity cannot be satisfied in general, since the term $r(t) - P(t)u(t)$ in Assumption 2.2 has to satisfy additional smoothness requirements, compare [10, Theorem 3.4] and [80, Theorem 2.52].

Since the adjoint DAE (2.6) has a leading term structure as well, the existence results in [10, Theorems 3.2, 3.4] can be applied to the adjoint DAE in order to guarantee that the adjoint DAE admits a solution $\lambda \in W^{1,2}_{A^\top}(I,\mathbb{R}^{n_x})$. In fact, it was shown in [80, Proposition 11.6,Theorem 11.9] that properties of the DAE (2.1) like the "properly stated leading term" and index-1 and index-2 tractability are inherited by the adjoint DAE.

2.2 Sufficient Conditions for Linear-Quadratic DAE Optimal Control Problems

The derivation of necessary conditions was subject to additional assumptions that needed to be imposed. However, if Q and R are symmetric and positive semi-definite, it is straightforward to show that the solvability of the "optimality system" (2.1), (2.5), (2.6), and (2.7) is already sufficient for optimality without any further assumptions.

Theorem 2.4 (Sufficient Condition) *Consider the linear-quadratic optimal control problem LQOCP. Let Q and R be symmetric and uniformly positive semi-definite on I. Let $(\hat{x}, \hat{u}) \in X \times U$ and $\lambda \in W^{1,2}_{A^\top}(I, \mathbb{R}^{n_x})$ on I satisfy*

$$A(t)(D(t)\hat{x}(t))' + B(t)\hat{x}(t) + P(t)\hat{u}(t) = q(t),\ D(t_0)\hat{x}(t_0) = x_0, \tag{2.8}$$

$$-D(t)^\top(A(t)^\top\lambda(t))' + Q(t)\hat{x}(t) + B(t)^\top\lambda(t) = 0,\ D(t_f)^\top A(t_f)^\top\lambda(t_f) = 0, \tag{2.9}$$

$$R(t)^\top\hat{u}(t) + P(t)^\top\lambda(t) = 0. \tag{2.10}$$

Then $(\hat{x}, \hat{u})$ is a global minimizer of LQOCP.

Proof Let (x, u) be feasible for LQOCP. Exploitation of the assumptions and neglecting the explicit time dependence for notational convenience yield

$$\begin{aligned}
J(x,u) - J(\hat{x},\hat{u}) &= \int_I \frac{1}{2}x^\top Qx + \frac{1}{2}u^\top Ru - \frac{1}{2}\hat{x}^\top Q\hat{x} - \frac{1}{2}\hat{u}^\top R\hat{u}\, dt \\
&= \int_I \frac{1}{2}x^\top Qx + \frac{1}{2}u^\top Ru - \frac{1}{2}\hat{x}^\top Q\hat{x} - \frac{1}{2}\hat{u}^\top R\hat{u} \\
&\qquad + \lambda^\top\left(A(Dx)' + Bx + Pu - q\right) \\
&\qquad - \lambda^\top\left(A(D\hat{x})' + B\hat{x} + P\hat{u} - q\right)\, dt \\
&= \int_I \frac{1}{2}x^\top Qx + \frac{1}{2}u^\top Ru - \frac{1}{2}\hat{x}^\top Q\hat{x} - \frac{1}{2}\hat{u}^\top R\hat{u} \\
&\qquad + \lambda^\top B(x-\hat{x}) + \lambda^\top P(u-\hat{u}) + (A^\top\lambda)^\top\left((Dx)' - (D\hat{x})'\right)\, dt \\
&= \int_I \frac{1}{2}x^\top Qx + \frac{1}{2}u^\top Ru - \frac{1}{2}\hat{x}^\top Q\hat{x} - \frac{1}{2}\hat{u}^\top R\hat{u} \\
&\qquad + \lambda^\top B(x-\hat{x}) + \lambda^\top P(u-\hat{u}) - \left((A^\top\lambda)'\right)^\top(Dx - D\hat{x})\, dt \\
&= \int_I \frac{1}{2}x^\top Qx + \frac{1}{2}u^\top Ru - \frac{1}{2}\hat{x}^\top Q\hat{x} - \frac{1}{2}\hat{u}^\top R\hat{u} \\
&\qquad + \lambda^\top B(x-\hat{x}) + \lambda^\top P(u-\hat{u}) - \hat{x}^\top Q(x-\hat{x}) - \lambda^\top B(x-\hat{x})\, dt
\end{aligned}$$

$$
\begin{aligned}
&= \int_I \frac{1}{2}x^\top Qx + \frac{1}{2}u^\top Ru - \frac{1}{2}\hat{x}^\top Q\hat{x} - \frac{1}{2}\hat{u}^\top R\hat{u} - \hat{u}^\top R(u-\hat{u}) \\
&\qquad -\hat{x}^\top Q(x-\hat{x})\, dt \\
&= \frac{1}{2}\int_I (x-\hat{x})^\top Q(x-\hat{x}) + (u-\hat{u})^\top R(u-\hat{u})\, dt \\
&\geq 0,
\end{aligned}
$$

since Q and R are supposed to be uniformly positive semi-definite. □

The theorem states the following: If the optimality system (2.8)–(2.10) has a solution, then this solution is optimal. It is important to point out, that in this context the solvability of the overall optimality system (2.8)–(2.10) viewed as one single DAE is important, not the solvability of the individual DAEs (2.8) and (2.9) appearing in the optimality system. In general it is not guaranteed that the optimality system has a solution, see [8, Beispiel 3.16] for a counterexample. Sufficient conditions for solvability of the optimality system (2.8)–(2.10) can be found in [76, Theorem 5.5] or [8, Satz 3.22].

Let us finally state a sufficient condition for LQOCP in the presence of control-state constraints of type

$$
S(t)x(t) + F(t)u(t) - r(t) \leq 0 \tag{2.11}
$$

with matrix functions $S \in L^\infty(I, \mathbb{R}^{\ell \times n_x})$, $F \in L^\infty(I, \mathbb{R}^{\ell \times n_u})$, and $r \in L^\infty(I, \mathbb{R}^\ell)$. The investigation of necessary conditions subject to restrictions similar to those in Sect. 2.1 leads to the following optimality system:

$$
A(t)(D(t)\hat{x}(t))' + B(t)\hat{x}(t) + P(t)\hat{u}(t) = q(t), \tag{2.12}
$$

$$
-D(t)^\top (A(t)^\top \lambda(t))' + Q(t)\hat{x}(t) + B(t)^\top \lambda(t) + S(t)^\top \eta(t) = 0, \tag{2.13}
$$

$$
R(t)^\top \hat{u}(t) + P(t)^\top \lambda(t) + F(t)^\top \eta(t) = 0, \tag{2.14}
$$

$$
D(t_0)\hat{x}(t_0) = x_0, \qquad D(t_f)^\top A(t_f)^\top \lambda(t_f) = 0, \tag{2.15}
$$

$$
0 \leq \eta(t) \quad \perp \quad -(S(t)\hat{x}(t) + F(t)\hat{u}(t) - r(t)) \geq 0, \tag{2.16}
$$

where $0 \leq a \perp b \geq 0$ is an abbreviation for the complementarity conditions $a \geq 0, b \geq 0, a^\top b = 0$. Solvability of this complementarity system is again sufficient for optimality:

Theorem 2.5 (Sufficient Condition in the Presence of Control-State Constraints) *Consider the linear-quadratic optimal control problem LQOCP subject to the control-state constraint (2.11). Let Q and R be symmetric and uniformly positive* *semi-definite on I. Let $(\hat{x}, \hat{u}) \in X \times U$, $\lambda \in W^{1,2}_{A^\top}(I, \mathbb{R}^{n_x})$, and $\eta \in L^2(I, \mathbb{R}^\ell)$ satisfy (2.12)–(2.16) on I.*

Then $(\hat{x}, \hat{u})$ is a global minimizer of LQOCP subject to (2.11).

The proof can be found in Appendix 7. The investigation of sufficient conditions for the solvability of (2.12)–(2.16) is the subject of future research.

2.3 Problems in Descriptor Form

Let the DAE in LQOCP be given in descriptor form (1.4) with a singular matrix function E on $I = [t_0, t_f]$:

Problem 2.6 (LQOCP-DF) Minimize

$$\frac{1}{2} \int_I x(t)^\top Q(t)x(t) + u(t)^\top R(t)u(t)dt$$

subject to the constraints

$$\begin{aligned} E(t)x'(t) &= A(t)x(t) + B(t)u(t) + q(t), \qquad (2.17) \\ x(t_0) &= x_0. \end{aligned}$$

Remark 2.1 The assignment $x(t_0) = x_0$ in LQOCP-DF, i.e., fixing the entire initial state vector, is used for notational convenience only. In fact it is misleading since in general it is not possible to fix the entire initial state vector $x(t_0)$ in advance (if continuous controls are considered). Some components may depend implicitly on the control. For illustration consider the DAE

$$x_1'(t) = x_2(t), \qquad x_2'(t) = x_3(t) + u(t), \qquad 0 = x_2(t) - t.$$

The initial value of x_1 can be arbitrary whereas $x_2(t_0)$ and $x_3(t_0)$ have to be consistent, that is $x_2(t_0) = t_0$ and $x_3(t_0) = 1 - u(t_0)$. To this end, if the problem was considered in the space of continuous controls, then LQOCP-DF might fail to have a solution if the entire vector $x(t_0)$ is fixed a priori. However, if LQOPC-DF is considered in the L^2-space, then LQOCP-DF may still have a solution but with a discontinuous control at t_0.

Owing to the singularity of E not all components of x need to be differentiable. But for the correct definition of the function spaces in LQOCP-DF it is necessary to identify the differentiable components and those with lower differentiability requirements. A concept that is capable to identify such components is the behavior approach and the strangeness index, see [68, Definition 3.15]. Herein, states and controls are unified in one state vector $z := (x, u)^\top$ without imposing a priori assumptions on the smoothness of its components. The DAE (2.17) is then equivalently written as the DAE

$$\mathscr{E}(t)z'(t) = \mathscr{A}(t)z(t) + q(t) \tag{2.18}$$

with $\mathscr{E}(t) := \big(E(t)\big|0\big)$, $\mathscr{A}(t) := \big(A(t)\big|B(t)\big)$.

Assuming the existence of the strangeness index, a canonical form of type

$$\begin{aligned} z_1'(t) &= \mathscr{A}_{13}(t)z_3(t) + q_1(t), \\ 0 &= z_2(t) + q_2(t), \\ 0 &= q_3(t) \end{aligned}$$

can be derived using suitable projectors for a suitable partition of z and q, compare [68, Theorem 3.17]. This canonical form allows to identify the smoothness requirements of the components of z. The components of z_2 are fixed by the inhomogeneity q_2 and thus they possess the same smoothness properties as q_2. An initial value $z_2(t_0)$ is consistent if and only if $z_2(t_0) = -q_2(t_0)$. The smoothness of z_1 is determined by the smoothness of z_3 and q_1, that is, if z_3 and q_1 are L^1-integrable function, then z_1 is absolutely continuous. The last equation $0 = q_3(t)$ is a measure of inconsistency of the descriptor system, i.e., a solution exists if and only if $q_3 \equiv 0$.

Once this partitioning of the descriptor system is known, it is possible to consider optimization problems with the appropriate function spaces. However, this approach does not distinguish states and controls and may require a higher smoothness of a control than it is actually realistic from an application point of view. Hence, for control problems a refined analysis as in [68, Sect. 3.6] is necessary. Moreover, the strangeness index requires E and A to be sufficiently smooth, which might be a restriction if the linear DAE (2.17) results from a linearization of the nonlinear DAE (1.1) along an optimal solution.

We omit the details and summarize necessary and sufficient conditions for LQOCP-DF. It was shown in [67, Theorems 2,3] (for a more general setting but with $q \equiv 0$) that the solvability of the linear BVP

$$\begin{pmatrix} E(t) & 0 & 0 \\ 0 & -E(t)^\top & 0 \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} x'(t) \\ \lambda'(t) \\ u'(t) \end{pmatrix} = \begin{pmatrix} A(t) & 0 & B(t) \\ Q(t) & A(t)^\top + E'(t)^\top & 0 \\ 0 & B(t)^\top & R(t) \end{pmatrix} \begin{pmatrix} x(t) \\ \lambda(t) \\ u(t) \end{pmatrix},$$

$$x(t_0) = x_0, \qquad E(t_f)^\top \lambda(t_f) = 0,$$

is a necessary condition and a sufficient condition for optimality, if Q and R are symmetric and positive semi-definite. A characterization for the strangeness index to be zero is provided in [67, Proposition 4]. Further solution properties are discussed as well. Optimal control problems with autonomous descriptor systems are considered in [87].

3 Necessary Optimality Conditions for Nonlinear DAE Optimal Control Problems

The Fritz John conditions and the KKT conditions in Theorems 1.3 and 1.4, respectively, are the basic tools for the derivation of necessary conditions for nonlinear control and state constrained DAE optimal control problems. In order to avoid technical matters with regard to the proper identification of function spaces, as it was outlined for the linear-quadratic case in Sect. 2, we restrict the discussion to semi-explicit DAEs of index two and consider the following autonomous problem on the compact time interval $I = [t_0, t_f]$ with fixed time points $t_0 < t_f$, the control set $\mathscr{U} \subseteq \mathbb{R}^{n_u}$, and functions

$$\begin{aligned} \varphi &: \mathbb{R}^{n_x} \times \mathbb{R}^{n_x} \longrightarrow \mathbb{R}, \\ f_0 &: \mathbb{R}^{n_x} \times \mathbb{R}^{n_y} \times \mathbb{R}^{n_u} \longrightarrow \mathbb{R}, \\ f &: \mathbb{R}^{n_x} \times \mathbb{R}^{n_y} \times \mathbb{R}^{n_u} \longrightarrow \mathbb{R}^{n_x}, \\ g &: \mathbb{R}^{n_x} \longrightarrow \mathbb{R}^{n_y}, \\ s &: \mathbb{R}^{n_x} \longrightarrow \mathbb{R}^{n_s}, \\ \psi &: \mathbb{R}^{n_x} \times \mathbb{R}^{n_x} \longrightarrow \mathbb{R}^{n_\psi}. \end{aligned}$$

φ, f_0, f, s, ψ are supposed to be continuously differentiable and g is supposed to be twice continuously differentiable.

Problem 3.1 (OCP-SE) Minimize

$$\varphi(x(t_0), x(t_f)) + \int_I f_0(x(t), y(t), u(t))\, dt$$

w.r.t. $x \in W^{1,\infty}(I, \mathbb{R}^{n_x})$, $y \in L^\infty(I, \mathbb{R}^{n_y})$, $u \in L^\infty(I, \mathbb{R}^{n_u})$ subject to the constraints

$$\begin{aligned} x'(t) &= f(x(t), y(t), u(t)) && \text{a.e. in } I, \\ 0 &= g(x(t)) && \text{in } I, \\ s(x(t)) &\le 0 && \text{in } I, \\ 0 &= \psi(x(t_0), x(t_f)), && \\ u(t) &\in \mathscr{U} && \text{a.e. in } I. \end{aligned}$$

This sufficiently simple problem class already exhibits the main difficulties in deriving necessary conditions. Moreover, OCP-SE contains practically important problem classes like mechanical multi-body systems in Gear-Gupta-Leimkuhler formulation, see [43]. For extensions towards more general systems with properly stated leading terms we refer to [8, Kapitel 5] and [80, Sect. 11.2] and for general nonlinear descriptor systems to [69].

Let $X := W^{1,\infty}(I, \mathbb{R}^{n_x})$, $Y := L^{\infty}(I, \mathbb{R}^{n_y})$, $U := L^{\infty}(I, \mathbb{R}^{n_u})$, $V := L^{\infty}(I, \mathbb{R}^{n_x}) \times W^{1,\infty}(I, \mathbb{R}^{n_y}) \times \mathbb{R}^{n_\psi}$, $W := C(I, \mathbb{R}^{n_s})$, $K := \{k \in C(I, \mathbb{R}^{n_s}) \mid k(t) \leq 0 \text{ in } I\}$, $Z := X \times Y \times U$, and $S := \{(x, y, u) \in Z \mid u(t) \in \mathscr{U} \text{ a.e. in } I\}$. Define $J : Z \longrightarrow \mathbb{R}$, $H : Z \longrightarrow V$, and $G : Z \longrightarrow W$ by

$$J(x, y, u) := \varphi(x(t_0), x(t_f)) + \int_I f_0(x(t), y(t), u(t))\, dt,$$

$$H(x, y, u) := \begin{pmatrix} x'(\cdot) - f(x(\cdot), y(\cdot), u(\cdot)) \\ -g(x(\cdot)) \\ \psi(x(t_0), x(t_f)) \end{pmatrix},$$

$$G(x, y, u) := s(x(\cdot)).$$

With these definitions and $z = (x, y, u)$, OCP-SE fits into the problem class of Problem 1.2, i.e.,

$$\text{Minimize} \quad J(z) \quad \text{s.t.} \quad z \in S,\ G(z) \in K,\ H(z) = 0.$$

In the sequel, $\hat{z} = (\hat{x}, \hat{y}, \hat{u})$ denotes a local minimum of OCP-SE. Throughout we assume that the DAE has index two:

Assumption 3.2 *Let the matrix*

$$M(t) := g_x'(\hat{x}(t)) f_y'(\hat{x}(t), \hat{y}(t), \hat{u}(t))$$

be non-singular almost everywhere in I and let $M(\cdot)^{-1}$ be essentially bounded in I.

3.1 A Local (or Weak) Minimum Principle

The local minimum principle (or weak minimum principle) requires a convex control set $\mathscr{U}$ with non-empty interior and it provides a necessary condition for a local (or weak) minimum $\hat{z}$ of OCP-SE. Local minimality means that $\hat{z} = (\hat{x}, \hat{y}, \hat{u})$ minimizes J w.r.t. to all feasible $z = (x, y, u)$ with

$$\|z - \hat{z}\|_Z = \max\{\|x - \hat{x}\|_{1,\infty}, \|y - \hat{y}\|_{\infty}, \|u - \hat{u}\|_{\infty}\} < \varepsilon$$

for some $\varepsilon > 0$. Note that this neighborhood contains comparatively few functions. For instance, if $\hat{u}$ is a bang–bang control, then the above (weak) neighborhood only contains controls u with the same points of discontinuity as of $\hat{u}$. This weak neighborhood will be enlarged in Sect. 3.2, which eventually results in stronger necessary conditions.

In the sequel we only outline the main steps to prove a local minimum principle. We omit technical difficulties and technical assumptions, which can be found in [48, Chap. 4] and [46, 47]. We emphasize that the same steps essentially can be followed for more general DAEs, see [69]. It turns out that the linearized DAE along the local minimum plays an important role and the existence and uniqueness results mentioned in Sect. 2 re-enter the scene.

The first step towards necessary conditions is to apply Theorem 1.3 to OCP-SE, which under appropriate assumptions yields the existence of multipliers $\ell_0 \geq 0$, $\lambda^* \in V^*$, and $\mu^* \in W^*$ such that the complementarity conditions

$$\mu^* \in K^- \quad \text{and} \quad \mu^*(G(\hat{x}, \hat{y}, \hat{u})) = 0, \tag{3.1}$$

and the variational inequality

$$0 \leq \ell_0 J'(\hat{x}, \hat{y}, \hat{u})(x, y, u) + \mu^*(G'(\hat{x}, \hat{y}, \hat{u})(x, y, u)) + \lambda^*(H'(\hat{x}, \hat{y}, \hat{u})(x, y, u)) \tag{3.2}$$

hold for all $(x, y, u) \in S - \{(\hat{x}, \hat{y}, \hat{u})\}$.

The second step is to obtain useful representations of the multipliers $\lambda^* \in V^* = L^\infty(I, \mathbb{R}^{n_x})^* \times W^{1,\infty}(I, \mathbb{R}^{n_y})^* \times \mathbb{R}^{n_\psi}$ and $\mu^* \in W^* = C(I, \mathbb{R}^{n_s})^*$. Without such representations, conditions (3.1) and (3.2) are of little practical use. The derivation of suitable representation (especially for λ^*) is rather technical and we omit the details, which can be found in [47] or [48, Chap. 3]. The analysis exploits the linearized DAE along the local minimum and results in the following representations with functions $\lambda_f \in BV(I, \mathbb{R}^{n_x})$, $\lambda_g \in L^\infty(I, \mathbb{R}^{n_y})$, $\zeta \in \mathbb{R}^{n_y}$, and $\mu \in NBV(I, \mathbb{R}^{n_s})$, compare [48, Corollary 3.2.4]:

$$\lambda_f^*(h_1) = -\int_I \left(\lambda_f(t)^\top + \lambda_g(t)^\top g_x'[t]\right) h_1(t)dt \qquad (h_1 \in L^\infty(I, \mathbb{R}^{n_x})),$$

$$\lambda_g^*(h_2) = -\zeta^\top h_2(t_0) - \int_I \lambda_g(t)^\top h_2'(t)dt \qquad (h_2 \in W^{1,\infty}(I, \mathbb{R}^{n_y})),$$

$$\mu^*(h) = \int_I h(t)^\top d\mu(t) \qquad (h \in C(I, \mathbb{R}^{n_s})).$$

Introducing these representations into (3.1)–(3.2) allows to deduce three variational inequalities and equalities for x, y, and u, respectively. Application of a variation lemma, compare [48, Lemma 3.1.9], eventually yields the following local minimum principle, compare [48, Theorem 3.2.7], which uses the Hamilton function

$$\mathscr{H}(x, y, u, \lambda_f, \lambda_g, \ell_0) := \ell_0 f_0(x, y, u) + \lambda_f^\top f(x, y, u) + \lambda_g^\top g_x'(x) f(x, y, u).$$

Theorem 3.3 (Local Minimum Principle for OCP-SE) *Let $(\hat{x}, \hat{y}, \hat{u})$ be a local minimum of OCP-SE. Let $\mathscr{U}$ be a closed and convex set with non-empty interior. Let Assumption 3.2 be valid and let the functions in OCP-SE be sufficiently regular, see [48, Assumption 2.2.8].*

Then there exist multipliers

$$\ell_0 \in \mathbb{R},\ \lambda_f \in BV(I, \mathbb{R}^{n_x}),\ \lambda_g \in L^\infty(I, \mathbb{R}^{n_y}),\ \mu \in NBV(I, \mathbb{R}^{n_s}),\ \zeta \in \mathbb{R}^{n_y},\ \sigma \in \mathbb{R}^{n_\psi}$$

such that the following conditions are satisfied:

(a) $\ell_0 \geq 0$, $(\ell_0, \zeta, \sigma, \lambda_f, \lambda_g, \mu) \neq 0$,
(b) Adjoint equations: Almost everywhere in I we have

$$\begin{aligned}\lambda_f(t) = \lambda_f(t_f) &+ \int_t^{t_f} \mathscr{H}_x'(\hat{x}(\tau), \hat{y}(\tau), \hat{u}(\tau), \lambda_f(\tau), \lambda_g(\tau), \ell_0)^\top d\tau, \\ &+ \int_t^{t_f} s_x'(\hat{x}(\tau))^\top d\mu(\tau) \end{aligned} \tag{3.3}$$

$$0 = \quad \mathscr{H}_y'(\hat{x}(t), \hat{y}(t), \hat{u}(t), \lambda_f(t), \lambda_g(t), \ell_0)^\top. \tag{3.4}$$

(c) Transversality conditions:

$$\begin{aligned}\lambda_f(t_0)^\top = -\Big(&\ell_0 \varphi_{x_0}'(\hat{x}(t_0), \hat{x}(t_f)) + \sigma^\top \psi_{x_0}'(\hat{x}(t_0), \hat{x}(t_f)) \\ &+ \zeta^\top g_x'(\hat{x}(t_0))\Big),\end{aligned} \tag{3.5}$$

$$\lambda_f(t_f)^\top = \quad \ell_0 \varphi_{x_f}'(\hat{x}(t_0), \hat{x}(t_f)) + \sigma^\top \psi_{x_f}'(\hat{x}(t_0), \hat{x}(t_f)). \tag{3.6}$$

(d) Stationarity of Hamilton function: Almost everywhere in I we have

$$\mathscr{H}_u'(\hat{x}(t), \hat{y}(t), \hat{u}(t), \lambda_f(t), \lambda_g(t), \ell_0)(u - \hat{u}(t)) \geq 0. \tag{3.7}$$

for all $u \in \mathscr{U}$.
(e) Complementarity condition: μ_i, $i \in \{1, \ldots, n_s\}$, is non-decreasing on I and constant on every interval (t_1, t_2) with $t_1 < t_2$ and $s_i(\hat{x}(t)) < 0$ for all $t \in (t_1, t_2)$.

Normality of the multiplier ℓ_0 (meaning that $\ell_0 = 1$ can be chosen) requires an additional constraint qualification, for instance the linear independence constraint qualification or the Mangasarian-Fromowitz constraint qualification, compare Theorem 1.4. In practice, it is often assumed that $\ell_0 = 1$ holds and with this assumption one tries to satisfy the necessary conditions either numerically or analytically.

The adjoint integral equation (3.3) with the Riemann–Stieltjes integral implies that the adjoint λ_f in general is of bounded variation only and hence λ_f may be discontinuous. The complementarity condition in (e) implies that the discontinuities may occur on active arcs of the state constraint only and the discontinuities are triggered by the multiplier μ. One can show that λ_f in between two discontinuities satisfies the differential equation

$$\lambda_f'(t) = -\mathscr{H}_x'(\hat{x}(t), \hat{y}(t), \hat{u}(t), \lambda_f(t), \lambda_g(t), \ell_0)^\top - s_x'(\hat{x}(t))^\top \mu'(t),$$

and at every point of discontinuity $t \in (t_0, t_f)$, λ_f satisfies the jump condition

$$\lambda_f(t) - \lambda_f(t-) = -s_x'(\hat{x}(t))^\top (\mu(t) - \mu(t-)),$$

where $\lambda_f(t-)$ and $\mu(t-)$ denote the left-sided limits at t.

Further local minimum principles for smooth problems with mixed control-state constraints and a combination of pure state constraints and mixed control-state constraints are derived in [46, Theorem 3.2].

A weak (or local) minimum principle for non-smooth optimal control problems with mixed control-state constraints and semi-explicit DAEs is proved in [33, Theorems 3.1,3.2].

A constructive way to prove a local minimum principle for higher index DAEs by means of first-order approximations using adjoint equations is described in [93, 94].

Remark 3.1 The local minimum principle contains some hidden index reduction which is visible in the Hamilton function through the term $g_x' f$.

This raises the question whether an analog local minimum principle holds for the Hamilton function

$$\tilde{\mathscr{H}}(x, y, u, \lambda_f, \lambda_g, \ell_0) := \ell_0 f_0(x, y, u) + \lambda_f^\top f(x, y, u) + \lambda_g^\top g(x) \,?$$

Using $\tilde{\mathscr{H}}$ instead of $\mathscr{H}$ in Theorem 3.3 yields the so-called formal necessary conditions. In general, these conditions do not constitute necessary optimality conditions, hence the terminology "formal necessary condition" is used. However, there are cases where the formal necessary conditions are actually necessary optimality conditions and can be related to the true necessary conditions, compare [70] for details in the linear case.

3.2 A Global (or Strong) Minimum Principle

In contrast to the local (or weak) minimum principle, the global minimum principle (or strong minimum principle) states necessary conditions for a strong local minimum $\hat{z}$ of J, which means that $\hat{z} = (\hat{x}, \hat{y}, \hat{u})$ minimizes J w.r.t. to all feasible $z = (x, y, u)$ with $\|x - \hat{x}\|_\infty < \varepsilon$ for some $\varepsilon > 0$. This neighborhood is comparatively large, as the distances of u and y to $\hat{u}$ and $\hat{y}$ are not taken into account explicitly. This allows to relax the assumptions on the control set $\mathscr{U}$, which in the sequel is merely supposed to be a bounded measurable subset of $\mathbb{R}^{n_u}$. $\mathscr{U}$ may even be a discrete set.

The following theorem is taken from [48, Theorem 7.1.6] and applies to OCP-SE without pure state constraints. An analog result holds for semi-explicit index-1 problems, see [52, Theorem 9.7]. Similar results are obtained in [97, Propositions 2–4] for semi-explicit Hessenberg DAEs up to index 3. The proof technique in [97] applies the minimum principle from ODE theory to the underlying ODE of the Hessenberg DAEs, while the proof technique in [48, 52] exploits a variable time transformation technique in combination with the local minimum principle.

Theorem 3.4 (Global Minimum Principle) *Let $(\hat{x}, \hat{y}, \hat{u})$ be a strong local minimum of OCP-SE (without pure state constraints $s(x(t)) \leq 0$). Let Assumption 3.2 be valid and let the functions in OCP-SE be sufficiently regular, see [48, Assumption 2.2.8].*

Then there exist multipliers

$$\ell_0 \in \mathbb{R},\ \lambda_f \in W^{1,\infty}(I, \mathbb{R}^{n_x}),\ \lambda_g \in L^\infty(I, \mathbb{R}^{n_y}),\ \zeta \in \mathbb{R}^{n_y},\ \sigma \in \mathbb{R}^{n_\psi}$$

such that the following conditions are satisfied:

(a) $\ell_0 \geq 0$, $(\ell_0, \zeta, \sigma, \lambda_f, \lambda_g) \neq 0$

(b) Adjoint equations: Almost everywhere in I we have

$$\begin{aligned} \lambda_f'(t) &= -\mathscr{H}_x'(\hat{x}(t), \hat{y}(t), \hat{u}(t), \lambda_f(t), \lambda_g(t), \ell_0)^\top, \\ 0 &= \mathscr{H}_y'(\hat{x}(t), \hat{y}(t), \hat{u}(t), \lambda_f(t), \lambda_g(t), \ell_0)^\top. \end{aligned}$$

(c) Transversality conditions:

$$\begin{aligned} \lambda_f(t_0)^\top &= -\left(\ell_0 \varphi_{x_0}'(\hat{x}(t_0), \hat{x}(t_f)) + \sigma^\top \psi_{x_0}'(\hat{x}(t_0), \hat{x}(t_f)) + \zeta^\top g_x'(\hat{x}(t_0))\right), \\ \lambda_f(t_f)^\top &= \ell_0 \varphi_{x_f}'(\hat{x}(t_0), \hat{x}(t_f)) + \sigma^\top \psi_{x_f}'(\hat{x}(t_0), \hat{x}(t_f)). \end{aligned}$$

(d) Optimality condition: Almost everywhere in I we have

$$\mathscr{H}(\hat{x}(t), \hat{y}(t), \hat{u}(t), \lambda_f(t), \lambda_g(t), \ell_0) \leq \mathscr{H}(\hat{x}(t), y, u, \lambda_f(t), \lambda_g(t), \ell_0)$$

for all $(u, y) \in \Omega(\hat{x}(t))$, where

$$\Omega(x) = \{(u, y) \in \mathscr{U} \times \mathbb{R}^{n_y} \mid g_x'(x) f(x, y, u) = 0\}.$$

(e) The Hamilton function is constant with respect to time:

$$\mathscr{H}(\hat{x}(t), \hat{y}(t), \hat{u}(t), \lambda_f(t), \lambda_g(t), \ell_0) \equiv const.$$

Note that the stationarity condition (3.7) in the local minimum principle can be seen as a necessary condition for the optimality condition (d) in the global minimum principle (if $\mathscr{U}$ is convex). Hence, the global minimum principle is a much stronger statement as it requires global minimality of the Hamilton function on Ω. The set $\Omega(x)$ contains feasible controls and algebraic variables that obey not only the explicit control constraints $u \in \mathscr{U}$ but also the hidden algebraic constraint $g'_x(x)f(x, y, u) = 0$.

The minimization on the set Ω is essential and it was observed in [34, Example, page 495] that a global minimum principle without this restriction may fail to hold, while a local minimum principle still holds, see [34, Theorem 3.2]. A global minimum principle for non-smooth optimal control problems was obtained in [34, Theorem 3.1] under a convexity assumption for the velocity set of a semi-explicit index-1 DAE.

In [36] a global minimum principle is derived for optimal control problems subject to implicit differential inequalities and control and state constraints under an analog of the Mangasarian-Fromowitz constraint qualification.

3.3 *Indirect Methods and Boundary Value Problems*

The indirect approach for optimal control problems is based on the semi-analytic exploitation of the necessary optimality conditions and its transformation to a multi-point boundary value problem. For simplicity we neglect state constraints in order to illustrate the basic approach and discuss an example first.

Example 3.5 Let constants $\alpha_1, \ldots, \alpha_4 > 0$ be given.

Minimize

$$\alpha_1 x_1(1)^2 + \alpha_2(x_2(1) + 1)^2 + \int_0^1 \alpha_3 u(t)^2 + \alpha_4 x_1(t)^2 \, dt$$

subject to the constraints

$$\begin{aligned} x_1'(t) &= u(t) - y(t), & x_1(0) &= 0, \\ x_2'(t) &= u(t), & x_2(0) &= 1, \\ x_3'(t) &= -x_2(t), & x_3(0) &= 0, \\ 0 &= x_1(t) + x_3(t). \end{aligned}$$

Differentiation of the algebraic constraint yields $0 = u(t) - y(t) - x_2(t)$ and the DAE has index two. The Hamilton function (with $\ell_0 = 1$, $x = (x_1, x_2, x_3)^\top$, $\lambda_f = (\lambda_1, \lambda_2, \lambda_3)^\top$) is defined by

$$\mathscr{H}(x, y, u, \lambda_f, \lambda_g, \ell_0) = \alpha_3 u^2 + \alpha_4 x_1^2 + \lambda_1(u - y) + \lambda_2 u - \lambda_3 x_2 + \lambda_g(u - y - x_2).$$

Let $(\hat{x}, \hat{u})$ be a local minimum. Then the local minimum principle in Theorem 3.3 yields the conditions

$$
\begin{aligned}
0 &= \mathscr{H}'_u = 2\alpha_3 \hat{u} + \lambda_1 + \lambda_2 + \lambda_g, && \\
\lambda_1' &= -\mathscr{H}'_{x_1} = -2\alpha_4 \hat{x}_1, && \lambda_1(1) = 2\alpha_1 \hat{x}_1(1), \\
\lambda_2' &= -\mathscr{H}'_{x_2} = \lambda_3 + \lambda_g, && \lambda_2(1) = 2\alpha_2(\hat{x}_2(1) + 1), \\
\lambda_3' &= -\mathscr{H}'_{x_3} = 0, && \lambda_3(1) = 0, \\
0 &= \mathscr{H}'_y = -\lambda_1 - \lambda_g. &&
\end{aligned}
$$

The first equation can be solved for $\hat{u}$:

$$
\hat{u} = -\frac{1}{2\alpha_3}\left(\lambda_1 + \lambda_2 + \lambda_g\right).
$$

Introducing this expression into the DAE yields the following optimality system, which is a linear DAE boundary value problem with the index-2 algebraic variable $\hat{y}$ and the index-1 variable λ_g:

$$
\begin{aligned}
\hat{x}_1' &= -\frac{1}{2\alpha_3}\left(\lambda_1 + \lambda_2 + \lambda_g\right) - \hat{y}, && \hat{x}_1(0) = 0, \\
\hat{x}_2' &= -\frac{1}{2\alpha_3}\left(\lambda_1 + \lambda_2 + \lambda_g\right), && \hat{x}_2(0) = 1, \\
\hat{x}_3' &= -\hat{x}_2, && \hat{x}_3(0) = 0, \\
\lambda_1' &= -2\alpha_4 \hat{x}_1, && \lambda_1(1) = 2\alpha_1 \hat{x}_1(1), \\
\lambda_2' &= \lambda_3 + \lambda_g, && \lambda_2(1) = 2\alpha_2(\hat{x}_2(1) + 1), \\
\lambda_3' &= 0, && \lambda_3(1) = 0, \\
0 &= \hat{x}_1 + \hat{x}_3, && \\
0 &= -\lambda_1 - \lambda_g. &&
\end{aligned}
$$

In this case the linear BVP can be solved analytically, and we leave the details to the reader. In general, however, the BVP will be nonlinear and numerical methods are required to solve it. Observe that the index of the overall optimality system is still 2 with y being the index-2 algebraic variable and λ_g being an index-1 algebraic variable. □

The key step in Example 3.5 was to express the control $\hat{u}$ not as a function of time but in feedback form $\hat{u} = u(\hat{x}, \hat{y}, \lambda_f, \lambda_g, \ell_0)$ (with $\ell_0 = 1$). Typically, this feedback form is obtained by solving the stationarity condition

$$
\mathscr{H}'_u(\hat{x}, \hat{y}, \hat{u}, \lambda_f, \lambda_g, \ell_0) = 0
$$

for $\hat{u}$, which is possible according to the implicit function theorem, if the Hessian matrix $\mathscr{H}''_{uu}$ is uniformly positive definite along the optimal solution. Note that the introduction of $\hat{u} = u(\hat{x}, \hat{y}, \lambda_f, \lambda_g, \ell_0)$ into the state and adjoint DAEs might change the index of these equations. Hence, it makes sense to consider and to analyze the overall optimality system as a coupled DAE with the additional algebraic constraint $\mathscr{H}'_u \equiv 0$ and u being the corresponding algebraic variable, see e.g., [9, 10, 67] for optimality systems arising in linear-quadratic optimal control problems.

If $\mathscr{H}'_u \equiv 0$ cannot be solved for u, the situation is more complicated. We illustrate the complications by a modification of Example 3.5.

Example 3.6 Consider again the optimal control problem in Example 3.5, but assume that $\alpha_3 = 0$.

In this case, we need to add constraints on u in order to obtain a meaningful optimization problem. So, suppose u is bound to the set

$$\mathscr{U} := [u_{min}, u_{max}] \qquad (u_{min} < u_{max}).$$

The global minimum principle in Theorem 3.4 states that the optimal control $\hat{u}$ minimizes the Hamilton function on the set

$$\Omega(\hat{x}(t)) = \{(u, y) \mid u \in [u_{min}, u_{max}], u - y - \hat{x}_2(t) = 0\}$$

for a.e. t. Minimizing the Hamilton function on $\Omega(\hat{x}(t))$ (observe $u - y = \hat{x}_2(t)$) yields:

$$\hat{u}(t) = \begin{cases} u_{min}, & \text{if } \lambda_2(t) > 0, \\ u_{max}, & \text{if } \lambda_2(t) < 0, \\ \text{singular}, & \text{if } \lambda_2(t) = 0 \text{ in some interval } [t_1, t_2] \text{ with } t_1 < t_2 \end{cases}$$

This determines the optimal control in feedback form, i.e., as a function of the adjoint λ_2. In the singular case we obtain the algebraic constraint $\lambda_2(t) = 0$ on the interval $[t_1, t_2]$. Differentiation yields $0 = \lambda_3(t) + \lambda_g(t)$. Since $\lambda_3 \equiv 0$ and $\lambda_g = -\lambda_1$ we find $\lambda_1(t) = 0$. Differentiation implies $\hat{x}_1(t) = 0$ and another differentiation yields $0 = \hat{u}(t) - \hat{y}(t) = \hat{x}_2(t)$ on $[t_1, t_2]$. By differentiation the latter holds if $\hat{u}(t) = 0$ on $[t_1, t_2]$, i.e., the control is zero on singular arcs. In order to obtain this singular control law on the interval $[t_1, t_2]$, we needed 4 differentiations of the algebraic constraint $\lambda_2 = 0$ and some algebraic manipulations to finally obtain the condition $\hat{u} = 0$ on $[t_1, t_2]$. Hence, the (differentiation) index is five on a singular subarc. On non-singular subarcs, $\hat{u}$ is explicitly given by u_{min} or u_{max}. Introducing this into the state DAE and the adjoint DAE yields a DAE of index two on non-singular subarcs, with y being the index-two algebraic variable and λ_g being the index-one algebraic variable, but an index-5 DAE on singular subarcs. □

Example 3.6 illustrates the difficulties that arise in the presence of control or state constraints. It is easy to imagine that the situation can be very involved if many control or state constraints are present in a nonlinear problem. Moreover, we have analyzed singular and non-singular arcs in Example 3.6, but we still do not know the time intervals on which the constraints are active or inactive/singular. Singular arcs may not even exist in Example 3.6. Apparently, singular subarcs cannot occur in Example 3.6 if $0 \notin [u_{min}, u_{max}]$.

In general a good intuition, a sound knowledge of the underlying physical problem, or good homotopy methods, see [35], are needed to recognize the switching structure of the optimal solution, i.e., the sequence of active, inactive, or singular arcs of the inequality constraints. On active arcs the optimality system can be interpreted as a DAE which consists of the original DAE, the adjoint DAE, the active control-state constraint (viewed as an algebraic equation), and the stationarity condition $\mathscr{H}_u' = 0$ (if $\mathscr{U} = \mathbb{R}^{n_u}$). Herein, the control vector u and the multipliers for the constraints serve as algebraic variables. On inactive arcs the optimality system can be viewed as a DAE as well but without the algebraic constraints resulting from the active inequality constraints. Hence, the overall optimality system can be viewed as a piecewise defined DAE with appropriate coupling conditions at the junction points of the different arcs. The index of the piecewise defined DAE may switch at the junction points. The overall system is a multi-point DAE boundary value problem. Its numerical solution requires a very good initial guess for the switching structure and the adjoints. For complicated problems this is hard to realize and for that reason other methods like direct discretization methods or function space methods are usually preferred. Note that also for the simpler problems in [8, 80] it may happen, that the overall optimality DAE fails to have index one around the solution, see e.g., [80, Example 11.19, Sect. 11.3].

A detailed overview on collocation methods and shooting methods for boundary value problems is provided by the monographs [6] and [68, Chap. 7]. Collocation methods for DAE boundary value problems can be found in [7, 65, 71, 73, 104]. Shooting methods are discussed in [72, 78, 79]. A parallel multiple shooting algorithm is developed in [63]. A damped Newton method and finite difference approximations are used in [13] to solve the BVP, which is formulated for mechanical multi-body systems using symbolic computations. [100] use a piecewise defined boundary value problem to solve optimal control problems with miniaturized manipulators. An algorithm for 2-point boundary value problems arising in economic problems with an infinite time horizon is discussed in [74].

4 Direct Discretization Methods for DAE Optimal Control Problems

Direct discretization methods have a long tradition in solving optimal control problems subject to ODEs and many extensions to DAEs exist as well, see, e.g., [12, 17, 20, 25, 27, 39, 40, 57, 64, 84, 88, 90–92, 95, 102, 103, 111]. Direct discretization methods can be grouped into collocation methods, compare [14, 60, 112], and direct (single or multiple) shooting methods, see, e.g., [19,23,44,53,105]. Both approaches have in common that the infinite dimensional optimal control problem is discretized and transformed into a finite dimensional nonlinear optimization problem. The approaches differ in the way the optimal control problem is discretized. Depending on the discretization the resulting optimization problems exhibit a small but dense structure or a large-scale but sparse structure. The sparse structure needs to be exploited in order to obtain an efficient numerical method. We do not focus on these algorithmic details since state-of-the-art nonlinear programming solvers are able to handle all these issues.

Consider the following optimal control problem on $I = [t_0, t_f]$ and note that more general problems like in Problem 1.1 can be transformed to this form by standard techniques.

Problem 4.1 Minimize

$$\varphi(x(t_0), x(t_f))$$

subject to the constraints

$$\begin{aligned} F(t, x(t), x'(t), u(t)) &= 0 && \text{a.e. in } I, \\ c(t, x(t), u(t)) &\leq 0 && \text{a.e. in } I, \\ \psi(x(t_0), x(t_f)) &= 0. \end{aligned}$$

4.1 The Full Discretization (Full Transcription)

Define the (for simplicity) equidistant grid

$$\mathbb{G}_N := \{t_i \mid t_i = t_0 + ih, i = 0, 1, \ldots, N\} \qquad (N \in \mathbb{N}),$$

with step-size $h = (t_f - t_0)/N$ and approximate the DAE on $\mathbb{G}_N$ by a suitable discretization method. Essentially any suitable discretization scheme for DAEs can be used for discretization, see [21, 58, 59] for an overview on BDF methods and Runge–Kutta methods. For notational simplicity we use the implicit Euler method

$$F\left(t_{i+1}, x_{i+1}, \frac{x_{i+1} - x_i}{h}, u_{i+1}\right) = 0, \qquad i = 0, 1, \ldots, N-1, \tag{4.1}$$

with approximations $x_i \approx x(t_i)$, $i = 0, \ldots, N$, and $u_i \approx u(t_i)$, $i = 1, \ldots, N$.

If the initial value x_0 is not fixed but contains degrees of freedom that are to be exploited in the optimization, a procedure is necessary to ensure consistency of the initial value. Consistent initial values can be achieved numerically, e.g., by adding algebraic constraints and hidden constraints at x_0 explicitly to the discretized problem, by projection, see [49] or [48, Sect. 4.5.1], or by relaxation, see [103] or [48, Sect. 4.5.2]. Alternate methods have been suggested by [5, 22, 28, 54, 82, 89].

The projection method projects a possibly inconsistent initial value x_0 onto algebraic constraints and yields a consistent value $\tilde{x}_0 = X_0(x_0, u_h)$ with a differentiable function X_0 and the control parameterization $u_h = (u_1, \ldots, u_N)^\top$. We impose the constraint $x_0 = X_0(x_0, u_h)$ to ensure that x_0 in the optimal solution is actually consistent. For semi-explicit Hessenberg-DAEs the function X_0 can be realized by solving a least squares problem.

In contrast to the projection method, the relaxation technique does not modify the initial value x_0 within each iteration of the numerical procedure to solve the optimization problem but instead it modifies the DAE such that x_0 becomes consistent for the modified DAE. Therefore additional consistency constraints have to be added to the optimization problem to ensure equivalence of the original DAE and the modified DAE in the optimal solution. This technique is mainly used in shooting methods.

An approximation of Problem 4.1 with the projection method for consistent initialization then reads as follows:

Problem 4.2 (DOCP) Minimize

$$\varphi(x_0, x_N)$$

with respect to $x_h := (x_0, \ldots, x_N)^\top$ and $u_h := (u_1, \ldots, u_N)^\top$ subject to the constraints (4.1) and

$$\begin{aligned} x_0 - X_0(x_0, u_h) &= 0, \\ c(t_i, x_i, u_i) &\leq 0, \qquad\qquad i = 0, \ldots, N, \text{ with } u_0 := u_1, \\ \psi(x_0, x_N) &= 0. \end{aligned}$$

DOCP is a finite dimensional optimization problem of type NLP, which is large-scale but exhibits a sparse structure in the Jacobian of the constraints and the Hessian matrix of the Lagrange function. It can be solved by any optimization method that is able to handle large-scale and sparse structures. The most frequently used paradigms are sequential quadratic programming (SQP), interior-point methods, or multiplier methods. The sparsity patterns have to be exploited in the computation of derivatives and on linear algebra level, where linear equations with saddle point matrices (KKT matrices) need to be solved, compare [14] or [102] for a reduced SQP method.

The accuracy of the solution of DOCP can be increased by grid refinement techniques. These techniques often use the local discretization error of the discretization (implicit Euler in our case) to measure accuracy, compare [15]. A grid refinement strategy conceptionally works as follows:

Algorithm 4.3 (Full Discretization Method)

(0) Init: Choose $N \in \mathbb{N}$, $tol > 0$.
(1) Solve DOCP by a suitable optimization method.

(2) Estimate the local discretization error of the discrete solution.
(3) If the local discretization error is less than *tol*, STOP.
(4) Refine the grid based on the local discretization error and go to (1) with the refined grid.

It was observed in [17, 39] that full discretization methods are often able to solve constrained optimal control problems whose index on active state constraints, if viewed as a DAE, is high (in other words: the order of the state constraint is high). An example is a state constrained optimal control problem subject to a method-of-lines discretization of a heat conduct equation, where the index on active arcs depends on the PDE discretization parameters and can be arbitrarily high. Full discretization methods are still able to solve such problems. This effect was analyzed further in [27, 64]. It is argued that shooting methods are likely to fail in this case. This is certainly true, if one attempts to solve the high index DAE on active arcs explicitly, which can be the case in the classic indirect method. Direct shooting methods, however, would not do this, since they work with discretized state constraints as well and impose them as inequality constraints in the optimization problem. Hence, direct shooting methods are able to solve many problems with higher order state constraints as well.

4.2 The Reduced Discretization (Direct Shooting Methods)

The reduced discretization approach (or shooting method) aims to reduce the size of Problem DOCP by elimination of the equations in (4.1) from DOCP. Suppose Eq. (4.1) can be solved for x_{i+1} step by step. This is guaranteed by the implicit function theorem (provided a solution exists), if the so-called iteration matrix

$$F'_x + \frac{1}{h} F'_{x'}$$

is non-singular (this requires regular local pencils). By solving the equations step by step we obtain

$$\begin{aligned}
\tilde{x}_0 &= X_0(x_0, u_h), \\
x_1 &= \bar{X}_1(\tilde{x}_0, u_1) = \bar{X}_1(X_0(x_0, u_h), u_1) =: X_1(x_0, u_h), \\
&\vdots \\
x_{i+1} &= \bar{X}_{i+1}(x_i, u_{i+1}) = \bar{X}_{i+1}(X_i(x_0, u_h), u_{i+1}) =: X_{i+1}(x_0, u_h), \\
&\vdots \\
x_N &= X_N(x_0, u_h),
\end{aligned}$$

where the value x_0 is projected onto a consistent initial value $\tilde{x}_0$ using the function X_0. Clearly, solving Eq. (4.1) in the above way is just the single shooting idea, where the initial value problem $F(t, x(t), x'(t), u(t)) = 0$, $x(t_0) = \tilde{x}_0$ is solved by the implicit Euler method for a consistent initial value $\tilde{x}_0$. In case of unique solvability the solution will depend on the initial value and the control input only. That is what the functions $X_i(x_0, u_h)$ indicate.

Additional intermediate shooting nodes could be introduced in order to obtain a multiple shooting method but we prefer to focus on the single shooting case for simplicity and leave the details to the reader.

Introducing the implicitly defined values $x_i = X_i(x_0, u_h)$ into DOCP yields an optimization problem of reduced size with considerably fewer constraints and optimization variables.

Problem 4.4 (R-DOCP) Minimize

$$\varphi(X_0(x_0, u_h), X_N(x_0, u_h))$$

with respect to $z := (x_0, u_h)^\top$, $u_h = (u_1, \dots, u_N)^\top$ subject to the constraints

$$\begin{aligned} c(t_i, X_i(x_0, u_h), u_i) &\le 0, \qquad i = 0, \dots, N,, \text{ with } u_0 := u_1, \\ \psi(X_0(x_0, u_h), X_N(x_0, u_h)) &= 0. \end{aligned}$$

Let

$$\begin{aligned} J(z) &:= \varphi(X_0(z), X_N(z)), \\ H(z) &:= \psi(X_0(z), X_N(z)), \\ G(z) &:= \begin{pmatrix} c(t_0, X_0(z), u_1) \\ c(t_1, X_1(z), u_1) \\ \vdots \\ c(t_N, X_N(z), u_N) \end{pmatrix}. \end{aligned}$$

With these definitions R-DOCP fits into the problem class NLP. Compared to DOCP the reduced problem R-DOCP is comparatively small but it has a dense structure (apart from some minor sparsity introduced by control approximations with local support). Hence standard nonlinear programming methods using dense linear algebra are sufficient to solve R-DOCP. However, most nonlinear programming solvers require to evaluate the gradient of the objective function $J'(z^k)$ and the Jacobians of the constraints $H'(z^k)$ and $G'(z^k)$ at some intermediate iterate z^k. These derivatives can be computed in various ways. A simple but often inefficient and inaccurate approach is to use finite difference approximations.

Instead the expressions

$$J'(z^k) = \varphi'_{x_0}[z^k] X'_0(z^k) + \varphi'_{x_f}[z^k] X'_N(z^k),$$

$$H'(z^k) = \psi'_{x_0}[z^k]X'_0(z^k) + \psi'_{x_f}[z^k]X'_N(z^k),$$

$$G'(z^k) = \begin{pmatrix} c'_x[t_0]X'_0(z^k) + c'_u[t_0]\frac{\partial u_1(z^k)}{\partial z} \\ c'_x[t_1]X'_1(z^k) + c'_u[t_1]\frac{\partial u_1(z^k)}{\partial z} \\ \vdots \\ c'_x[t_N]X'_N(z^k) + c'_u[t_N]\frac{\partial u_N(z^k)}{\partial z} \end{pmatrix},$$

are useful, where the notations $[z^k]$ and $[t_i]$ indicate that the respective functions are evaluated at $X_i(z^k)$ and at the grid points t_i, $i = 0, \ldots, N$. Herein, it is convenient to view the control value u_i as a function of z^k, i.e., $u_i = u_i(z^k)$. The sensitivities $S_i := X'_i(z^k)$, $i = 0, 1, \ldots, N$ need to be computed. That is, the numerical solution of the initial value problem needs to be differentiated w.r.t. the optimization vector z. This can be achieved by internal numerical differentiation (IND), compare [18]. The idea is to differentiate the numerical discretization scheme w.r.t. the optimization variables. Application of this idea to the implicit Euler discretization in (4.1) yields the linearized equations

$$\left(F'_x[z^k] + \frac{1}{h}F'_{x'}[z^k]\right) X'_{i+1}(z^k) - \frac{1}{h}F'_{x'}[z^k]X_i(z^k) + F'_u[z^k]\frac{\partial u_{i+1}(z^k)}{\partial z} = 0$$

for $i = 0, 1, \ldots, N-1$. The IND approach coincides with the sensitivity equation approach, if the sensitivity equation (or variational equation)

$$F'_x[t]S(t) + F'_{x'}[t]S'(t) + F'_u[t]\frac{\partial u(t; z^k)}{\partial z} = 0$$

with a control parameterization $u = u(t; z^k)$ (e.g., a B-spline representation) is discretized by the same numerical method with the same step-sizes as for the nonlinear DAE $F(t, x(t), x'(t), u(t; z^k)) = 0$. Extensions of this approach can be found in [11, 30, 41, 86]. These numerical procedures often re-use the iteration matrix $F'_x + \frac{1}{h}F'_{x'}$ for several integration steps in order to save computation time. A drawback of these sensitivity equation approaches is that the dimension of the sensitivity matrix $S_i = X'_i(z^k)$ grows with the dimension of the optimization vector z. Hence, the approach is not very efficient if many optimization variables but few constraints are present.

In this case the adjoint equation approach in [29] is more efficient. Herein, an adjoint equation has to be solved for each constraint of the optimization problem. The dimension of the adjoint equation does not depend on the number of optimization variables and hence the adjoint equation approach is more efficient if few constraints but many optimization variables are present. The adjoint method for gradient computations will be used in Sect. 5.1 to compute the gradient of a reduced objective functional in a projected gradient method.

Finally, an accurate and efficient approach with provable efficiency bounds is to use tools from algorithmic differentiation in combination with checkpointing strategies, compare [55, 56]. Checkpointing is a way to reduce the storage requirements. Note that the adjoint equation requires either to store the state at all grid points or to recompute it whenever it is needed in the adjoint system. The idea of a checkpointing strategy is to introduce a suitable number of intermediate time points at which the state is stored and from which the state is recomputed by forward integration if the state is needed by the adjoint scheme at intermediate time points. This technique allows to balance storage requirements and computing effort.

The following numerical experiments illustrate the reduced discretization approach. We used the software OCPID-DAE1 by the author, which is available for academic use on the webpage http://www.optimal-control.de\.

Example 4.5 We revisit Example 3.5:

Minimize

$$\alpha_1 x_1(1)^2 + \alpha_2(x_2(1)+1)^2 + \int_0^1 \alpha_3 u(t)^2 + \alpha_4 x_1(t)^2\,dt$$

subject to the constraints

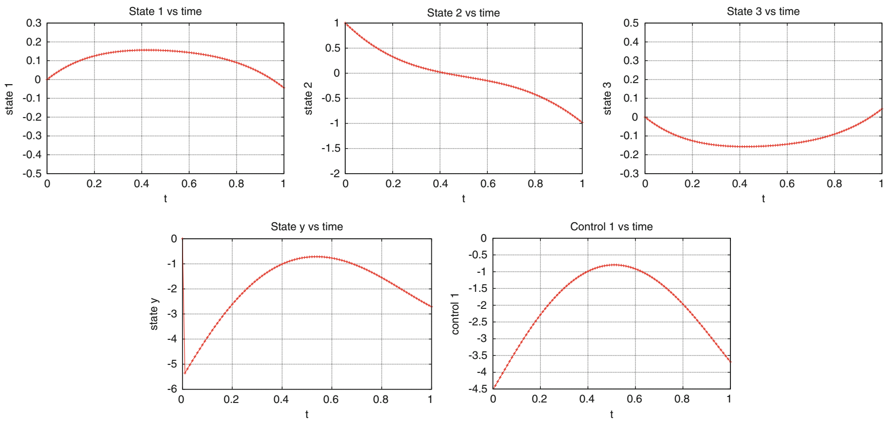
$$\begin{aligned}
x_1'(t) &= u(t) - y(t), & x_1(0) &= 0,\\
x_2'(t) &= u(t), & x_2(0) &= 1,\\
x_3'(t) &= -x_2(t), & x_3(0) &= 0,\\
0 &= x_1(t) + x_3(t).
\end{aligned}$$

The direct (single) shooting method with tolerance $tol = 10^{-8}$, $\alpha_1 = \alpha_2 = \alpha_4 = 1$, $\alpha_3 = 0.5 \cdot 10^{-2}$, $N = 100$, and initial guess $u_h^0 \equiv -3$ produces the following iterates:

```
=== sqpfiltertoolbox  (C) MATTHIAS GERDTS, UNIVERSITAET DER BUNDESWEHR   ====
-----------------------------------------------------------------------------
ITER    QPIT   ALPHA                OBJ                   CV           KKT
-----------------------------------------------------------------------------
0        0    0.0000E+00      0.1328333044250002E+01   0.0000E+00   0.3103E-01
1        1    0.1000E+01      0.1261996137706250E+01   0.0000E+00   0.3018E-01
2        1    0.1000E+01      0.9645290326151866E+00   0.0000E+00   0.2600E-01
3        1    0.1000E+01      0.1626445121083435E+00   0.0000E+00   0.7893E-02
4        1    0.1000E+01      0.5933569494404990E-01   0.0000E+00   0.1340E-02
5        1    0.1000E+01      0.5929137763126855E-01   0.0000E+00   0.1340E-02
...
74       1    0.1000E+01      0.4105117130358388E-01   0.0000E+00   0.2923E-07
75       1    0.1000E+01      0.4105117130166638E-01   0.0000E+00   0.2956E-07
76       1    0.1000E+01      0.4105117129766830E-01   0.0000E+00   0.2720E-07
77       1    0.1000E+01      0.4105117129130897E-01   0.0000E+00   0.1935E-07
78       1    0.1000E+01      0.4105117128571807E-01   0.0000E+00   0.8277E-08
=============================================================================
END OF SQP METHOD
=============================================================================
KKT CONDITIONS SATISFIED TO THE REQUESTED ACCURACY (IER=          0 )!
```

The column “ITER” shows the major iteration index of a filter and linesearch SQP method, “QPIT” indicates the iterations needed to solve a linear-quadratic optimization problem within each major iteration, “ALPHA” is the step-size used in a globalization procedure, “OBJ” is the objective function value, “CV” denotes the constraint violation, and “KKT” contains the error in the optimality conditions (KKT condition).

The Following Pictures Show The Converged Solution Of The Direct Shooting Method: □



Example 4.6 We revisit Example 3.5 with additional control constraints and $\alpha_3 > 0$:

Minimize

$$\alpha_1 x_1(1)^2 + \alpha_2(x_2(1)+1)^2 + \int_0^1 \alpha_3 u(t)^2 + \alpha_4 x_1(t)^2 \, dt$$

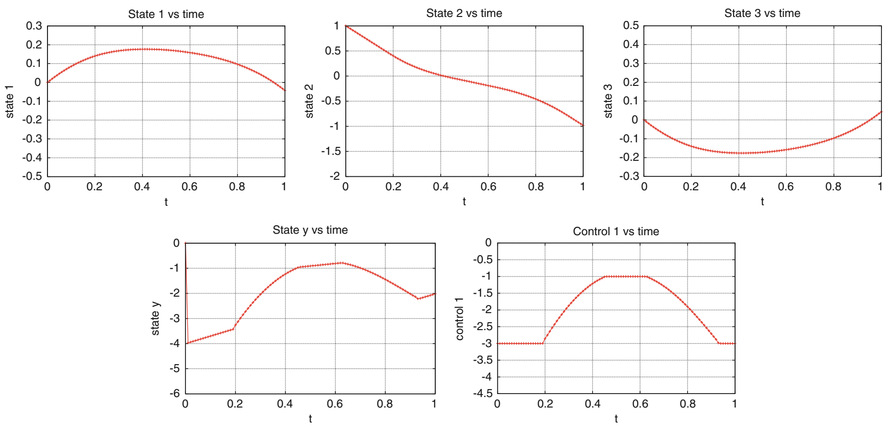
subject to the constraints

$$\begin{aligned}
x_1'(t) &= u(t) - y(t), & x_1(0) &= 0,\\
x_2'(t) &= u(t), & x_2(0) &= 1,\\
x_3'(t) &= -x_2(t), & x_3(0) &= 0,\\
0 &= x_1(t) + x_3(t), & &\\
u(t) &\in [-3, -1]. & &
\end{aligned}$$

The direct (single) shooting method with optimality and feasibility tolerance $tol = 10^{-8}$, $\alpha_1 = \alpha_2 = \alpha_4 = 1$, $\alpha_3 = 0.5 \cdot 10^{-2}$, $N = 100$, and initial guess $u_h^0 \equiv -3$ produces the following iterates. Please note the high number 202 of QP iterations needed in iteration 1. The QP is being solved by a primal active set method and the high number of iterations indicates that the initial guess corresponds to an active set which is far away from the optimal active set. Hence, the QP needs quite a lot of iterations to identify the active constraints correctly.

```
=== sqpfiltertoolbox  (C) MATTHIAS GERDTS, UNIVERSITAET DER BUNDESWEHR   ====
-----------------------------------------------------------------------------
ITER    QPIT   ALPHA                  OBJ                   CV            KKT
-----------------------------------------------------------------------------
0         0    0.0000E+00     0.1328333044250002E+01   0.0000E+00   0.3103E-01
1       202    0.1000E+01     0.1261996137706250E+01   0.0000E+00   0.3018E-01
2         1    0.1000E+01     0.9645290326151866E+00   0.0000E+00   0.2600E-01
3         1    0.1000E+01     0.1626445121083435E+00   0.0000E+00   0.7893E-02
4         1    0.1000E+01     0.5933569494404990E-01   0.0000E+00   0.1340E-02
5         1    0.1000E+01     0.5929137763126855E-01   0.0000E+00   0.1340E-02
...
270       1    0.1000E+01     0.4202430002584630E-01   0.0000E+00   0.2972E-07
271       1    0.1000E+01     0.4202430002537009E-01   0.0000E+00   0.2943E-07
272       1    0.1000E+01     0.4202430002306404E-01   0.0000E+00   0.2807E-07
273       1    0.1000E+01     0.4202430001330967E-01   0.0000E+00   0.2154E-07
274       1    0.1000E+01     0.4202429999601267E-01   0.0000E+00   0.8365E-08
=============================================================================
END OF SQP METHOD
=============================================================================
KKT CONDITIONS SATISFIED TO THE REQUESTED ACCURACY (IER=           0 )!
```

The following pictures show the converged solution of the direct shooting method: □



Example 4.7 We revisit Example 3.6 and choose $\alpha_3 = 0$. In this case, the optimal solution is a bang–bang-solution and singular subarcs cannot appear owing to the box constraints for u.

Minimize

$$\alpha_1 x_1(1)^2 + \alpha_2(x_2(1)+1)^2 + \int_0^1 \alpha_3 u(t)^2 + \alpha_4 x_1(t)^2 \, dt$$

subject to the constraints

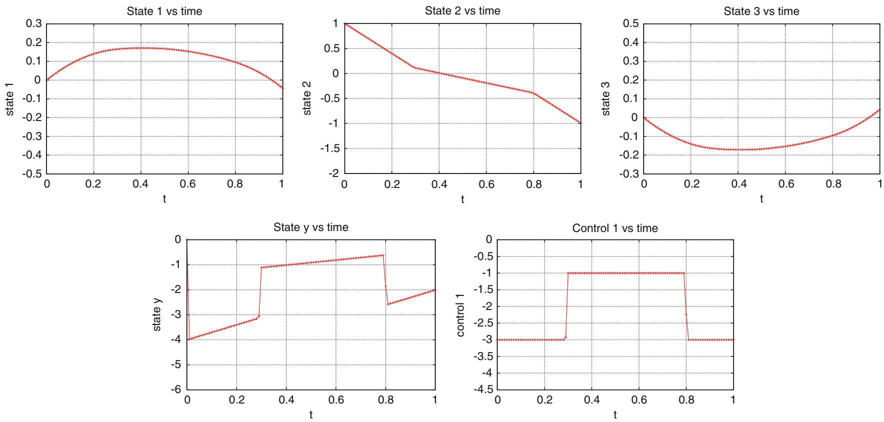
$$\begin{aligned} x_1'(t) &= u(t) - y(t), & x_1(0) &= 0, \\ x_2'(t) &= u(t), & x_2(0) &= 1, \\ x_3'(t) &= -x_2(t), & x_3(0) &= 0, \\ 0 &= x_1(t) + x_3(t), \\ u(t) &\in [-3, -1]. \end{aligned}$$

The direct (single) shooting method with optimality and feasibility tolerance $tol = 10^{-8}$, $\alpha_1 = \alpha_2 = \alpha_4 = 1$, $\alpha_3 = 0$, $N = 100$, and initial guess $u_h^0 \equiv -3$ produces the following iterates:

```
=== sqpfiltertoolbox  (C) MATTHIAS GERDTS, UNIVERSITAET DER BUNDESWEHR   ====
------------------------------------------------------------------------------
ITER    QPIT    ALPHA                    OBJ                  CV          KKT
------------------------------------------------------------------------------
0        0    0.0000E+00      0.1283333044250000E+01   0.0000E+00   0.3073E-01
1      202    0.1000E+01      0.1218503970294439E+01   0.0000E+00   0.2989E-01
2        1    0.1000E+01      0.9276782329801730E+00   0.0000E+00   0.2577E-01
3        1    0.1000E+01      0.1415878077993118E+00   0.0000E+00   0.7918E-02
4        1    0.1000E+01      0.3865667516225475E-01   0.0000E+00   0.1287E-02
5        1    0.1000E+01      0.3861717769109438E-01   0.0000E+00   0.1287E-02
...
437      1    0.1000E+01      0.1817325950042694E-01   0.0000E+00   0.3984E-05
438      1    0.1000E+01      0.1817323931406664E-01   0.0000E+00   0.3878E-05
439      1    0.1000E+01      0.1817314890395615E-01   0.0000E+00   0.3359E-05
440      1    0.1000E+01      0.1817290710543137E-01   0.0000E+00   0.1110E-05
441      1    0.1000E+01      0.1817287743385263E-01   0.0000E+00   0.2496E-10
==============================================================================
END OF SQP METHOD
==============================================================================
KKT CONDITIONS SATISFIED TO THE REQUESTED ACCURACY (IER=           0 )!
```

The following pictures show the converged solution of the direct shooting method: □

Finally, a more challenging problem with control and state constraints is discussed.



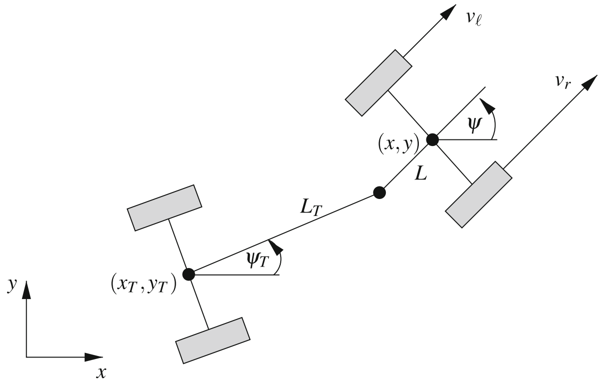


Fig. 1 Configuration of a vehicle and a trailer

Example 4.8 Consider a vehicle with two wheels and a trailer, which is attached to the vehicle, see Fig. 1.

Herein, (x, y) denotes the center of gravity of the vehicle, (x_T, y_T) the center of gravity of the trailer, ψ the yaw angle of the vehicle, ψ_T the yaw angle of the trailer, $B = 0.11$ the width of the vehicle and the trailer, $L = 0.1$ the distance of the center of gravity of the vehicle to the attachment point for the trailer, and $L_T = 0.2$ the distance of the center of gravity of the trailer to the attachment point of the vehicle. The velocities of the vehicle's wheels are denoted by v_ℓ (left) and v_r (right) and are subject to state constraints $v_\ell, v_r \in [-0.3, 0.3]$. The acceleration of each wheel of the vehicle can be controlled by controls u_ℓ and u_r subject to box constraints $u_\ell, u_r \in [-0.5, 0.5]$. The velocities of the wheels of the trailer serve as algebraic variables y_ℓ and y_r in the following optimal control problem. The task is to perform a reverse parking maneuver from a given initial position to a given terminal position in minimal time. This leads to the following optimal control problem.

Minimize t_f subject to the index-2 DAE

$$
\begin{aligned}
x'(t) &= \frac{v_\ell(t) + v_r(t)}{2} \cos \psi(t), \\
y'(t) &= \frac{v_\ell(t) + v_r(t)}{2} \sin \psi(t), \\
\psi'(t) &= \frac{v_r(t) - v_\ell(t)}{B}, \\
v_\ell(t) &= u_\ell(t), \\
v_r(t) &= u_r(t), \\
x_T'(t) &= \frac{y_\ell(t) + y_r(t)}{2} \cos \psi_T(t), \\
y_T'(t) &= \frac{y_\ell(t) + y_r(t)}{2} \sin \psi_T(t), \\
\psi_T'(t) &= \frac{y_r(t) - y_\ell(t)}{B}, \\
0 &= x_T(t) + L_T \cos \psi_T(t) - (x(t) - L \cos \psi(t)), \\
0 &= y_T(t) + L_T \sin \psi_T(t) - (y(t) - L \sin \psi(t)),
\end{aligned}
$$

the control and state constraints

$$u_\ell(t), u_r(t) \in [-0.5, 0.5], \qquad v_\ell(t), v_r(t) \in [-0.3, 0.3],$$

the initial conditions

$$x(0) = y(0) = \psi(0) = y_T(0) = \psi_T(0) = v_\ell(0) = v_r(0) = 0, x_T(0) = -0.3,$$

and the terminal conditions

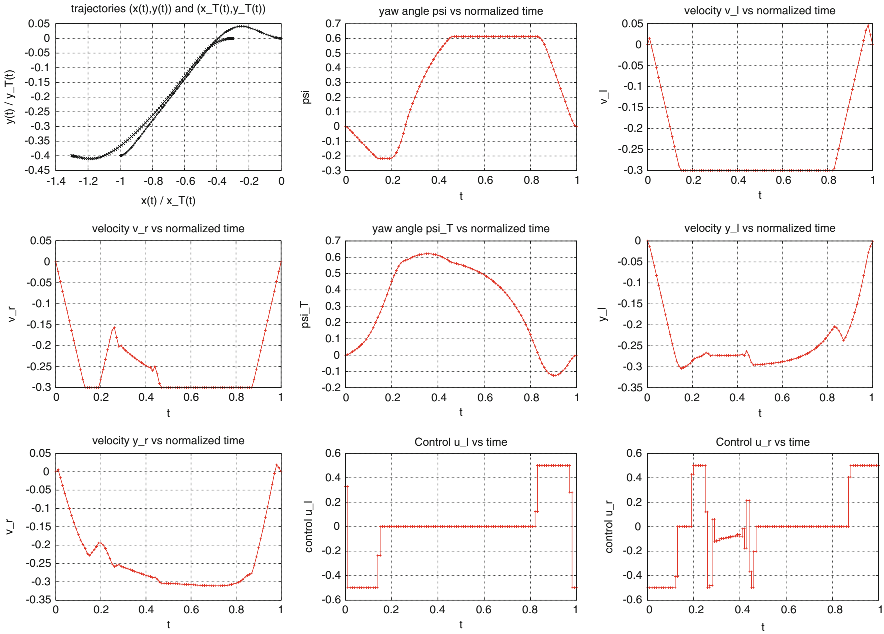
$$x(t_f) = -1, y(t_f) = -0.4, \psi(t_f) = v_\ell(t_f) = v_r(t_f)) = \psi_T(t_f) = 0.$$

The direct (single) shooting method with optimality and feasibility tolerance $tol = 10^{-8}$, $N = 100$, and initial guess $u_\ell, u_r \equiv -0.3$ produces the following iterates (note that the objective function was scaled by a factor of 10):

```
=== sqpfiltertoolbox  (C) MATTHIAS GERDTS, UNIVERSITAET DER BUNDESWEHR   ====
----------------------------------------------------------------------------
ITER     QPIT   ALPHA                      OBJ                  CV          KKT
----------------------------------------------------------------------------
0         0    0.0000E+00      0.4000000000000000E+02    0.9000E+00    0.1000E+02
1       503    0.1000E+01      0.4035136156884651E+02    0.1477E+00    0.4500E+01
2       323    0.1000E+01      0.4319188910480073E+02    0.1478E+00    0.6860E+01
3        38    0.1000E+01      0.4617600877472075E+02    0.5227E-01    0.6438E+01
4        78    0.1000E+01      0.4691915302534527E+02    0.5860E-02    0.2459E+01
```

```
5      111     0.1000E+01       0.4691471552645523E+02    0.1142E-03    0.2211E+01
...
298      8     0.1000E+01       0.4683007498066451E+02    0.3274E-09    0.1572E-06
299      5     0.1000E+01       0.4683007498043936E+02    0.2709E-09    0.3665E-07
300      7     0.1000E+01       0.4683007498037029E+02    0.5909E-09    0.3183E-07
301      7     0.1000E+01       0.4683007498046145E+02    0.2047E-09    0.5966E-08
==============================================================================
END OF SQP METHOD
==============================================================================
KKT CONDITIONS SATISFIED TO THE REQUESTED ACCURACY (IER=           0 )!
```

The following pictures show the converged solution of the direct shooting method on a normalized time scale. The final time amounts to $t_f \approx 4.683$: □



Direct discretization methods are frequently applied in model-predictive control, compare [37, 38], and extensions towards real-time optimal control by means of a parametric sensitivity analysis can be found in [24].

Direct discretization methods have been used successfully to solve mixed-integer optimal control problems with a partially discrete control set $\mathscr{U}$ in Problem 1.1. To this end the mixed-integer optimal control problem is either relaxed and combined with an appropriate rounding strategy as in [98, 99] or transformed by a time transformation technique as in [45, 81].

5 Function Space Methods

Function space methods apply solution methods in the same function spaces where the optimal control problem lives. This has the advantage that discretization errors are not introduced immediately. Moreover, structures of the optimal control problem can be exploited efficiently. However, a detailed functional analytic background is necessary to set up the methods and the analysis becomes particularly challenging in the presence of pure state constraints as the Lagrange multipliers are measures in this case. Function space methods are frequently used in PDE constrained optimal control, see the monographs [61, 62, 107] for the state-of-the-art in this field. However, function space methods are less frequently used in ODE or DAE constrained optimal control problems since these problems typically exhibit strong nonlinearities, non-convexity, and complicated state and control constraints. Direct discretization methods and especially the underlying state-of-the-art nonlinear programming solvers are able to handle these difficulties since they use sophisticated globalization strategies and measures to deal with inconsistencies, ill-conditioning, rank deficiencies etc. Without these additional measures, conceptual function space methods like gradient methods, interior-point methods, or sequential-quadratic programming (SQP) methods are often less robust for highly nonlinear problems. Nevertheless, they can perform very well for well-behaved problems. In order to illustrate the working principle of function space methods we discuss a gradient method and a Lagrange–Newton method.

5.1 Gradient Method

The gradient method and its extension, the projected gradient method, are the most simple gradient-based optimization methods for unconstrained problems or problems with sufficiently simple constraints like box constraints.

The projected gradient method is demonstrated for the following DAE optimal control problem subject to simple bounds, where $I := [t_0, t_f]$ is a compact interval, $\bar{x} \in \mathbb{R}^{n_x}$ is a given vector, $\varphi : \mathbb{R}^{n_x} \longrightarrow \mathbb{R}$, $f : \mathbb{R}^{n_x} \times \mathbb{R}^{n_y} \times \mathbb{R}^{n_u} \longrightarrow \mathbb{R}^{n_x}$ are continuously differentiable functions, $g : \mathbb{R}^{n_x} \longrightarrow \mathbb{R}^{n_y}$ is a twice continuously differentiable function, and $\mathcal{U} \subseteq \mathbb{R}^{n_u}$ is a closed convex set.

Problem 5.1 (OCP-SB) Minimize

$$\Gamma(x, y, u) := \varphi(x(t_f))$$

with respect to $x \in W^{1,\infty}(I, \mathbb{R}^{n_x})$, $y \in L^{\infty}(I, \mathbb{R}^{n_y})$, $u \in L^{\infty}(I, \mathbb{R}^{n_u})$ subject to the constraints

$$x'(t) = f(x(t), y(t), u(t)) \qquad \text{a.e. in } I, \tag{5.1}$$

$$0 = g(x(t)) \qquad \text{in } I, \tag{5.2}$$

$$x(t_0) = \bar{x}, \tag{5.3}$$

$$u(t) \in \mathscr{U} \qquad \text{a.e. in } I. \tag{5.4}$$

The DAE (5.1)–(5.2) is supposed to be of index two, see Assumption 3.2, and $\bar{x}$ is supposed to be consistent, i.e., $g(\bar{x}) = 0$. Moreover, in order to allow for the elimination of the equality constraints we assume the following:

Assumption 5.2

(a) The initial value problem (5.1)–(5.3) possesses a unique solution $(x(u), y(u)) \in W^{1,\infty}(I, \mathbb{R}^{n_x}) \times L^\infty(I, \mathbb{R}^{n_y})$ *for every control input* $u \in L^\infty(I, \mathbb{R}^{n_u})$.

(b) The control-to-state mapping $L^\infty(I, \mathbb{R}^{n_u}) \ni u \mapsto (x(u), y(u)) \in W^{1,\infty}(I, \mathbb{R}^{n_x}) \times L^\infty(I, \mathbb{R}^{n_y})$ *is continuously Fréchet-differentiable.*

Remark 5.1 The idea of considering the control-to-state mapping in Assumption 5.2 is exactly the single shooting idea. The realization requires to solve the initial value problem (5.1)–(5.3) for a given control input u by some suitable discretization scheme, amongst them are the implicit Euler method, BDF methods, and implicit Runge–Kutta methods. The existence of solutions in Assumption 5.2 (a) can be shown for ODEs (Carathéodory solutions) or under standard assumptions in the case that f and g in (5.1)–(5.2) are linear. General existence and uniqueness results can be found in [96], but for L^∞-inputs existence and uniqueness is not fully understood up to the knowledge of the author. Hence we merely assume that a unique solution exists for a given control input.

Exploitation of Assumption 5.2 allows to eliminate the equality constraints in Problem 5.1 and to consider an equivalent minimization problem for the reduced functional

$$J(u) := \Gamma(x(u), y(u), u) \tag{5.5}$$

subject to the simple bounds $u(t) \in \mathscr{U}$ only.

Problem 5.3 (Reduced Problem)

Minimize $J(u)$ with respect to $u \in L^\infty(I, \mathbb{R}^{n_u})$ subject to $u(t) \in \mathscr{U}$ a.e. in I.

Let $\hat{u}$ be a local minimum of Problem 5.3. Then the first order necessary optimality condition reads

$$J'(\hat{u})(u - \hat{u}) \geq 0 \qquad \forall u \in \mathscr{U}_{ad}, \tag{5.6}$$

where the admissible set $\mathscr{U}_{ad}$ is defined by

$$\mathscr{U}_{ad} := \{u \in L^\infty(I, \mathbb{R}^{n_u}) \mid u(t) \in \mathscr{U} \text{ a.e. in } I\}.$$

The variational inequality (5.6) with $\nabla J(\hat{u})$ being the Riesz representation of the functional $J'(\hat{u})$) (in a Hilbert space) is equivalent with the condition

$$\hat{u} = \Pi_{\mathscr{U}_{ad}}(\hat{u} - \nu\nabla J(\hat{u})) \quad (\nu > 0)$$

that has to hold a.e. in I, where $\Pi_{\mathscr{U}_{ad}} : L^\infty(I, \mathbb{R}^{n_u}) \longrightarrow \mathscr{U}_{ad}$ is the projection onto the admissible set $\mathscr{U}_{ad}$. For box constraints

$$\mathscr{U} = \{u \in \mathbb{R} \mid a \leq u \leq b\}$$

the projection of u at t computes to

$$\Pi_{\mathscr{U}_{ad}}(u)(t) = \max\{a, \min\{b, u(t)\}\} = \begin{cases} a, & \text{if } u(t) < a, \\ u(t), & \text{if } a \leq u(t) \leq b, \\ b, & \text{if } u(t) > b. \end{cases}$$

In the sequel we assume that the projection onto $\mathscr{U}_{ad}$ is easy to compute like it is in the box-constrained case. Then, a conceptual projected gradient method reads as follows:

Algorithm 5.4 (Projected Gradient Method)

(0) Choose $u^0 \in \mathscr{U}_{ad}$, $\beta \in (0, 1)$, $\sigma \in (0, 1)$, $tol > 0$, and set $k := 0$.
(1) If $\|u^k - \Pi_{\mathscr{U}_{ad}}\left(u^k - \nabla J(u^k)\right)\|_\infty \leq tol$, STOP.
(2) Set

$$\tilde{d}^k := -\nabla J(u^k),$$

compute

$$\tilde{u}^k := \Pi_{\mathscr{U}_{ad}}\left(u^k + \tilde{d}^k\right),$$

and set

$$d^k := \tilde{u}^k - u^k.$$

(4) Perform an Armijo line-search: Find smallest $j \in \{0, 1, 2, \ldots\}$ with

$$J(u^k + \beta^j d^k) \leq J(u^k) + \sigma\beta^j J'(u^k)(d^k)$$

and set $\alpha_k := \beta^j$.
(5) Set $u^{k+1} := u^k + \alpha_k d^k$, $k := k + 1$, and go to (1).

Remark 5.2 An alternate version of the projected gradient method does not use the projection in step (2), but instead uses the projection directly in the line-search in step (4) as follows

$$J\left(\Pi_{\mathscr{U}_{ad}}\left(u^k+\beta^j d^k\right)\right) \le J(u^k)+\sigma\beta^j J'(u^k)(d^k),$$

compare [107, Sect. 3.7.1]. The new iterate in step (5) is then given by $u^{k+1} := \Pi_{\mathscr{U}_{ad}}\left(u^k+\alpha_k d^k\right)$.

It remains to answer one question: How does the gradient $\nabla J(u)$ look like?

In a Hilbert space U, this question is easy to answer, because the Fréchet derivative $J'(\tilde{u})$ of J at $\tilde{u}$ is a linear and continuous functional and by the Riesz theorem it possesses the representation $J'(\tilde{u})(u) = \langle \eta, u\rangle_U$ with some $\eta \in U$. Hence, the element η can be interpreted as the gradient of J at $\tilde{u}$. But Riesz' Theorem does not hold in general Banach spaces. However, we will make use of a formal Lagrange technique to obtain a similar representation in our setting. To this end define the auxiliary functional (with $\ell_0 = 1$)

$$\begin{aligned}\tilde{J}(\tilde{u}) &:= J(\tilde{u}) + \left\langle \lambda_f(\cdot), f(\tilde{x}(\cdot),\tilde{y}(\cdot),\tilde{u}(\cdot)) - \tilde{x}'(\cdot)\right\rangle_{L^2}\\ &\qquad + \left\langle \lambda_g(\cdot), g_x'(\tilde{x}(\cdot)) f(\tilde{x}(\cdot),\tilde{y}(\cdot),\tilde{u}(\cdot))\right\rangle_{L^2}\\ &= \varphi(\tilde{x}(t_f)) + \int_I \mathscr{H}(\tilde{x}(t),\tilde{y}(t),\tilde{u}(t),\lambda_f(t),\lambda_g(t),\ell_0) - \lambda_f(t)^\top \tilde{x}'(t)dt,\end{aligned}$$

where $\lambda_f \in W^{1,\infty}(I,\mathbb{R}^{n_x})$ and $\lambda_g \in L^\infty(I,\mathbb{R}^{n_y})$ are functions to be specified later and $\tilde{x} := x(\tilde{u})$, $\tilde{y} := y(\tilde{u})$ are Fréchet differentiable functions of u. Partial integration of the last term yields

$$\begin{aligned}\tilde{J}(\tilde{u}) &= \varphi(\tilde{x}(t_f)) - \left[\lambda_f(t)^\top \tilde{x}(t)\right]_{t_0}^{t_f}\\ &\qquad + \int_I \mathscr{H}(\tilde{x}(t),\tilde{y}(t),\tilde{u}(t),\lambda_f(t),\lambda_g(t),\ell_0) + \lambda_f'(t)^\top \tilde{x}(t)dt.\end{aligned}$$

Formal differentiation of $\tilde{J}$ at $\tilde{u}$ in the direction u together with the Fréchet derivatives $S^x := x'(\tilde{u})(u)$ and $S^y := y'(\tilde{u})(u)$ yields

$$\begin{aligned}\tilde{J}'(\tilde{u})(u) &= \left(\varphi'(\tilde{x}(t_f)) - \lambda_f(t_f)^\top\right) S^x(t_f)\\ &\qquad + \int_I \left(\mathscr{H}_x'[t] + \lambda_f'(t)^\top\right) S^x(t) + \mathscr{H}_y'[t] S^y(t) + \mathscr{H}_u'[t] u(t)dt,\end{aligned}$$

where we exploited that the initial value of x does not depend on u and $[t]$ is an abbreviation for $(\tilde{x}(t),\tilde{y}(t),\tilde{u}(t),\lambda_f(t),\lambda_g(t),\ell_0)$.

As the derivatives S^x and S^y are expensive to compute, λ_f and λ_g are chosen in such a way that the terms involving S^x and S^y vanish. This yields the initial value problem with the index-one adjoint DAE

$$\lambda_f'(t) = -\mathscr{H}_x'(\tilde{x}(t), \tilde{y}(t), \tilde{u}(t), \lambda_f(t), \lambda_g(t), \ell_0)^\top, \tag{5.7}$$

$$0 = \mathscr{H}_y'(\tilde{x}(t), \tilde{y}(t), \tilde{u}(t), \lambda_f(t), \lambda_g(t), \ell_0)^\top, \tag{5.8}$$

$$\lambda_f(t_f) = \varphi'(\tilde{x}(t_f))^\top, \tag{5.9}$$

and $\tilde{J}'(\tilde{u})(u)$ reduces to

$$\tilde{J}'(\tilde{u})(u) = \int_I \mathscr{H}_u'[t]u(t)dt.$$

The adjoint DAE (5.7)–(5.9) is a linear semi-explicit DAE of index one and thus it is well-defined and possesses a unique solution.

One can show with similar techniques as in [48, Theorem 8.1.6] that $\tilde{J}'(\tilde{u})(u)$ and $J'(\tilde{u})(u)$ in fact coincide and thus

$$J'(\tilde{u})(u) = \tilde{J}'(\tilde{u})(u) = \int_I \mathscr{H}_u'[t]u(t)dt. \tag{5.10}$$

The representation in (5.10) reminds of the Riesz representation of a continuous linear functional and thus we define the gradient as follows:

Definition 5.1 (Gradient of Reduced Functional) The gradient $\nabla J(\tilde{u})$ of the reduced objective functional J in (5.5) at $\tilde{u}$ is defined by

$$\nabla J(\tilde{u})(\cdot) := \nabla_u \mathscr{H}(\tilde{x}(\cdot), \tilde{y}(\cdot), \tilde{u}(\cdot), \lambda_f(\cdot), \lambda_g(\cdot), \ell_0),$$

where $\ell_0 = 1$, $\tilde{x} = x(\tilde{u})$, $\tilde{y} = y(\tilde{u})$, and λ_f and λ_g solve the adjoint DAE (5.7)–(5.9).

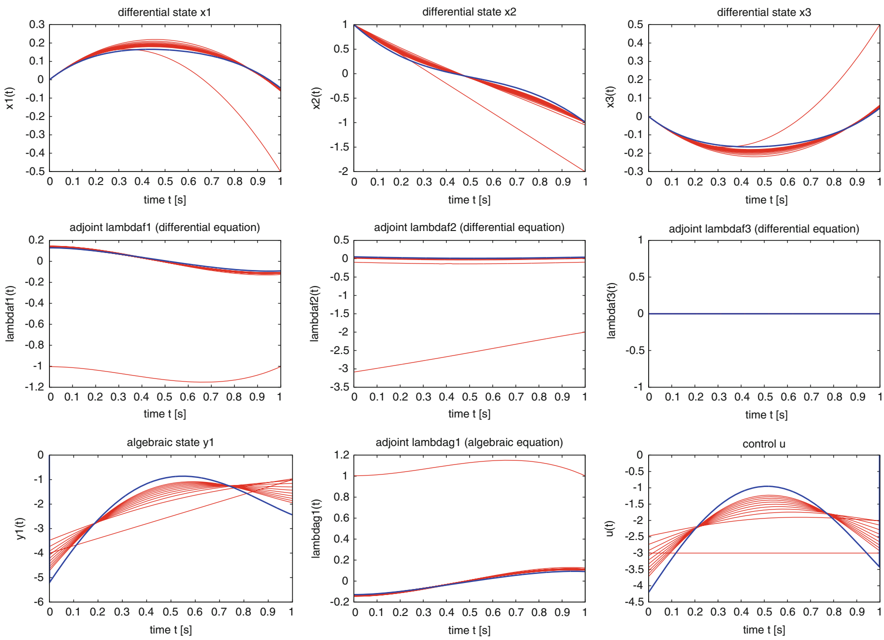
In fact it is easy to verify that the normed direction $d = -\nabla J(\tilde{u})/\|\nabla J(\tilde{u})\|_2$ minimizes the directional derivative $J'(\tilde{u})(u)$ w.r.t. all directions u with $\|u\|_2 = 1$. This property justifies the alternate name "steepest descent method" for the gradient method.

Example 5.5 Consider Example 4.5. Since u is not restricted, i.e., $\mathscr{U} = \mathbb{R}$, the projected gradient method reduces to the classic gradient method. The gradient method with tolerance $tol = 10^{-5}$, $\alpha_1 = \alpha_2 = \alpha_4 = 1$, $\alpha_3 = 0.5 \cdot 10^{-2}$, $N = 1000$ and initial guess $u^0 \equiv -3$ produces the following iterates:

A look at the iterates reveals a major drawback of the gradient method: The convergence rate is only linear and it is rather slow in this example. Moreover, the gradient method can be quite sensitive w.r.t. to scaling and tolerances. For instance, if we reduce the tolerance tol to 10^{-6}, then the line-search procedure terminates with a step-size close to zero.

k	α_k	$J(u^k)$	$\Vert u^k - \Pi_{\mathscr{U}}\left(u^k - \nu J'(u^k)\right)\Vert_\infty$ $\nu = 10^{-3}$	$J'(u^k)(d^k)$
0	0.00000000E+00	0.13300873E+01	0.31148251E−02	−0.67634180E+01
1	0.65610000E+00	0.76882228E+00	0.25684209E−02	−0.37878631E+01
2	0.65610000E+00	0.45335163E+00	0.17268254E−02	−0.21216493E+01
3	0.65610000E+00	0.27650174E+00	0.14715161E−02	−0.11885594E+01
4	0.65610000E+00	0.17683468E+00	0.99728958E−03	−0.66603951E+00
5	0.65610000E+00	0.12081438E+00	0.85221832E−03	−0.37332995E+00
…	…	…	…	…
195	0.81000000E+00	0.41473570E−01	0.10260497E−04	−0.18966824E−04
196	0.72900000E+00	0.41471467E−01	0.18804354E−04	−0.17294724E−04
197	0.72900000E+00	0.41469326E−01	0.10490706E−04	−0.15639555E−04
198	0.72900000E+00	0.41467372E−01	0.18067697E−04	−0.14314419E−04
199	0.81000000E+00	0.41466091E−01	0.98482036E−05	−0.17769042E−04

The following pictures show some intermediate iterates (thin lines) and the converged solution (thick lines) of the gradient method for the states, the adjoints, and the control. □

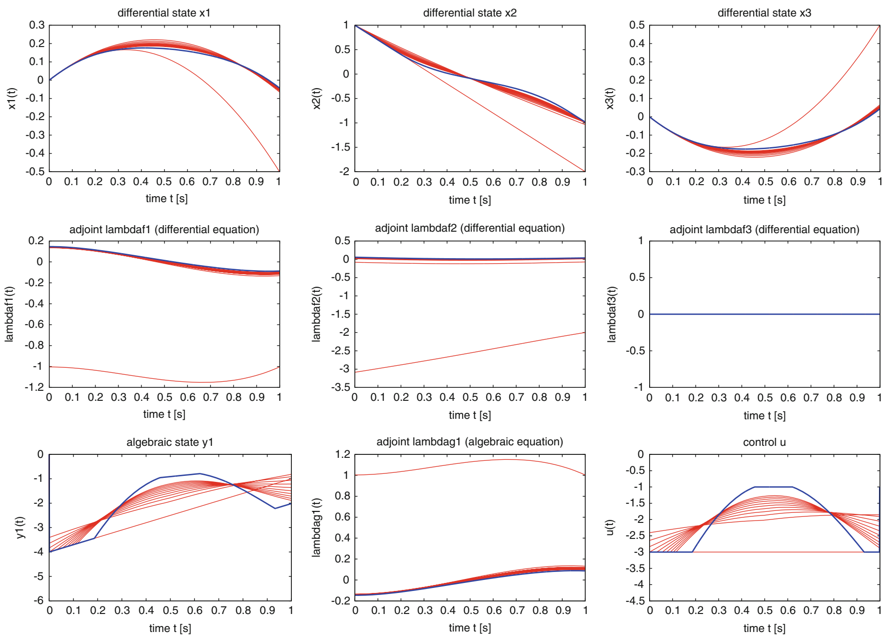


Example 5.6 Consider Example 4.6. The projected gradient method with tolerance $tol = 10^{-7}$, $\alpha_1 = \alpha_2 = \alpha_4 = 1$, $\alpha_3 = 0.5 \cdot 10^{-2}$, $N = 1000$ and initial guess

$u^0 \equiv -3$ produces the following iterates, which exhibit a slow linear convergence rate:

k	α_k	$J(u^k)$	$\|u^k - \Pi_{\mathscr{U}}\left(u^k - \nu J'(u^k)\right)\|_\infty$ $\nu = 10^{-3}$	$J'(u^k)(d^k)$
0	0.00000000E+00	0.13300873E+01	0.31148251E−02	−0.51621641E+01
1	0.81000000E+00	0.57297403E+00	0.21639411E−02	−0.25254696E+01
2	0.72900000E+00	0.35775984E+00	0.15304789E−02	−0.16252587E+01
3	0.65610000E+00	0.22253942E+00	0.12832913E−02	−0.91034675E+00
4	0.65610000E+00	0.14643376E+00	0.89053644E−03	−0.51008708E+00
5	0.65610000E+00	0.10367291E+00	0.74329723E−03	−0.28584962E+00
…	…	…	…	…
471	0.10000000E+01	0.42028359E−01	0.10342884E−06	−0.13237960E−08
472	0.10000000E+01	0.42028358E−01	0.10233230E−06	−0.12956173E−08
473	0.10000000E+01	0.42028356E−01	0.10124469E−06	−0.12680419E−08
474	0.10000000E+01	0.42028355E−01	0.10017421E−06	−0.12410509E−08
475	0.10000000E+01	0.42028354E−01	0.99108933E−07	−0.12146379E−08

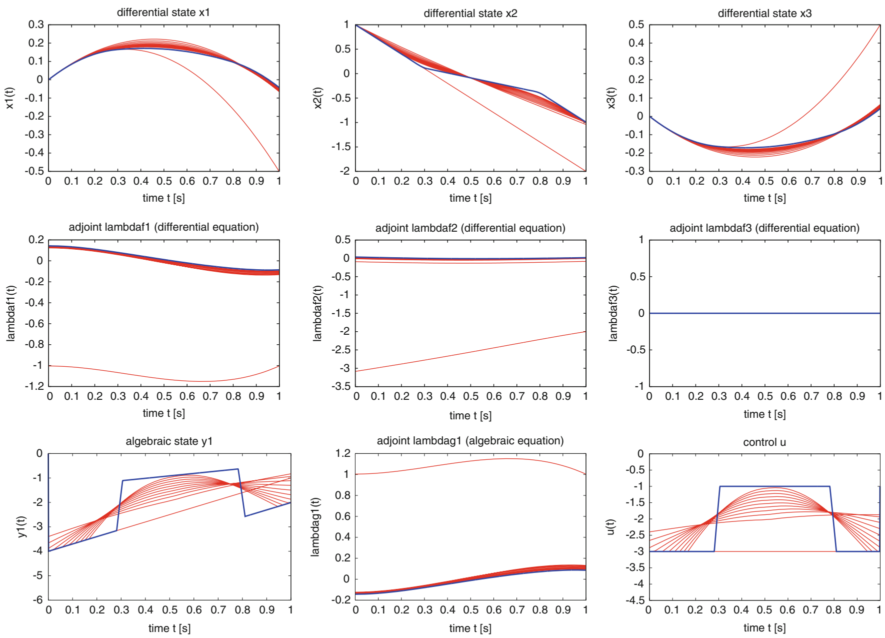
The following pictures show some intermediate iterates (thin lines) and the converged solution (thick lines) of the projected gradient method for the states, the adjoints, and the control. □



Example 5.7 Consider Example 4.7. The projected gradient method with tolerance $tol = 10^{-6}$, $\alpha_1 = \alpha_2 = \alpha_4 = 1$, $\alpha_3 = 0$, $N = 1000$ and initial guess $u^0 \equiv -3$ produces the following iterates with a slow linear convergence rate:

k	α_k	$J(u^k)$	$\|u^k - \Pi_{\mathscr{U}}\left(u^k - \nu J'(u^k)\right)\|_\infty$ $\nu = 10^{-3}$	$J'(u^k)(d^k)$
0	0.00000000E+00	0.12850873E+01	0.30848252E−02	−0.51021641E+01
1	0.81000000E+00	0.56345203E+00	0.21777410E−02	−0.25559953E+01
2	0.72900000E+00	0.33237684E+00	0.15172054E−02	−0.15910525E+01
3	0.65610000E+00	0.19663752E+00	0.12574239E−02	−0.87563698E+00
4	0.65610000E+00	0.12158166E+00	0.87048761E−03	−0.48210072E+00
5	0.65610000E+00	0.80129201E−01	0.71767043E−03	−0.26547456E+00
…	…	…	…	…
1000	0.10000000E+01	0.18185375E−01	0.10092448E−05	−0.18871142E−07
1001	0.10000000E+01	0.18185356E−01	0.10091735E−05	−0.18871079E−07
1002	0.10000000E+01	0.18185337E−01	0.10091040E−05	−0.18871008E−07
1003	0.10000000E+01	0.18185318E−01	0.10090356E−05	−0.18066969E−07
1004	0.10000000E+01	0.18185300E−01	0.99357979E−06	−0.17849778E−07

The following pictures show some intermediate iterates (thin lines) and the converged solution (thick lines) of the projected gradient method for the states, the adjoints, and the control. Note that the control is a bang–bang control. □



5.2 Lagrange–Newton Method

The Lagrange–Newton method and its extension to problems with inequality constraints, the SQP method, are analyzed in a Banach space setting in [1, 2]. The application of SQP methods to optimal control problems subject to ODEs can be found in [3, 4] and [85].

The basic idea of the Lagrange–Newton method is to solve the optimality system provided by the local minimum principle by Newton's method. Note that, although the global minimum principle provides stronger necessary conditions than the local one, the global minimum principle is difficult to exploit for numerical algorithms, because the optimality condition in (d) of Theorem 3.4 requires to find a global minimum of the Hamilton function on the set Ω. Since global minimization is expensive, we use the local minimum principle. To this end consider OCP-SE without control constraints and pure state constraints:

Problem 5.8 Minimize

$$\varphi(x(t_0), x(t_f)) + \int_I f_0(x(t), y(t), u(t))\, dt$$

w.r.t. $x \in W^{1,\infty}(I, \mathbb{R}^{n_x})$, $y \in L^{\infty}(I, \mathbb{R}^{n_y})$, $u \in L^{\infty}(I, \mathbb{R}^{n_u})$ subject to the constraints

$$\begin{aligned} x'(t) &= f(x(t), y(t), u(t)) && \text{a.e. in } I, \\ 0 &= g(x(t)) && \text{in } I, \\ 0 &= \psi(x(t_0), x(t_f)). \end{aligned}$$

The local minimum principle in Theorem 3.3 (assuming $\ell_0 = 1$) yields the necessary conditions

$$T(x, y, u, \lambda_f, \lambda_g, \sigma, \zeta) := \begin{pmatrix} x'(\cdot) - f(x(\cdot), y(\cdot), u(\cdot)) \\ g(x(\cdot)) \\ \lambda_f'(\cdot) + \mathscr{H}_x'(x(\cdot), y(\cdot), u(\cdot), \lambda_f(\cdot), \lambda_g(\cdot), \ell_0)^\top \\ \mathscr{H}_y'(x(\cdot), y(\cdot), u(\cdot), \lambda_f(\cdot), \lambda_g(\cdot), \ell_0)^\top \\ \mathscr{H}_u'(x(\cdot), y(\cdot), u(\cdot), \lambda_f(\cdot), \lambda_g(\cdot), \ell_0)^\top \\ \psi(x(t_0), x(t_f)) \\ \lambda_f(t_0) + \kappa_{x_0}'(x(t_0), x(t_f), \sigma, \zeta)^\top \\ \lambda_f(t_f) - \kappa_{x_f}'(x(t_0), x(t_f), \sigma, \zeta)^\top \end{pmatrix} = 0, \tag{5.11}$$

where $\kappa(x_0, x_f, \sigma, \zeta) := \varphi(x_0, x_f) + \sigma^\top \psi(x_0, x_f) + \zeta^\top g(x_0)$.

Let the operator T be Fréchet-differentiable and let T' be surjective. Then Newton's method can be applied to the nonlinear equation $T(\eta) = 0$ with $\eta = (x, y, u, \lambda_f, \lambda_g, \sigma, \zeta)$. The resulting method is called Lagrange–Newton method and reads as follows:

Algorithm 5.9 (Lagrange–Newton Algorithm)

(0) Choose η^0, $tol > 0$, and set $k := 0$.
(1) If $\|T(\eta^k)\| \leq tol$, STOP.
(2) Solve the linear operator equation $T'(\eta^k)(d) = -T(\eta^k)$ for d and denote the solution by d^k.
(3) Set $\eta^{k+1} := \eta^k + d^k$, $k := k + 1$, and go to (1).

The standard convergence results on Newton's method apply under standard assumptions and globalized (or damped) versions can be considered. The linear operator equation in step (2) with $d = (x, y, u, \lambda_f, \lambda_g, \sigma, \zeta)$ corresponds to the linear DAE boundary value problem

$$
\begin{pmatrix} x' \\ \lambda_f' \\ 0 \\ 0 \\ 0 \end{pmatrix} + \begin{pmatrix} -f_x' & 0 & -f_y' & 0 & -f_u' \\ \mathscr{H}_{xx}'' & \mathscr{H}_{x\lambda_f}'' & \mathscr{H}_{xy}'' & \mathscr{H}_{x\lambda_g}'' & \mathscr{H}_{xu}'' \\ g_x' & 0 & 0 & 0 & 0 \\ \mathscr{H}_{yx}'' & \mathscr{H}_{y\lambda_f}'' & \mathscr{H}_{yy}'' & \mathscr{H}_{y\lambda_g}'' & \mathscr{H}_{yu}'' \\ \mathscr{H}_{ux}'' & \mathscr{H}_{u\lambda_f}'' & \mathscr{H}_{uy}'' & \mathscr{H}_{u\lambda_g}'' & \mathscr{H}_{uu}'' \end{pmatrix} \begin{pmatrix} x \\ \lambda_f \\ y \\ \lambda_g \\ u \end{pmatrix}
$$

$$
= - \begin{pmatrix} (x^k)' - f \\ (\lambda_f^k)' + \left(\mathscr{H}_x'\right)^\top \\ g \\ \left(\mathscr{H}_y'\right)^\top \\ \left(\mathscr{H}_u'\right)^\top \end{pmatrix} \tag{5.12}
$$

with boundary conditions

$$
\psi_{x_0}' x(t_0) + \psi_{x_f}' x(t_f) = -\psi, \tag{5.13}
$$

$$
\lambda_f(t_0) + \kappa_{x_0,x_0}'' x(t_0) + \kappa_{x_0,x_f}'' x(t_f) + \kappa_{x_0,\sigma}'' \sigma + \kappa_{x_0,\zeta}'' \zeta = -\left(\lambda_f^k(t_0) + (\kappa_{x_0}')^\top\right), \tag{5.14}
$$

$$
\lambda_f(t_f) - \kappa_{x_f,x_0}'' x(t_0) - \kappa_{x_f,x_f}'' x(t_f) - \kappa_{x_f,\sigma}'' \sigma = -\left(\lambda_f^k(t_f) - (\kappa_{x_f}')^\top\right), \tag{5.15}
$$

where all functions are evaluated at η^k. The components σ and ζ are treated via the trivial differential equations $\sigma' = 0$ and $\zeta' = 0$.

Since the boundary value problem (5.12)–(5.15) arose from a linearization of a nonlinear equation around some (arbitrary) iterate η^k, existence of a solution is not guaranteed. In particular it happens that the linearized boundary conditions are inconsistent. Moreover, the multiplier ζ might be redundant in the minimum principle and can be set to zero, e.g., if the initial value of $x(t_0)$ is fixed. This redundancy leads to rank deficiencies in the linear BVP. Regularization methods become necessary in these cases, compare [51]. For index one DAEs the situation is less involved, compare [48, Sect. 8.2].

A straightforward calculation shows that the index of the DAE in (5.12) is two, if the matrix

$$\begin{pmatrix} g_x' f_y' & 0 & g_x' f_u' \\ \mathscr{H}_{yy}'' & \mathscr{H}_{y\lambda_g}'' & \mathscr{H}_{yu}'' \\ \mathscr{H}_{uy}'' & \mathscr{H}_{u\lambda_g}'' & \mathscr{H}_{uu}'' \end{pmatrix}$$

is non-singular a.e. on I with an essentially bounded inverse on I.

The outlined Lagrange–Newton method can be applied to more general DAEs. Again, results for linear DAEs whether in leading term formulation or in descriptor form can be applied to the resulting boundary value problems in step (2) of the algorithm.

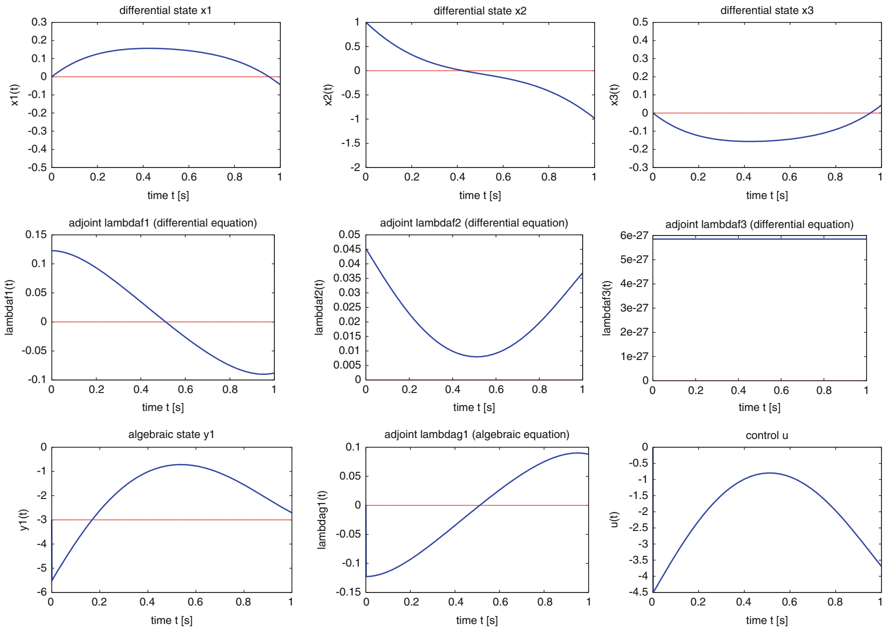
Example 5.10 Consider again Example 3.5 resp. Example 4.5. The Lagrange–Newton method with tolerance $tol = 10^{-15}$, $\alpha_1 = \alpha_2 = \alpha_4 = 1$, $\alpha_3 = 0.5 \cdot 10^{-2}$, $N = 1000$ (number of steps in the shooting method used for the numerical solution of BVP), and initial guess $x^0 \equiv 0$, $y^0 \equiv 0$, $u^0 \equiv -3$, $\lambda_f^0 \equiv 0$, $\lambda_g^0 \equiv 0$, $\sigma^0 \equiv 0$, $\zeta^0 \equiv 0$ converges in one step:

k	α_k	$\Vert T(\eta^k)\Vert_2^2$	$\Vert d^k\Vert_2^2$
0	0.000000E+00	0.140000E+02	0.271697E+04
1	0.100000E+01	0.172345E−26	0.438543E−09

This is not surprising since the optimal control problem is a linear-quadratic problem and the necessary optimality conditions form a linear operator equation.

The following pictures show the initial guess (constant lines) and the solution (thick lines) of the Lagrange–Newton method for the states, the adjoints, and the control.

□



5.3 Treatment of Inequality Constraints

Inequality constraints can be handled conceptually by, e.g., SQP methods, see [3, 4, 85], interior-point methods, see [101, 110, 113], penalty methods, or semi-smooth Newton methods, see [31, 51, 62, 108, 109].

We focus on semi-smooth Newton methods and outline the main ideas. Semi-smooth Newton methods require the reformulation of the necessary optimality conditions in terms of a nonlinear equation. This can be achieved in several ways and we discuss two commonly used approaches.

Firstly, consider OCP-SE without pure state constraints but with control constraints $u(t) \in \mathscr{U}$, where $\mathscr{U}$ is a closed and convex set. In this case we have to deal with the variational inequality

$$\mathscr{H}_u'(\hat{x}(t), \hat{y}(t), \hat{u}(t), \lambda_f(t), \lambda_g(t), \ell_0)(u - \hat{u}(t)) \geq 0 \qquad \forall u \in \mathscr{U}$$

in (d) of Theorem 3.3. Likewise as in Sect. 5.1 this variational inequality can be reformulated as the equation

$$0 = \hat{u} - \Pi_{\mathscr{U}_{ad}}(\hat{u} - \nu \nabla_u \mathscr{H}) \quad (\nu > 0) \tag{5.16}$$

with

$$\mathscr{U}_{ad} := \{u \in L^\infty(I, \mathbb{R}^{n_u}) \mid u(t) \in \mathscr{U} \text{ a.e. in } I\}.$$

Herein, $\nabla_u \mathscr{H}$ is evaluated at $(\hat{x}, \hat{y}, \hat{u}, \lambda_f, \lambda_g, \ell_0)$ with $\ell_0 = 1$.

Replacing $\nabla_u \mathscr{H}$ in (5.11) by the right hand-side in (5.16) yields again a nonlinear equation similar to (5.11). Since the projection $\Pi_{\mathscr{U}_{ad}}$ is only Lipschitz continuous but not Fréchet differentiable, the nonlinear equation is non-smooth and modifications of Newton's method towards semi-smooth Newton methods are necessary. Herein, the Fréchet derivative $T'(\eta^k)$ has to be replaced by a suitably defined generalized Jacobian $\partial T(\eta^k)$, compare, e.g., [109] for details in the context of PDE constrained optimization.

Another transformation can be used, if the control constraints are expressed in terms of mixed control-state constraints of type $c(x(t), y(t), u(t)) \leq 0$. The resulting necessary optimality conditions then involve complementarity conditions of type

$$0 \leq \mu(t) \quad \perp \quad -c(x(t), y(t), u(t)) \geq 0.$$

These can be transformed to equivalent nonlinear and non-smooth equations by pointwise application of a suitable nonlinear complementarity function like the Fischer-Burmeister function $\phi(a, b) := \sqrt{a^2 + b^2} - a - b$. This Lipschitz-continuous function has the property that $\phi(a, b) = 0$ holds if and only if $0 \leq a \perp b \geq 0$. The resulting optimality system with the non-smooth equation

$$\phi(-c(x(t), y(t), u(t)), \mu(t)) = 0 \qquad \text{a.e. in } I$$

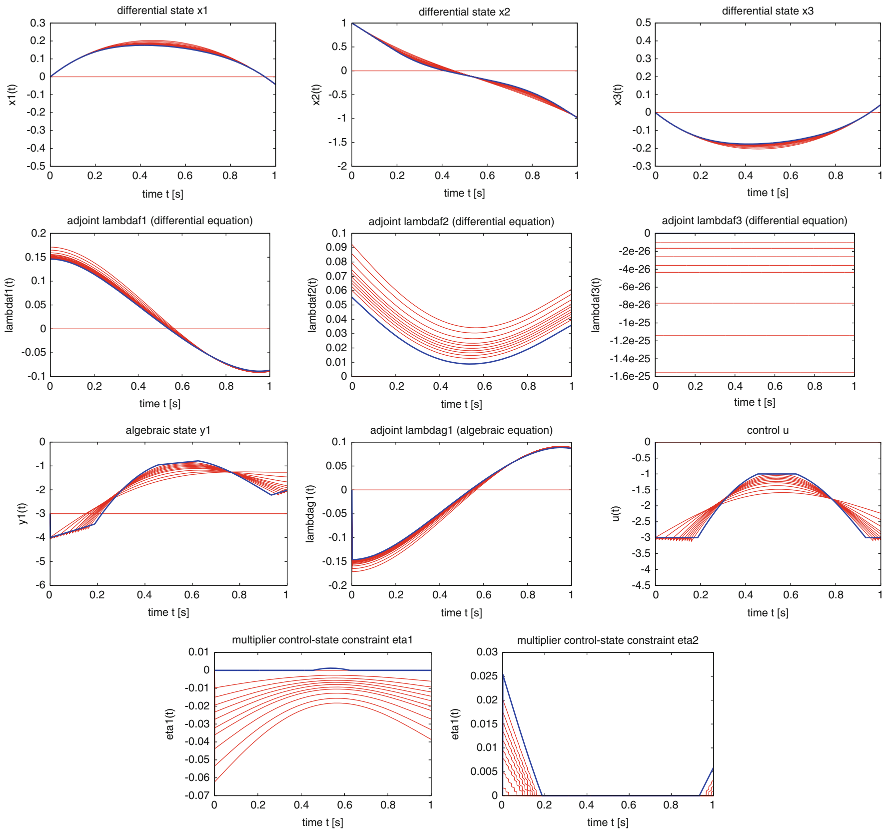
can be solved by a semi-smooth Newton method again, compare [31, 51]. We illustrate the performance of the semi-smooth Newton method, which we augmented by an Armijo line-search procedure, in the subsequent example.

Example 5.11 Consider again Example 5.6 resp. Example 4.6. The semi-smooth Newton method in [51] with tolerance $tol = 10^{-15}$, $\alpha_1 = \alpha_2 = \alpha_4 = 1$, $\alpha_3 = 0.5 \cdot 10^{-2}$, $N = 1000$ (number of steps in the shooting method used for the numerical solution of BVP), and initial guess $x^0 \equiv 0$, $y^0 \equiv 0$, $u^0 \equiv -3$, $\lambda_f^0 \equiv 0$, $\lambda_g^0 \equiv 0$, $\sigma^0 \equiv 0$, $\zeta^0 \equiv 0$ produces the following iterates, which exhibit a superlinear convergence rate:
The following pictures show some intermediate iterates (thin lines) and the converged solution (thick lines) of the semi-smooth Newton method for the states, the adjoints, the control, and the multipliers for the control constraints. □

Pure state constraints in function space methods are often handled by relaxation or penalization, compare the virtual control concept in [32, 50, 66]. The idea of the virtual control concept is to introduce an artificial control $v \in L^\infty(I, \mathbb{R})$ (for a single state constraint) and to consider the relaxed state constraint

$$s(x(t)) - \gamma(\alpha) v(t) \leq 0$$

k	α_k	$\|F(z^k)\|_2^2$	$\|d\|_2^2$
0	0.000000E+00	0.180000E+02	0.136708E+05
1	0.100000E+01	0.343312E+01	0.880798E+04
2	0.100000E+01	0.910739E−01	0.965659E+05
3	0.100000E+01	0.108791E−02	0.385528E+04
4	0.523348E−01	0.107136E−02	0.281572E+04
5	0.471013E−01	0.104974E−02	0.433688E+04
...	...	...	...
19	0.100000E+01	0.214659E−03	0.113684E+02
20	0.100000E+01	0.989223E−08	0.106969E+01
21	0.100000E+01	0.532519E−10	0.425010E−02
22	0.100000E+01	0.502770E−13	0.108164E−03
23	0.100000E+01	0.720014E−19	0.470676E−06



with a regularization parameter $\alpha > 0$ and some suitable positive function γ. In order to drive v to zero as $\alpha \to 0$, the term

$$\frac{\phi(\alpha)}{2} \int_I \|v(t)\|^2 dt$$

is added to the objective function, where ϕ is some suitable positive function. For any positive α the regularized problem has only mixed control-state constraints and no pure state constraints. It can be solved by the aforementioned methods. Under suitable conditions convergence of the regularized solutions can be shown. In fact, the virtual control concept is a penalty method since the optimal $\hat{v}_\alpha$ for $\alpha > 0$ satisfies

$$\hat{v}_\alpha(t) = \frac{1}{\gamma(\alpha)} \max\{0, s(\hat{x}_\alpha(t))\}$$

and instead of considering the relaxed state constraint one could add the penalty term

$$\frac{\phi(\alpha)}{2\gamma(\alpha)^2} \int_I \max\{0, s(x(t))\}^2 dt$$

to the objective function.

6 Conclusions and Future Directions

The paper aims to provide an overview on theoretical results and numerical techniques for optimal control problems subject to differential-algebraic equations. Naturally this is a vast area and not all topics could be covered in detail. Special attention was put on necessary and—whenever available—sufficient conditions of optimality for linear-quadratic and nonlinear optimal control problems and on numerical techniques. Although many theoretical and numerical issues in DAE optimal control have been addressed and solved today, there are several topics of interest with little attention so far. These topics, to the author's opinion, deserve more attention in the future. Amongst them are:

Sufficient conditions for nonlinear optimal control problems: Sufficient conditions of optimality are well-known for linear-quadratic DAE optimal control problems and for optimal control problems subject to explicit ODEs. However, sufficient conditions of optimality have not been obtained so far for optimal control problems subject to nonlinear DAEs with possibly higher index.

Sufficient conditions of optimality typically appear as well in the study of convergence properties of discretizations and parametric sensitivity analysis. Hence, they are of fundamental importance and should be investigated in more detail.

Parametric sensitivity analysis: Numerical techniques and theoretical properties with regard to the dependence of optimal solutions with respect to parameters are well established for finite dimensional optimization problems and hence on a discretization level, a parametric sensitivity analysis for DAE optimal control problems can be performed. The mathematically thorough function space counterpart for parametric DAE optimal control problems is missing so far. The task is to derive conditions that guarantee that the solution of a DAE optimal control problem is continuous, Lipschitz-continuous, or Fréchet-differentiable, respectively, with respect to some parameter entering the problem formulation. This analysis has to be carried out in a proper function space setting, which is suitable for the DAE optimal control problem.

Convergence properties of discretizations: Despite the fact that there are many sophisticated algorithms around with the ability to numerically solve discretized DAE optimal control problems, the convergence of discretizations of DAE optimal control problems has not been established so far. For semi-explicit DAEs of index one convergence proofs for ODE optimal control problems could be extended in a straightforward way. For higher index DAEs one is typically faced with a structural gap between the necessary conditions on discretization level, which usually do not involve index reduction, and on function space level, where some implicit index reduction takes place as explained in Sect. 3 and Remark 3.1.

Existence of optimal solutions: A fundamental question is the question of existence of an optimal solution for reasonable initial conditions. Apart from general existence results up to the author's knowledge there are no particular existence results for nonlinear (non-convex) DAE optimal control problems.

Optimal control of coupled DAE-PDE systems: Many practically important applications naturally lead to coupled systems of DAEs and partial differential equations, for instance if a truck, modeled by a mechanical multi-body system, carries some water tank, modeled by the Navier–Stokes equations. Such coupled systems have not been investigated systematically, neither from a numerical point of view nor from a theoretical point of view. Hence, the (optimal) control of coupled DAE-PDE systems provides a huge area for future research with regard to necessary and sufficient conditions, existence of solutions, and efficient structure exploiting numerical methods (both, discretization based and function space based). Extensions of the index concept towards PDAEs can be found in [26].

The above topics possess counterparts in ODE optimal control and for such problems most of the above issues have been solved to some satisfactory level, except for coupled ODE-PDE systems. It is expected that well-known ODE techniques and results regarding existence, sufficient conditions, and parametric sensitivity analysis can be extended in a more or less straightforward way to DAEs with a special structure like Hessenberg DAEs. More general DAEs, however, are likely to require new techniques. This is particularly true for the convergence analysis of higher index DAE optimal control problems owing to the gap between the necessary conditions for the discretized problem and those for the continuous problem.

7 Appendix: Auxiliary Results

Theorem 7.1 *Let $D : I \longrightarrow \mathbb{R}^{m\times n}$ be an essentially bounded matrix function in $L^\infty(I,\mathbb{R}^{m\times n})$. Then,*

$$W_D^{1,2}(I,\mathbb{R}^n) = \{x \in L^2(I,\mathbb{R}^n) \mid Dx \in W^{1,2}(I,\mathbb{R}^m)\}$$

is a Hilbert space with scalar product

$$\langle x, y\rangle_{W_D^{1,2}(I,\mathbb{R}^n)} = \langle x, y\rangle_{L^2(I,\mathbb{R}^n)} + \langle (Dx)', (Dy)'\rangle_{L^2(I,\mathbb{R}^m)}.$$

Proof Let $\{x_k\}$ be a Cauchy sequence in $W_D^{1,2}(I,\mathbb{R}^n)$. Then, $\{x_k\}$ is a Cauchy sequence in $L^2(I,\mathbb{R}^n)$ and $\{y_k'\}$ with $y_k := Dx_k$ is a Cauchy sequence in $L^2(I,\mathbb{R}^m)$. Since L^2 is complete, there exist limits $x \in L^2(I,\mathbb{R}^n)$ and $g \in L^2(I,\mathbb{R}^m)$ with $\lim_{k\to\infty} x_k = x$ and $\lim_{k\to\infty} y_k' = g$.

Moreover continuity of the mapping $x \mapsto Dx$ yields

$$\lim_{k\to\infty} y_k = \lim_{k\to\infty} Dx_k = D(\lim_{k\to\infty} x_k) = Dx =: y.$$

It remains to show that $y \in W^{1,2}(I,\mathbb{R}^m)$ and $y' = (Dx)' = g$. To this end for any $\phi \in C_0^\infty(I,\mathbb{R}^m)$ we find by partial integration

$$\begin{aligned} 0 &= \lim_{k\to\infty} \int_I (y_k'(t) - g(t))^\top \phi(t)\, dt \\ &= -\lim_{k\to\infty} \int_I \left(y_k(t) - \int_{t_0}^t g(s)ds \right)^\top \phi'(t)\, dt \\ &= -\int_I \left(y(t) - \int_{t_0}^t g(s)ds \right)^\top \phi'(t)\, dt. \end{aligned}$$

Application of a variation lemma, e.g. [48, Lemma 3.1.9], yields a constant C with

$$y(t) = \int_{t_0}^t g(s)ds + C \qquad (a.e.\ in\ I).$$

Hence $y = Dx \in W^{1,2}(I,\mathbb{R}^m)$ and $y' = g$. Thus, $x \in W_D^{1,2}(I,\mathbb{R}^n)$ which shows the completeness of $W_D^{1,2}(I,\mathbb{R}^n)$. □

Proof of Theorem 2.5:

Proof Let (x, u) be feasible for LQOCP and (2.11). Exploitation of the assumptions and neglecting the explicit time dependence for notational convenience yields

$$
\begin{aligned}
J(x,u) - J(\hat{x},\hat{u}) &= \int_I \frac{1}{2}x^\top Qx - \frac{1}{2}u^\top Ru - \frac{1}{2}\hat{x}^\top Q\hat{x} - \frac{1}{2}\hat{u}^\top R\hat{u}\,dt \\
&= \int_I \frac{1}{2}x^\top Qx + \frac{1}{2}u^\top Ru - \frac{1}{2}\hat{x}^\top Q\hat{x} - \frac{1}{2}\hat{u}^\top R\hat{u} \\
&\qquad +\lambda^\top \left(A(Dx)' + Bx + Pu - q\right) \\
&\qquad -\lambda^\top \left(A(D\hat{x})' + B\hat{x} + P\hat{u} - q\right)\,dt \\
&= \int_I \frac{1}{2}x^\top Qx + \frac{1}{2}u^\top Ru - \frac{1}{2}\hat{x}^\top Q\hat{x} - \frac{1}{2}\hat{u}^\top R\hat{u} \\
&\qquad +\lambda^\top B(x-\hat{x}) + \lambda^\top P(u-\hat{u}) + (A^\top\lambda)^\top \left((Dx)' - (D\hat{x})'\right)\,dt \\
&= \int_I \frac{1}{2}x^\top Qx + \frac{1}{2}u^\top Ru - \frac{1}{2}\hat{x}^\top Q\hat{x} - \frac{1}{2}\hat{u}^\top R\hat{u} \\
&\qquad +\lambda^\top B(x-\hat{x}) + \lambda^\top P(u-\hat{u}) - \left((A^\top\lambda)'\right)^\top (Dx - D\hat{x})\,dt \\
&= \int_I \frac{1}{2}x^\top Qx + \frac{1}{2}u^\top Ru - \frac{1}{2}\hat{x}^\top Q\hat{x} - \frac{1}{2}\hat{u}^\top R\hat{u} \\
&\qquad +\lambda^\top B(x-\hat{x}) + \lambda^\top P(u-\hat{u}) \\
&\qquad -\hat{x}^\top Q(x-\hat{x}) - \lambda^\top B(x-\hat{x}) - \eta^\top S(x-\hat{x})\,dt \\
&= \int_I \frac{1}{2}x^\top Qx + \frac{1}{2}u^\top Ru - \frac{1}{2}\hat{x}^\top Q\hat{x} - \frac{1}{2}\hat{u}^\top R\hat{u} \\
&\qquad -\hat{u}^\top R(u-\hat{u}) - \eta^\top F(u-\hat{u}) - \hat{x}^\top Q(x-\hat{x}) - \eta^\top S(x-\hat{x})\,dt \\
&= \int_I \frac{1}{2}(x-\hat{x})^\top Q(x-\hat{x}) + \frac{1}{2}(u-\hat{u})^\top R(u-\hat{u}) \\
&\qquad - \underbrace{\eta^\top}_{\geq 0}\underbrace{(Sx + Fu - r)}_{\leq 0} + \underbrace{\eta^\top(S\hat{x} + F\hat{u} - r)}_{=0}\,dt \\
&\geq 0,
\end{aligned}
$$

since Q and R are supposed to be uniformly positive semidefinite. □

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