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Differentiability of Consistency Functions

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Differentiability of Consistency Functions for DAE Systems

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Abstract. In the present paper, parametric initial-value problems for differential–algebraic (DAE) systems are investigated. It is known that initial values of DAE systems must satisfy not only the original equations in the system but also derivatives of these equations with respect to time. Whether or not this actually imposes additional constraints on the initial values depends on the particular problem.

Often the initial values are not determined uniquely, so that the resulting degrees of freedom can be used to optimize a given performance index. For this purpose, a class of functions is defined which will be called consistency functions. These functions map a set of parameters, which also include those undetermined initial values, to consistent initial values for the DAE system.

Because of frequent gradient evaluations of the performance index and the constraints with respect to these system parameters needed by many optimization procedures, we state conditions such that the consistency functions represent differentiable functions with respect to these parameters.

Several examples are provided to illustrate the verification of the theoretical assumptions and their differentiability properties.
Key Words. Parametric DAE systems, consistent initial values, sensitivity analysis.

1 Introduction

Many engineering and scientific problems are described by systems of *differential–algebraic equations* (DAEs). Typical applications for such DAE systems arise in multi–body dynamics, process engineering, electric circuit simulation, robot path planning problems or singular and constrained arcs in optimal control problems. Though DAE systems are easy to formulate and are close to the *'engineer's way of thinking'*, they pose several numerical problems: *DAE's are not ODE's*; see Ref. 1.

Besides ill-conditioning, stiffness and stability problems in the numerical solution of such DAE systems, the calculation of *consistent initial values* for nonlinear DAE systems is a demanding problem. Several methods are proposed in the literature. Among others, techniques are discussed that are based on index reduction methods, artificial integration steps (Ref. 2), Taylor series expansions (Ref. 3), graph theoretic algorithms (Ref. 4), projection methods (Ref. 5), or methods that set up the derivative array equations (Refs. 6-7). In all of these articles, a unique solution for the consistent initial values is assumed.

In Büskens and Gerdts (Refs. 8-9), numerical methods are discussed where consistent initial values can be calculated even in the case that no unique solution exists. The proposed methods are based on finite dimensional optimization, where the non–uniqueness is used for an optimal exploitation of the degrees of freedom left in the consistent initial values. An objective function to be defined and certain equality constraints are introduced to guarantee both consistency and optimality of the free initial values. In this article we generalize the numerical investigations of Ref. 8 to a more general class of *consistency functions*. Hereby, a consistency function will be defined as a function which maps a set of parameters or variables to a locally uniquely defined consistent initial value for a given DAE system.

Sensitivity analysis is concerned with the behavior of solutions of a given problem with respect to parameter variations or uncertainties. *Solution differentiability*, i.e., the differentiability w.r.t. these parameters, is of particular importance. The theoretical framework for a sensitivity analysis of optimization problems has been developed by Fiacco (Ref. 10). In this book, the main result on solution differentiability is based on second order sufficient conditions (SSC) and their numerical verification. Since the computation of consistency functions is phrased in terms of an optimization problem, we shall be able to derive conditions which ensure, roughly speaking, that the consistency functions become differentiable functions of special parameters. Second order sufficient conditions (SSC) are used to proof the stability of the solution and the existence of *sensitivity differentials*.

The verification of SSC and the calculation of sensitivity differentials with respect to the parameters by numerical methods, has been proven to be a very powerful and helpful instrument for a multitude of mathematical problems, see Büskens (Ref. 11). The investigation of differentiability properties of consistent initial values with respect to parameters is not only an interesting problem on its own, but also in combination with direct shooting methods for the numerical solution of DAE optimal control problems these sensitivity differentials play a substantial role, see Gerdts (Ref. 12). The intention of this paper is to give the theoretical basis for the applicability of the numerical methods mentioned before.

The paper is organized as follows: First we give a short overview on DAE systems and some of their formulations (Section 2). The index of DAE systems and the consistency of their initial values are discussed in order to define consistency functions. This leads to a nonlinear programming problem (NLP). Well-known necessary and second order sufficient conditions for NLPs are presented in Section 3 in order to establish conditions such that solutions of the NLPs are locally unique. Furthermore, strong differentiability conditions for consistency functions are formulated by applying these results. By extracting relevant information, these conditions can be weakened as described in Section 4. Several examples are discussed in Section 5, which show the applicability of the proposed ideas. A short conclusion completes the paper.

2 Overview and Formulation of the Problem

In the following we investigate parametric DAE systems in the most general *implicit form.* Without loss of generality, we restrict the discussion to autonomous problems:

$$F(x(t), \dot{x}(t), p) = 0, \qquad \text{for all} \quad t \in [t_0, t_f], \tag{1}$$

with a sufficiently smooth function $F : \mathbb{R}^n \times \mathbb{R}^n \times P \to \mathbb{R}^n$, $P \subseteq \mathbb{R}^m$. The argument $x(t) \in \mathbb{R}^n$ denotes the state of the dynamical system (1) at time $t \in [t_0, t_f]$, $\dot{x}(t)$ its derivative w.r.t. t, while p represents an additional (fixed) parameter.

If the Jacobian $F_{\dot{x}} := \partial F / \partial \dot{x}$ is nonsingular for all $t \in [t_0, t_f]$, equation (1) describes an *implicit ordinary differential equation system* (IODE system). In the following we confine the discussion to problems with singular Jacobian $F_{\dot{x}}$ (Refs. 1,13). In this case, Eq. (1) contains differential equations as well as algebraic equations and is called a *differential-algebraic equation system.*

DAE systems arising from engineering applications often have a special structure. For instance dynamic models of chemical engineering processes and electric circuits are described by DAE systems, which are linear in $\dot{x}$:

$$M(x(t), p)\, \dot{x}(t) = f(x(t), p), \tag{2}$$

where $M(x(t), p)$ is singular. Mechanical multi–body systems can be transformed to *semi-explicit* DAE systems:

$$\begin{pmatrix} I & 0 \\ 0 & 0 \end{pmatrix} \begin{pmatrix} \dot{x}(t) \\ \dot{y}(t) \end{pmatrix} = \begin{pmatrix} \dot{x}(t) \\ 0 \end{pmatrix} = \begin{pmatrix} f(x(t), y(t), p) \\ g(x(t), y(t), p) \end{pmatrix} \tag{3}$$

where the matrix M in (2) is characterized by a special structure. Note that only for the differential variables $x(t) \in \mathbb{R}^{n_x}$ a differential equation $\dot{x}(t) = f(x(t), y(t), p)$ is given explicitly and that the dimensions of $y(t)$ and $g(x(t), y(t), p)$ are the same. The *algebraic variable* $y(t) \in \mathbb{R}^{n_y}$ is implicitly given by the *algebraic constraint* $0 = g(x(t), y(t), p)$ or their derivatives w.r.t. time. Therefore in contrast to ODE systems initial value problems for a semi-explicit DAE system with initial values $x(t_0) = x_0$ and $y(t_0) = y_0$ are in general not solvable for arbitrary values (x_0, y_0). This holds for problems of form (1) as well as of form (2). Since the more common formulations (2) and (3) are only special cases of (1), we restrict our considerations to the more general implicit form (1).

The *differentiation index* describes a measure how hard the calculation of consistent initial values is (Ref. 14):

Definition 2.1 (Differentiation Index and Consistency) A natural number $k \in \mathbb{N}_0$ is called the differentiation index of the DAE (1) if it is the smallest number such that from

$$\begin{aligned} F(x(t), \dot{x}(t), p) &= 0, \quad &(4a) \\ \frac{d}{dt} F(x(t), \dot{x}(t), p) &= 0, \quad &(4b) \\ &\vdots \\ \frac{d^k}{dt^k} F(x(t), \dot{x}(t), p) &= 0, \quad &(4c) \end{aligned}$$

an explicit ODE system of type

$$\dot{x}(t) = \Psi(x(t), p) \tag{5}$$

can be derived by algebraic manipulations. A set of initial values $(x_0, \dot{x}_0) \in \mathbb{R}^{2n}$ for the DAE system (1) of differentiation index k at $t = t_0$ is called consistent, if $(x_0, \dot{x}_0)$ fulfills Eqs. (4) and $\dot{x}_0 = \Psi(x_0, p)$. We call the DAE (1) solvable if there exist consistent initial values such that the ODE system (5) is solvable for each consistent initial value.

The derivatives in Eq. (4) are short-hand notations. For example, it holds

$$\frac{d}{dt} F(x(t), \dot{x}(t), p) = F_x(x(t), \dot{x}(t), p) \cdot \dot{x}(t) + F_{\dot{x}}(x(t), \dot{x}(t), p) \cdot \ddot{x}(t).$$

The higher order derivatives are defined recursively, as described in more detail in Leimkuhler et al. (Ref. 3). In particular, notice that the k^{th} derivative of F includes the derivatives $x, \dot{x}, \ddot{x}, \ldots, x^{(k+1)}$. Implicitly it is assumed that these derivatives actually exist. Furthermore, notice that a consistent initial value in general depends on the parameters p.

Note that an ODE system (the Jacobian $F_{\dot{x}}$ is nonsingular) has the differentiation index $k = 0$. Depending on the index, consistent initial values x_0 yield initial values $\dot{x}_0$ for the first derivatives by equation (5) and must satisfy (4):

$$\begin{aligned} F(x_0, \dot{x}_0, p) &= 0, \quad &(6a) \\ \frac{d}{dt} F(x_0, \dot{x}_0, p) &= 0, \quad &(6b) \\ &\vdots \\ \frac{d^k}{dt^k} F(x_0, \dot{x}_0, p) &= 0. \quad &(6c) \end{aligned}$$

In general, the user may have some information about the initial state. Hence the following problem can be stated:

Problem 2.1 (Consistent Initial Values) Find consistent initial values $(x(t_0), \dot{x}(t_0))$ such that the DAE system (1) can be solved subject to an additional set of equality constraints defined by the function $\varphi : \mathbb{R}^n \times \mathbb{R}^n \times P \to \mathbb{R}^r$, $r \leq n$:

$$\begin{aligned} F(x(t), \dot{x}(t), p) &= 0, \qquad \text{for all} \quad t \in [t_0, t_f], & \text{(7a)} \\ \varphi(x(t_0), \dot{x}(t_0), p) &= 0. & \text{(7b)} \end{aligned}$$

In the literature the special case $\varphi(x(t_0), \dot{x}(t_0), p) := x(t_0) - p$ often can be found.

Often, consistent initial values are determined uniquely by Eqs. (7). In this paper we are particularly interested in the case where consistent initial values are not uniquely determined for a given parameter p. For this purpose we introduce the concept of *consistency functions*.

Definition 2.2 (Consistency Function) Let $P \subseteq \mathbb{R}^m$ and $con : P \to \mathbb{R}^{2n}$ be a function with $con(p) = (con_1(p), con_2(p))$, $con_1, con_2 : P \to \mathbb{R}^n$, that solves Problem 2.1 for all $p \in P$, i.e., $F(con_1(p), con_2(p), p) = 0$ and $\varphi(con_1(p), con_2(p), p) = 0$. Then con is called a consistency function.

In the following we will concentrate on C^1-consistency functions which have a wide area of applications, e.g. in optimization problems and optimal control problems. Our intention is to define a class of consistency functions for problems with both non-unique and unique solutions. Hence our proposal is to investigate consistency functions which are defined by the solutions of nonlinear optimization problems, e.g.,

$$\begin{aligned} &\text{(NLP1(p))} \qquad \min_z \quad g(z, p), && \text{(8a)} \\ &\qquad\qquad\qquad \text{s.t.} \quad F(x(t_0), \dot{x}(t_0), p) = 0, && \text{(8b)} \\ &\qquad\qquad\qquad\qquad \frac{d}{dt} F(x(t_0), \dot{x}(t_0), p) = 0, && \text{(8c)} \\ &\qquad\qquad\qquad\qquad \vdots \\ &\qquad\qquad\qquad\qquad \frac{d^k}{dt^k} F(x(t_0), \dot{x}(t_0), p) = 0, && \text{(8d)} \\ &\qquad\qquad\qquad\qquad \varphi(x(t_0), \dot{x}(t_0), p) = 0. && \text{(8e)} \end{aligned}$$

The objective function $g(z, p)$ has to be defined here appropriately for $z := (x(t_0), \dot{x}(t_0), \ldots, x^{(k+1)}(t_0))$. Let $\bar{x}(p) = (\bar{x}_0(p), \ldots, \bar{x}_0^{(k+1)}(p))^T$ be an optimal solution of (8), then $con(p) := (\bar{x}_0(p), \dot{\bar{x}}_0(p))^T$ defines a consistency function.

In the sequel we will formulate conditions such that the consistency function defined by the solution of (8) is a C^1 function.

Please note that if no unique consistent initial value is given by the equality constraints in (8), we have to define the objective $g(z, p)$ in (8) such that the optimal solution of (NLP1(p)) results in a locally unique solution.

In the sequel we tacitly assume that problem 2.1 is solvable.

3 Strong Solution Differentiability of Consistency Functions

A first step for the solution of problem (8) is to formulate necessary conditions. Problem (8) represents a finite dimensional nonlinear optimization problem (NLP) with *equality* constraints. Hence let

$$G(z,p) \quad := \quad \begin{pmatrix} F(x(t_0),\dot{x}(t_0),p) \\ \frac{d}{dt}F(x(t_0),\dot{x}(t_0),p) \\ \vdots \\ \frac{d^k}{dt^k}F(x(t_0),\dot{x}(t_0),p) \\ \varphi(x(t_0),\dot{x}(t_0),p) \end{pmatrix} \tag{9}$$

for $G : \mathbb{R}^{(k+2)n} \times P \to \mathbb{R}^{(k+1)n+r}$, and z defined as in (8). Then Problem (8) is of form below:

$$\text{(NLP(p))} \qquad \min_z \quad g(z,p), \tag{10a}$$
$$\text{s.t.} \quad G(z,p) = 0. \tag{10b}$$

Definition 3.1 (Admissible Set, Local Minimum)

(a) The set

$$S(p) := \{z \in \mathbb{R}^{(k+2)n} | G(z,p) = 0\} \tag{11}$$

is called a set of admissible variables or admissible set. A variable $z \in S(p)$ is called admissible variable.

(b) A variable $\bar{z} \in S(p)$ is called a local, resp. strong local minimum of Problem (10), if a neighborhood $V \subseteq \mathbb{R}^{(k+2)n}$ of $\bar{z}$ exists, such that

$$g(\bar{z},p) \le g(z,p) \text{ for all } z \in S(p) \cap V$$

resp.

$$g(\bar{z},p) < g(z,p) \text{ for all } z \in S(p) \cap V, z \neq \bar{z}.$$

Let us introduce the Lagrangian function for the nonlinear optimization problem (NLP(p))

$$L \quad : \quad \mathbb{R}^{(k+2)n} \times \mathbb{R}^{(k+1)n+r} \times P \longrightarrow \mathbb{R}, \tag{12a}$$
$$L(z,\mu,p) \quad := \quad g(z,p) + \mu^T G(z,p), \tag{12b}$$

with multiplier $\mu \in \mathbb{R}^{(k+1)n+r}$, where $(\cdot)^T$ denotes the transpose. Herewith first order necessary optimality conditions can be formulated, cf., e.g., Fletcher (Ref. 15):

Theorem 3.1 (Strong Necessary Optimality Conditions for (NLP(p))) Let g and G be continuously differentiable with respect to z in a neighborhood of a local minimum $\bar{z}$ for Problem (10). Furthermore let the Jacobian $G_z(\bar{z}, p)$ be of full rank. Then there exist a uniquely determined multiplier $\mu \in \mathbb{R}^{(k+1)n+r}$ satisfying

$$L_z(\bar{z}, \mu, p) = g_z(\bar{z}, p) + \mu^T G_z(\bar{z}, p) = 0. \tag{13}$$

Besides necessary conditions, second order sufficient conditions (SSC) have to be checked to ensure the local optimality of solutions. These SSC play an important role for selecting optimal solutions. Another important aspect of SSC appears in the *sensitivity analysis* of Problem (10) where SSC are used to proof the existence of *sensitivity differentials*. SSC for problems of form (NLP(p)) can be validated numerically using linear algebra techniques.

Fiacco (Ref. 10) has derived conditions which ensure that solutions (z, μ) of Eq. (13) become differentiable functions of the parameter p. Let us fix a *reference* or *nominal* parameter p^0 to conduct a local sensitivity analysis. Furthermore let us consider problem (NLP(p^0)) as the *unperturbed* or *nominal* problem. We assume that there exists a local solution (z^0, μ^0) of the reference problem (NLP(p^0)) satisfying the necessary KKT conditions (13) for the nominal parameter p^0.

As a first step let us summarize different assumptions to formulate conditions for the solution differentiability of the optimal solutions of (8). We focus on the vector valued function $G(z, p)$ in Eq. (9).

Assumption 3.1

(i) Let the functions $G(z, p)$ and $g(z, p)$ be twice continuously differentiable with respect to z in a neighborhood of $z_0 := (x_0, \dot{x}_0, \ldots, x_0^{(k+1)})$ for the nominal parameter $p = p^0$.

(ii) Let the rank of the Jacobian of G be maximal, i.e.,

$$\operatorname{rank}(G_z(x_0, \dot{x}_0, \ldots, x_0^{(k+1)}, p^0)) = (k+1)n + r. \tag{14}$$

(iii) Assume that there exists a multiplier $\mu_0 \in \mathbb{R}^{(k+1)n+r}$, such that z_0 and μ_0 satisfy the necessary optimality conditions of Theorem (3.1) with the Lagrangian

$$L(z_0, \mu_0, p^0) = g(x_0, \dot{x}_0, \ldots, x_0^{(k+1)}, p^0) + \mu_0^T G(x_0, \dot{x}_0, \ldots, x_0^{(k+1)}, p^0). \tag{15}$$

(iv) Let the functions $g_z(z, p)$, $G_z(z, p)$ and $G(z, p)$ be continuously differentiable with respect to p in a neighborhood of z_0 and p^0.

(v) The Hessian of the Lagrangian is positive definite on

$$\operatorname{Ker}(G_z(x_0, \dot{x}_0, \ldots, x_0^{(k+1)}, p^0)). \tag{16}$$

Due to the special structure of the derivatives in Eq. (4) we find that Assumption 3.1 (i) is equivalent to

Assumption 3.1 (i') Let the DAE in (1) be of index k. Moreover let the function $F(x,\dot{x},p)$ be $k+2$ times continuously differentiable with respect to x and $\dot{x}$, let the function $\varphi(x,\dot{x},p)$ be twice continuously differentiable with respect to x and $\dot{x}$ and let the function $g(z,p)$ be twice continuously differentiable with respect to z in a neighborhood of z_0 for the nominal parameter $p=p^0$.

Similarly, Assumption 3.1 (iv) can be expressed in terms of the components of G in (9).

Note, that if Assumptions 3.1 (i)-(iii) hold, $z_0 = (x_0, \dot{x}_0, \ldots, x_0^{(k+1)})$ and μ_0 satisfy the conditions of Theorem 3.1, especially μ_0 is unique.

Then it holds, cf. Fiacco (Ref. 10):

Theorem 3.2 (Strong Sensitivity Analysis for Solutions of (NLP1(p))) Let Assumption 3.1 be fulfilled for the NLP (8). Then,

(a) $z_0 = (x_0, \dot{x}_0, \ldots, x_0^{(k+1)})$ is a strong local minimum of (8) and fulfills Eqs. (6). In particular, $(x_0, \dot{x}_0)$ is a consistent initial value,

(b) there exists a neighborhood $P^0 \subseteq P$ of p^0 and unique continuously differentiable functions $x_0^i : P^0 \longrightarrow \mathbb{R}^n$, $i = 0, \ldots, k+1$, and $\mu_0 : P^0 \longrightarrow \mathbb{R}^{(k+1)n+r}$ with

  (i) $x_0^{(i)}(p^0) = x_0^{(i)}$, $i = 0, \ldots, k+1$,

  (ii) $\mu_0(p^0) = \mu_0$,

  (iii) $(x_0(p), \ldots, x_0^{(k+1)}(p))$, $\mu_0(p)$ satisfy the conditions in Assumption 3.1 for the perturbed problem (NLP1(p)) for all $p \in P^0$.
  In particular $(x_0(p), \ldots, x_0^{(k+1)}(p), \mu_0(p))$ is a unique strong local minimum of (NLP1(p)),

c) the first order derivatives of $(x_0(p), \ldots, x_0^{(k+1)}(p))$ and $\mu_0(p)$ are given by

$$\begin{pmatrix} \frac{dx_0}{dp}(p^0) \\ \vdots \\ \frac{dx_0^{(k+1)}}{dp}(p^0) \\ \frac{d\mu_0}{dp}(p^0) \end{pmatrix} = - \begin{pmatrix} L_{zz}(z_0,\mu_0,p^0) & G_z(z_0,p^0)^\top \\ G_z(z_0,p^0) & 0 \end{pmatrix}^{-1} \begin{pmatrix} L_{zp}(z_0,\mu_0,p^0) \\ G_p(z_0,p^0) \end{pmatrix}. \tag{17}$$

As a direct consequence of Theorem 3.2 we find:

Theorem 3.3 (Strong Differentiability Conditions for the Consistency Function con(p)) Let Assumptions 3.1 be fulfilled for the NLP (8) with reference parameter $p = p^0$. Then, there exists a neighborhood $P^0 \subseteq P$ of p^0 such that $con(p) := (x_0(p), \dot{x}_0(p))^T$ defines a C^1 consistency function on P^0.

Assumption 3.1 describes sufficient conditions needed to proof the differentiability of consistency functions defined by (8). However, we can in general not expect that all of these conditions are fulfilled as the simple Example 3.1 shows:

Example 3.1 *Let* $z := (x_1(t_0), x_2(t_0), \ldots, x_1^{(k+1)}(t_0), x_2^{(k+1)}(t_0))$ *and* $t_0 = 0$*:*

$$\min_{z} \quad x_2^2(t_0), \tag{18a}$$

$$s.t. \quad \dot{x}_1(t) = \begin{cases} \frac{1}{6}x_2^3(t), & \text{if } x_2(t) \geq 0, \\ -\frac{1}{6}x_2^3(t), & \text{if } x_2(t) < 0, \end{cases} \tag{18b}$$

$$x_2(t) - t = 0, \tag{18c}$$

$$x_1(t_0) - p = 0. \tag{18d}$$

Obviously, the index of the DAE system in (18) is $k = 1$ and a unique solution is given by $x_2(t_0) = \dot{x}_1(t_0) = \ddot{x}_1(t_0) = \ddot{x}_2(t_0) = 0$, $x_1(t_0) = p$, $\dot{x}_2(t_0) = 1$.
Hence $z = (x_1(t_0), x_2(t_0), \dot{x}_1(t_0), \dot{x}_2(t_0), \ddot{x}_1(t_0), \ddot{x}_2(t_0))$, we find the (NLP1(p))

$$\min_{z} \quad x_2^2(t_0), \tag{19a}$$

$$\text{s.t.} \quad \dot{x}_1(t_0) = \begin{cases} \frac{1}{6}x_2^3(t_0), & \text{if } x_2(t_0) \geq 0, \\ -\frac{1}{6}x_2^3(t_0), & \text{if } x_2(t_0) < 0, \end{cases} \tag{19b}$$

$$x_2(t_0) = t_0, \tag{19c}$$

$$\ddot{x}_1(t_0) = \begin{cases} \frac{1}{2}x_2^2(t_0), & \text{if } x_2(t_0) \geq 0, \\ -\frac{1}{2}x_2^2(t_0), & \text{if } x_2(t_0) < 0, \end{cases} \tag{19d}$$

$$\dot{x}_2(t_0) = 1, \tag{19e}$$

$$x_1(t_0) = p. \tag{19f}$$

Since the equation for $\ddot{x}_1(t_0)$ in (19) is not twice continuously differentiable with respect to $x_2(t_0)$, Assumption 3.1 is not fulfilled. Hence Theorem 3.2 and Theorem 3.3 can not be applied. On the other hand, $\ddot{x}_1(t)$ is not used to find consistent initial values for the DAE system (18). Hence we can dispense with Eqs. (19) for $\ddot{x}_1(t_0)$.

4 Weak Solution Differentiability of Consistency Functions

Concerning the difficulties with Example 3.1 in applying Theorem 3.2 and Theorem 3.3 we will show in this section, that the differentiability assumption 3.1 can be appropriately weakened. The idea is to determine relevant equations for finding consistent initial values.

First we reorder the components of the vector $x(t_0)$ of initial values and then partition it as follows:

$$x(t_0) = (x^N(t_0), x^B(t_0))^T$$

with

$$\begin{aligned} x^N(t_0) &= (x_1^N(t_0), \dots, x_{n-q}^N(t_0))^T, \quad x_i^N(t_0) \in \{x_1(t_0), \dots, x_n(t_0)\}, \\ x^B(t_0) &= (x_1^B(t_0), \dots, x_q^B(t_0))^T, \quad x_i^B(t_0) \in \{x_1(t_0), \dots, x_n(t_0)\}. \end{aligned}$$

Here, $x^N(t_0)$ denotes the vector of initial values which can be expressed by the unspecified (free) initial values in the vector $x^B(t_0)$. In the following, we use the notation $\mathbb{N}_{\bar{n}} := \{1, 2, \dots, \bar{n}\}$, $\bar{n} \in \mathbb{N}$.

Definition 4.1 (Degree of Freedom) Suppose that (7) is solvable. A natural number $q \in \{1, \dots, n\}$ is called *degree of freedom* in the initial vector $x(t_0)$ of system (7), i.e., the dimension of $x^B(t_0)$, if it is the largest number, such that the following holds: $n_B^E \in \mathbb{N}_{(k+1)n+r}$ is the smallest number of equations, such that $\bar{G} = (\bar{G}_1, \dots, \bar{G}_{n_B^E})^T$ is a collection of equations of (9), and $\hat{z} = (\hat{z}_1, \dots, \hat{z}_{n_B^V})^T$ is a collection of variables, such that $\bar{G}(\hat{z}, p) = 0$ can be transformed into

$$\begin{pmatrix} x^N(t_0) \\ \dot{x}(t_0) \end{pmatrix} = \tilde{G}(x^B(t_0), p). \tag{20}$$

Remark 4.1 Herewith, the dependent initial values $x_i^N(t_0)$ are expressed as functions of the free initial values $x_j^B(t_0)$. The second equation in (20) corresponds to the underlying ODE (5) and since (7) is assumed to be solvable, there always exists a transformation like (20).

Definition 4.2 (Basis of Necessary Variables and Equations) Let $q \in \{1, \dots, n\}$ be the degree of freedom in (7). Let $\bar{G} = (\bar{G}_1, \dots, \bar{G}_{n_B^E})^T$ and $\hat{z} = (\hat{z}_1, \dots, \hat{z}_{n_B^V})^T$ be defined as in Definition 4.1. Furthermore let $z^* = (z_1^*, \dots z_{n_B^E}^*)^T$, $z_i^* \in \{\hat{z}_1, \dots, \hat{z}_{n_B^V}\}$, $i = 1, \dots, n_B^E$, with $\bar{G}_{z^*}$ nonsingular. We call the set $B^V \subseteq (\mathbb{N}_{k+2} \cup \{0\}) \times \mathbb{N}_n$ of tuples of indices *basis of necessary variables* for Problem 2.1 and $B^E \subseteq (\mathbb{N}_{k+1} \cup \{0\}) \times \mathbb{N}_n$ of tuples of indices *basis of necessary equations* for Problem 2.1 if

a) $(1, j) \in B^V$, if $x_j(t_0) \in \{x_1^N(t_0), \dots, x_{n-q}^N(t_0)\}$,
$(2, j) \in B^V$, for all $j \in \mathbb{N}_n$,
$(i, j) \in B^V$, if $x_j^{(i-1)} = \frac{d^{i-1}}{dt^{i-1}} x_j(t_0) \in \{z_1^*, \dots, z_{n_B^E}^*\}$, $i \geq 3$

b) $(0, j) \in B^E$, if $\varphi_j(t_0) \in \{\bar{G}_1, \ldots, \bar{G}_{n_B^E}\}$,
$(i, j) \in B^E$, if $\frac{d^{i-1}}{dt^{i-1}} F_j(x(t_0), \dot{x}(t_0), p) \in \{\bar{G}_1, \ldots, \bar{G}_{n_B^E}\}$.

Remark 4.2

- In the sets of tuples B^V and B^E, resp., the first index is associated with the derivative and the second with the component of the vector $x(t_0)$, resp., of the equation in (9).
- For a given problem the determination of a basis of necessary variables and a basis of necessary equations is a demanding task, since a carefully analysis of all functions in Problem 2.1 is necessary, compare Pantelides (Ref. 4). The intention of this paper is the analysis of differentiability properties of consistency functions, hence we do not discuss how to obtain these bases.

Those definitions ensure that if a basis of necessary variables and equations exist, the system (9) can be transformed into an ODE system like (5), where the maximal information on $x(t_0)$ is exploited by the consistency equations. Note, that neither the basis of necessary variables nor of equations need to be unique as well as their dimensions. Furthermore the regularity condition in Definition 4.2 ensures the applicability of the implicit function theorem and herewith the following

Theorem 4.1 (Weak Solution Differentiability) Let B^V be a basis of necessary variables of dimension n_B^E, and let B^E be a basis of necessary equations for Problem 2.1. Furthermore let $\hat{z} = (\hat{z}_1, \ldots, \hat{z}_{n_B^E})^T$ be necessary variables B^V and $\bar{G}$ necessary equations B^E. As collection of necessary variables and initial variables $x(t_0)$ we define $C := \{\hat{z}_1, \ldots, \hat{z}_{n_B^E}\} \cup \{x_1(t_0), \ldots, x_n(t_0)\} = \{z_1, \ldots, z_{\hat{n}}\}$, $\hat{n} = n_B^E + q$, and $z := (z_1, \ldots, z_{\hat{n}})^T$. Suppose that (z^0, μ^0) satisfies Assumption 3.1 for the problem

$$\text{(NLP2(p))} \qquad \min_z \quad g(z, p), \tag{21a}$$

$$\text{s.t.} \quad \bar{G}(z, p) = 0. \tag{21b}$$

Then

(a) (z^0, μ^0) is a strong local minimum of (NLP2(p^0)),

(b) there exists a neighborhood $P^0 \subseteq P$ of $p = p^0$ and unique continuously differentiable functions $z : P^0 \longrightarrow \mathbb{R}^{(k+2)n}$, $\mu : P^0 \longrightarrow \mathbb{R}^{(k+1)n+r}$ with the following:

 (i) $z(p^0) = z^0$,

 (ii) $\mu(p^0) = \mu^0$,

 (iii) for all $p \in P^0$: $z(p)$, $\mu(p)$ satisfy Assumption 3.1 for the perturbed problem (NLP2(p)). In particular $(z(p), \mu(p))$ is a unique strong local minimum of (NLP2(p)),

(c) the first order derivatives of $z(p)$ and $\mu(p)$ are given by

$$\begin{pmatrix} \frac{dz}{dp}(p^0) \\ \frac{d\mu}{dp}(p^0) \end{pmatrix} = - \begin{pmatrix} L_{zz}(z^0, \mu^0) & \bar{G}_z(z^0)^T \\ \bar{G}_z(z^0) & 0 \end{pmatrix}^{-1} \begin{pmatrix} L_{zp}(z^0, \mu^0) \\ \bar{G}_p(z^0) \end{pmatrix}, \tag{22}$$

where the Lagrangian L in (22) is given by

$$L(z, \mu, p) := g(z, p) + \mu^T \bar{G}(z, p). \tag{23}$$

The proof of this theorem is equivalent to that of Theorem 3.2 and will not be discussed here. Besides the weaker assumptions, this formulation is especially advantageous in practical applications, e.g., for semi-explicit DAE systems, since the number of variables and equations in (NLP2(p)) is generally (considerably) reduced in comparison to (NLP1(p)).

Again as a direct consequence we find:

Theorem 4.2 (Weak Differentiability Conditions for the Consistency Function con(p)) Suppose there exist consistent initial values for Problem 2.1 and the assumptions in Theorem 4.1 are fulfilled for a reference parameter $p = p^0$. Without loss of generality let $z_i = x_i(t_0)$, $z_{n+i} = \dot{x}_i(t_0)$ for $i = 1, \ldots, n$ and z as in Theorem 4.1. Then, for $x_0(t_0) = (x_1(t_0), \ldots, x_n(t_0))^T$, $\dot{x}_0(t_0) = (\dot{x}_1(t_0), \ldots, \dot{x}_n(t_0))^T$ there exists a neighborhood $P^0 \subseteq P$ of p^0 such that $con(p) := (x_0(p), \dot{x}_0(p))^T$ defines a C^1 consistency function on P^0.

This implies that for p near to p^0 the unperturbed solution (z^0, μ^0) can be embedded into a C^1–family of perturbed optimal solutions $(z(p), \mu(p))$ for (NLP(p)) with $(z(p_0), \mu(p_0)) = (z_0, \mu_0)$. Note again, that in general it is not an easy task to specify a basis of necessary variables and a basis of necessary equations. Hence a carefully analysis of all functions in Problem 2.1 is necessary.

5 Examples

Three different examples will be discussed in this section. In general the nominal perturbation parameter p^0 represents a fixed value. In the sequel we evaluate the theoretical results from the previous sections in an analytical way. This helps us to demonstrate, that the derivatives of the consistency function defined in Theorem 3.3 [resp. Theorem 4.2] calculated by formula (17) [resp. formula (22)] coincide with a direct differentiation of the solutions obtained after evaluating the necessary conditions (13).

Example 5.1 As the first example let us revisit Example 3.1, which could not be solved according to Theorem 3.2 [resp. Theorem 3.3] because of the too strong differentiability assumptions. By defining the basis of necessary variables and equations

$$
\begin{aligned}
B^V &:= \{(1,1),(1,2),(2,1),(2,2)\}, && (24a)\\
B^E &:= \{(0,1),(1,1),(1,2),(2,2)\} && (24b)
\end{aligned}
$$

we obtain for $t_0 = 0$:

$$
\begin{aligned}
z &:= (x_1(t_0), x_2(t_0), \dot{x}_1(t_0), \dot{x}_2(t_0))^T, && (25a)\\
\bar{G}(z,p^0) &:= \begin{pmatrix} \dot{x}_1(t_0) - \frac{1}{6}x_2(t_0)^3 \\ x_2(t_0) - t_0 \\ \dot{x}_2(t_0) - 1 \\ x_1(t_0) - p^0 \end{pmatrix} = 0, \qquad \text{if } x_2(t_0) \geq 0, && (25b)\\
\bar{G}(z,p^0) &:= \begin{pmatrix} \dot{x}_1(t_0) + \frac{1}{6}x_2(t_0)^3 \\ x_2(t_0) - t_0 \\ \dot{x}_2(t_0) - 1 \\ x_1(t_0) - p^0 \end{pmatrix} = 0, \qquad \text{if } x_2(t_0) < 0. && (25c)
\end{aligned}
$$

For $\mu \in \mathbb{R}^4$ the Lagrangian is given by $L(z,\mu,p^0) = x_2(t_0)^2 + \mu^T\bar{G}(z,p^0)$. Evaluating the necessary conditions of Theorem 3.1 yields $L_z(z,\mu,p^0) = (x_2(t_0)^2)_z + \mu^T\bar{G}_z(z,p^0) = 0$ and, together with the equality constraints (25), we obtain

$$
\begin{aligned}
\bar{z} &= (p^0,0,0,1)^T, && (26a)\\
\bar{\mu} &= (0,0,0,0)^T && (26b)
\end{aligned}
$$

as a candidate for an optimal solution of

$$
\begin{aligned}
\min_z \quad & x_2(t_0)^2, && (27a)\\
\text{s.t.} \quad & \bar{G}(z,p^0) = 0. && (27b)
\end{aligned}
$$

To check the second order sufficient conditions for $\bar{z}$ and $\bar{\mu}$ we calculate

$$
L_{zz}(\bar{z},\bar{\mu},p^0) = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 2 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix} \qquad (28)
$$

and

$$
\bar{G}_z(\bar{z},p^0) = \begin{pmatrix} 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 1 & 0 & 0 & 0 \end{pmatrix}. \qquad (29)
$$

Since $\bar{G}_z(\bar{z},p^0)$ is of full rank we find $\mathrm{Ker}(\bar{G}_z(\bar{z},p^0)) = (0,0,0,0)^T$ and the Hessian $L_{zz}(\bar{z},\bar{\mu},p^0)$ in (28) is positive definite on $\mathrm{Ker}(\bar{G}_z(\bar{z},p^0))\backslash\{0\}$ (compare Assumption 3.1.5).Hence $(\bar{z},\bar{\mu})$ is a strong local minimum of (27). Since all differentiability properties are fulfilled we can apply Theorem 4.1 and Theorem 4.2 and find that there exists a neighborhood $P(p^0)$ for any reference parameter $p = p^0$ and a unique C^1 consistency function $con : P(p^0) \longrightarrow \mathbb{R}^{2n}$:

$$
\mathrm{con(p) := (x_0(p), \dot{x}_0(p))^T = (z_1(p), z_2(p), z_3(p), z_4(p))^T}. \qquad (30)
$$

The derivative $\frac{d\text{con}}{dp}(p^0)$ can be calculated with

$$L_{zp}(\bar{z},\bar{\mu},p^0) = \begin{pmatrix} 0 \\ 0 \\ 0 \\ 0 \end{pmatrix}, \qquad \bar{G}_p(\bar{z},p^0) = \begin{pmatrix} 0 \\ 0 \\ 0 \\ -1 \end{pmatrix}, \tag{31}$$

and

$$\begin{pmatrix} L_{zz}(\bar{z},\bar{\mu},p^0) & \bar{G}_z(\bar{z},p^0)^T \\ \bar{G}_z(\bar{z},p^0) & 0 \end{pmatrix}^{-1} = \begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & -2 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix} \tag{32}$$

by applying Formula (22) as

$$\frac{d\text{con}}{dp}(p^0) = (1,0,0,0). \tag{33}$$

This coincides with the direct differentiation of $\bar{z}$ in (26) with respect to p^0.

Example 5.2 (Implicit Problem) Assume the following implicitly given problem of index $k = 1$:

$$\begin{pmatrix} x_2(t) & -x_3(t) & 0 \\ -x_2(t) & x_3(t) & 0 \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} \dot{x}_1(t) \\ \dot{x}_2(t) \\ \dot{x}_3(t) \end{pmatrix} - \begin{pmatrix} x_3(t) \\ x_1(t) \\ x_1(t) + x_2(t) \end{pmatrix} = 0. \tag{34}$$

We try to find consistent initial values for $(x_2(t_0), x_3(t_0))$ near to given values (p_1^0, p_2^0):

$$\begin{array}{ll} \min\limits_{\tilde{z}} & (x_2(t_0) - p_1^0)^2 + (x_3(t_0) - p_2^0)^2, \\ \text{subject to} & \text{the DAE system (34) and its first derivatives,} \end{array} \tag{35}$$

where $\tilde{z}$ is defined by

$$\tilde{z} := (x(t_0), \dots, x^{(k+1)}(t_0))^T. \tag{36}$$

All differentiability assumptions hold for Theorem 3.2 and Theorem 3.3. However we use Theorem 4.1 and Theorem 4.2 and follow the ideas of Section 4. A basis of necessary variables and equations is given by

$$B^V \;:=\; \{(1,1),(1,2),(2,1),(2,2),(2,3),(3,1)\}, \tag{37a}$$
$$B^E \;:=\; \{(1,1),(1,2),(1,3),(2,1),(2,2),(2,3)\}. \tag{37b}$$

This gives

$$z := (x_1(t_0), x_2(t_0), x_3(t_0), \dot{x}_1(t_0), \dot{x}_2(t_0), \dot{x}_3(t_0), \ddot{x}_1(t_0))^T,$$
$$\bar{G}(z,p^0) := \begin{pmatrix} x_2\dot{x}_1 - x_3 - x_3\dot{x}_2 \\ x_3\dot{x}_2 - x_1 - x_2\dot{x}_1 \\ x_2 + x_1 \\ \dot{x}_2\dot{x}_1 + x_2\ddot{x}_1 - \dot{x}_3 - \dot{x}_2\dot{x}_3 - x_3\ddot{x}_2 \\ \dot{x}_3\dot{x}_2 + x_3\ddot{x}_2 - \dot{x}_1 - \dot{x}_1\dot{x}_2 - x_2\ddot{x}_1 \\ \dot{x}_2 + \dot{x}_1 \end{pmatrix} = 0, \tag{38}$$

where all components in $\bar{G}(z,p^0)$ are evaluated at t_0. Please note, that the component $\ddot{x}_2$ occurs in (38). But, as we will see later, it turns out that this variable has no influence on the initial values $x(t_0)$ and $\dot{x}(t_0)$.

For $\mu \in \mathbb{R}^6$ the Lagrangian is given by $L(z,\mu,p^0) = (x_2(t_0)-p_1^0)^2+(x_3(t_0)-p_2^0)^2+\mu^T\bar{G}(z,p^0)$. The equality constraints from $\bar{G}(z,p^0) = 0$ in (38) and the necessary conditions in Theorem 3.1 yield

$$\begin{aligned} \bar{z} &:= (-\frac{1}{2}(p_1^0+p_2^0), \frac{1}{2}(p_1^0+p_2^0), \frac{1}{2}(p_1^0+p_2^0), \frac{1}{2}, -\frac{1}{2}, -\frac{1}{2}, \ddot{x}_2,)^T, && \text{(39a)} \\ \bar{\mu} &:= (p_1^0-p_2^0, p_1^0-p_2^0, p_1^0-p_2^0, 0, 0, 0,)^T. && \text{(39b)} \end{aligned}$$

The Hessian of the Lagrangian evaluated at $(\bar{z},\bar{\mu})$ is given by

$$L_{zz}(\bar{z},\bar{\mu},p^0) = \begin{pmatrix} 0&0&0&0&0&0&0 \\ 0&2&0&0&0&0&0 \\ 0&0&2&0&0&0&0 \\ 0&0&0&0&0&0&0 \\ 0&0&0&0&0&0&0 \\ 0&0&0&0&0&0&0 \\ 0&0&0&0&0&0&0 \end{pmatrix} \tag{40}$$

while the Jacobian of the constraints yield for $\beta = \frac{1}{2}(p_1^0+p_2^0)$,

$$\bar{G}_z(\bar{z},p^0) = \begin{pmatrix} 0 & \frac{1}{2} & -\frac{1}{2} & \beta & -\beta & 0 & 0 \\ -1 & -\frac{1}{2} & -\frac{1}{2} & -\beta & \beta & 0 & 0 \\ 1 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & \ddot{x}_2 & -\ddot{x}_2 & -\frac{1}{2} & 1 & -\frac{1}{2} & \beta \\ 0 & -\ddot{x}_2 & \ddot{x}_2 & -\frac{1}{2} & -1 & -\frac{1}{2} & -\beta \\ 0 & 0 & 0 & 1 & 1 & 0 & 0 \end{pmatrix}. \tag{41}$$

The Jacobian $\bar{G}_z(\bar{z},p^0)$ is of maximal rank, hence the dimension of the kernel is one. We find $\mathrm{Ker}(\bar{G}_z(\bar{z},p^0)) = \{v \in \mathbb{R}^7 : v = (-\alpha,\alpha,\alpha,0,0,0,0)^T,\ \alpha \in \mathbb{R}\}$ and thus obtain

$$v^T L_{zz}(\bar{z},\bar{\mu},p^0)v = 4\alpha^2 \tag{42}$$

for $v \in \mathrm{Ker}(\bar{G}_z(\bar{z},p^0))$. Hence, the Hessian is positive definite on $\mathrm{Ker}(\bar{G}_z(\bar{z},p^0))\backslash\{0\}$ (compare Assumption 3.1.5). Thus $(\bar{z},\bar{\mu})$ is a strong local minimum of (34). Since all differentiability properties are fulfilled we can apply Theorem 4.1 and Theorem 4.2 and find that there exists a neighborhood $P(p^0)$ for any reference parameter $p = p^0$ and a unique C^1 consistency function $con : P(p^0) \longrightarrow \mathbb{R}^{2n}$:

$$\mathrm{con(p)} := (\mathrm{x_0(p)}, \dot{\mathrm{x}}_0(\mathrm{p}))^{\mathrm{T}} = (\mathrm{z_1(p)}, \mathrm{z_2(p)}, \ldots, \mathrm{z_6(p)})^{\mathrm{T}}. \tag{43}$$

With

$$L_{zp}(\bar{z},\bar{\mu},p^0) = \begin{pmatrix} 0&0 \\ -2&0 \\ 0&-2 \\ 0&0 \\ 0&0 \\ 0&0 \\ 0&0 \end{pmatrix}, \qquad \bar{G}_p(\bar{z},p^0) = \begin{pmatrix} 0&0 \\ 0&0 \\ 0&0 \\ 0&0 \\ 0&0 \\ 0&0 \end{pmatrix}, \tag{44}$$

and by formula (22) the derivative $\frac{d\text{con}}{dp}(p^0)$ reads as

$$\frac{d\text{con}}{dp_1}(p_1^0) = \frac{d\text{con}}{dp_2}(p_2^0) = (-\frac{1}{2}, \frac{1}{2}, \frac{1}{2}, 0, 0, 0). \tag{45}$$

This indicates, that small deviations in $p = (p_1, p_2)$ cause the consistent initial values for $x(t_0)$ to change. Especially $x_1(t_0)$ is influenced by this perturbations even though the deviations are only directly coupled with $x_2(t_0)$ and $x_3(t_0)$ in the objective function. The derivative $\frac{d\text{con}}{dp}(p^0)$ coincides with a direct differentiation of the first six arguments of $\bar{z}$ in (39) with respect to p^0.

Example 5.3 (Mathematical Pendulum) The equations of motion of a mathematical pendulum with mass m and length $l = 1$ are given by

$$\begin{aligned}
\dot{x}_1(t) &= x_3(t), & \text{(46a)}\\
\dot{x}_2(t) &= x_4(t), & \text{(46b)}\\
m\dot{x}_3(t) &= \qquad - 2\,x_5(t)\,x_1(t), & \text{(46c)}\\
m\dot{x}_4(t) &= -mg_0 - 2\,x_5(t)\,x_2(t), & \text{(46d)}\\
0 &= x_1(t)^2 + x_2(t)^2 - 1. & \text{(46e)}
\end{aligned}$$

Here, $x_1(t), \ldots, x_4(t)$ denote the differential variables and $x_5(t)$ denotes the algebraic variable.

Threefold differentiation of the algebraic constraint $0 = x_1(t)^2 + x_2(t)^2 - 1$ w.r.t. time yields the possibility to transform (46) to an ODE system, hence the differentiation index is $k = 3$. Let additional initial values

$$\begin{aligned}
x_1(t_0) &= \frac{1}{\sqrt{2}}, & \text{(47a)}\\
x_2(t_0) &= -\frac{1}{\sqrt{2}} & \text{(47b)}
\end{aligned}$$

be given.
In the sequel we investigate the problem

$$\begin{aligned}
\min_{\hat{z}} \quad & (x_3(t_0) - s)^2 + (x_4(t_0) - s)^2, & \text{(48a)}\\
\text{s.t.} \quad & \text{equation (46), and its derivatives up to order 3, and (47)} & \text{(48b)}
\end{aligned}$$

with $\hat{z}$ defined by

$$\hat{z} := (x(t_0), \ldots, x^{(k+1)}(t_0))^T. \tag{49}$$

As perturbation parameter we choose $p = (m, g_0, s)$. Please note, that similar problems arise in connection with direct solution methods for optimal control problems with DAE systems of higher index and free initial values.

All differentiability assumptions hold for Theorem 3.2 and Theorem 3.3. However, due to the high dimension we favour Theorem 4.1 and Theorem 4.2 and follow the ideas of Section 4. A basis of necessary variables and equations is given by

$$
\begin{aligned}
B^V &:= \{(1,1),(1,2),(1,3),(1,4),(2,1),(2,2),(2,3),(2,4),(2,5),\\
&\quad (3,1),(3,2),(3,3),(3,4),(4,1),(4,2)\}, && \text{(50a)}\\
B^E &:= \{(0,1),(0,2),(1,1),(1,2),(1,3),(1,4),(2,1),(2,2),(2,3),\\
&\quad (2,4),(2,5),(3,1),(3,2),(3,5),(4,5)\}. && \text{(50b)}
\end{aligned}
$$

For a reference parameter $p^0 = (m^0, g_0^0, s^0)$ this leads to the optimization variables and equations, resp.,

$$
\begin{aligned}
z &:= (x_1,\dots,x_5,\dot{x}_1,\dots,\dot{x}_5,\ddot{x}_1,\dots,\ddot{x}_4,\dddot{x}_1,\dddot{x}_2)^T,\\
\bar{G}(z,p^0) &:= \begin{pmatrix}
\dot{x}_1 - x_3\\
\dot{x}_2 - x_4\\
m^0\dot{x}_3 + 2x_5x_1\\
m^0\dot{x}_4 + m^0 g_0^0 + 2x_5x_2\\
\ddot{x}_1 - \dot{x}_3\\
\ddot{x}_2 - \dot{x}_4\\
m^0\ddot{x}_3 + 2\dot{x}_1x_5 + 2x_1\dot{x}_5\\
m^0\ddot{x}_4 + 2\dot{x}_2x_5 + 2x_2\dot{x}_5\\
2x_1\dot{x}_1 + 2x_2\dot{x}_2\\
\dddot{x}_1 - \ddot{x}_3\\
\dddot{x}_2 - \ddot{x}_4\\
2\dot{x}_1^2 + 2x_1\ddot{x}_1 + 2\dot{x}_2^2 + 2x_2\ddot{x}_2\\
6\dot{x}_1\ddot{x}_1 + 2x_1\dddot{x}_1 + 6\dot{x}_2\ddot{x}_2 + 2x_2\dddot{x}_2\\
x_1 - \frac{1}{\sqrt{2}}\\
x_2 + \frac{1}{\sqrt{2}}
\end{pmatrix} = 0,
\end{aligned} \tag{51}
$$

where all components in z and $\bar{G}(z,p^0)$ are evaluated at t_0. For $\mu \in \mathbb{R}^{15}$ the Lagrangian is given by $L(z,\mu,p^0) = (x_3(t_0) - s^0)^2 + (x_4(t_0) - s^0)^2 + \mu^T \bar{G}(z,p^0)$. The equality constraints from $\bar{G}(z,p^0) = 0$ in (51) and the necessary conditions in Theorem 3.1 yield $\bar{\mu} = 0 \in \mathbb{R}^{15}$ and

$$
\bar{z} = \begin{pmatrix}
\frac{1}{\sqrt{2}}\\
-\frac{1}{\sqrt{2}}\\
s^0\\
s^0\\
\frac{1}{4}m^0(\sqrt{2}g_0^0 + 4(s^0)^2)\\
s^0\\
s^0\\
-\frac{1}{2}g_0^0 - \sqrt{2}(s^0)^2\\
-\frac{1}{2}g_0^0 + \sqrt{2}(s^0)^2\\
-\frac{3}{2}m^0 g_0^0 s^0\\
-\frac{1}{2}g_0^0 - \sqrt{2}(s^0)^2\\
-\frac{1}{2}g_0^0 + \sqrt{2}(s^0)^2\\
s^0(\sqrt{2}g_0^0 - 2(s^0)^2)\\
-2s^0(\sqrt{2}g_0^0 + (s^0)^2)\\
s^0(\sqrt{2}g_0^0 - 2(s^0)^2)\\
-2s^0(\sqrt{2}g_0^0 + (s^0)^2)
\end{pmatrix}. \tag{52}
$$

The Hessian of the Lagrangian is defined by $A := L_{zz}(\bar{z}, \bar{\mu}, m^0, g_0^0, s^0)$ with

$$A = (A)_{i,j} = \begin{cases} 2, & \text{if} \quad i = j = 3, \ \text{or } i = j = 4, \\ 0, & \text{else}, \end{cases} \tag{53}$$

while the Jacobian of the constraints yield

$$\bar{G}_z(\bar{z}, p^0) = \left(\begin{array}{cccccccccccccccc}
0 & 0 & -1 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & -1 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
\beta_1 & 0 & 0 & 0 & \frac{\sqrt{2}}{m^0} & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & \beta_1 & 0 & 0 & -\frac{\sqrt{2}}{m^0} & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & -1 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & -1 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\
-3s^0 g_0^0 & 0 & 0 & 0 & 2\frac{s^0}{m^0} & \beta_1 & 0 & 0 & 0 & \frac{\sqrt{2}}{m^0} & 0 & 0 & 1 & 0 & 0 & 0 \\
0 & -3s^0 g_0^0 & 0 & 0 & 2\frac{s^0}{m^0} & 0 & \beta_1 & 0 & 0 & -\frac{\sqrt{2}}{m^0} & 0 & 0 & 0 & 1 & 0 & 0 \\
2s^0 & 2s^0 & 0 & 0 & 0 & \sqrt{2} & -\sqrt{2} & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & -1 & 0 & 1 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & -1 & 0 & 1 \\
-\beta_2 & \beta_2 & 0 & 0 & 0 & 4s^0 & 4s^0 & 0 & 0 & 0 & \sqrt{2} & -\sqrt{2} & 0 & 0 & 0 & 0 \\
-\beta_3 & 2\beta_3 & 0 & 0 & 0 & -\beta_4 & \beta_4 & 0 & 0 & 0 & 6s^0 & 6s^0 & 0 & 0 & \sqrt{2} & -\sqrt{2} \\
1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0
\end{array} \right) \tag{54}$$

with

$$\beta_1 = 2(s^0)^2 + \frac{1}{\sqrt{2}} g_0^0, \qquad \beta_2 = 2\sqrt{2}(s^0)^2 - g_0^0, \tag{55a}$$

$$\beta_3 = -2s^0(\sqrt{2} g_0^0 - 2(s^0)^2), \qquad \beta_4 = 6\sqrt{2}(s^0)^2 - 3g_0^0. \tag{55b}$$

The Jacobian is of maximal rank hence the dimension of the kernel is one and given by

$$\begin{aligned} &\mathrm{Ker}(\bar{G}_z(\bar{z}, p^0)) = \{v \in \mathbb{R}^{16} : \\ &\quad v = (0, 0, c_2, c_2, c_3, c_2, c_2, -c_4, c_4, c_5, -c_4, c_4, \alpha, c_6, \alpha, c_6)^T, \ \alpha \in \mathbb{R}\} \end{aligned} \tag{56}$$

with

$$c_1 = g_0^0 - 3\sqrt{2}(s^0)^2, \quad c_2 = \frac{\alpha}{\sqrt{2} c_1}, \qquad c_3 = \frac{\alpha s^0 \sqrt{2} m^0}{c_1}, \tag{57a}$$

$$c_4 = 2\frac{\alpha s^0}{c_1}, \qquad c_5 = -\frac{3\alpha m^0 g_0^0 \sqrt{2}}{4c_1}, \quad c_6 = -\frac{\alpha(2g_0^0 + 3\sqrt{2}(s^0)^2)}{c_1}. \tag{57b}$$

Furthermore we get

$$v^T L_{zz}(\bar{z}, \bar{\mu}, p^0) v = \frac{2\alpha^2}{(g_0^0 - 3\sqrt{2}(s^0)^2)^2}, \tag{58}$$

independent on m^0, hence the Hessian is positive definite on $\mathrm{Ker}(\bar{G}_z(\bar{z}, p^0)) \backslash \{0\}$ (compare Assumption 3.1.5). Thus $(\bar{z}, \bar{\mu})$ is a strong local minimum of (34). Since all differentiability properties are fulfilled we can apply Theorem 4.1 and Theorem 4.2 and find that there exists a neighborhood $P(p^0)$ for any reference parameter $p = p^0$ and a unique C^1 consistency function $\mathrm{con} : \mathrm{P(p^0)} \longrightarrow \mathrm{I\!R^{2n}}$:

$$\mathrm{con(p)} := (\mathrm{x_0(p)}, \dot{\mathrm{x}}_0(\mathrm{p}))^{\mathrm{T}} = (\mathrm{z_1(p)}, \mathrm{z_2(p)}, \ldots, \mathrm{z_{10}(p)})^{\mathrm{T}}. \tag{59}$$

From $B := L_{zp}(\bar{z}, \bar{\mu}, m^0, g_0^0, s^0)$ with

$$B = (B)_{i,j} = \begin{cases} -2, & \text{if} \quad i = 3,\ j = 3,\ \text{or } i = 4,\ j = 3, \\ 0, & \text{else}, \end{cases} \tag{60}$$

and $C := \bar{G}_p(\bar{z}, m^0, g_0^0, s^0)$ with

$$C = (C)_{i,j} = \begin{cases} -\frac{\sqrt{2}g_0^0 + 4(s^0)^2}{2\sqrt{2}m^0}, & \text{if} \quad i = 3,\ j = 1, \\ \frac{\sqrt{2}g_0^0 + 4(s^0)^2}{2\sqrt{2}m^0}, & \text{if} \quad i = 4,\ j = 1, \\ 1, & \text{if} \quad i = 4,\ j = 2, \\ -\frac{s^0(\sqrt{2}g_0^0 + 4(s^0)^2) - 3\sqrt{2}g_0^0 s^0}{2m^0}, & \text{if} \quad i = 7,\ j = 1, \\ -\frac{s^0(\sqrt{2}g_0^0 + 4(s^0)^2) + 3\sqrt{2}g_0^0 s^0}{2m^0}, & \text{if} \quad i = 8,\ j = 1, \\ 0, & \text{else}, \end{cases} \tag{61}$$

the derivative $\frac{d\text{con}}{dp}(p^0)$ reads as

$$\frac{d\text{con}}{dp}(p^0) = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 0 & - \\ \frac{1}{4}\sqrt{2}(2\sqrt{2}(s^0)^2 + g_0^0) & -\frac{1}{4}\sqrt{2}m^0 & 2m^0 s \\ 0 & 0 & 1 \\ 0 & 0 & 1 \\ 0 & -\frac{1}{2} & -2\sqrt{2}s^0 \\ 0 & -\frac{1}{2} & 2\sqrt{2}s^0 \\ -\frac{3}{2}s^0 g_0^0 & -\frac{3}{2}m^0 s^0 & -\frac{3}{2}g_0^0 m^0 \end{pmatrix}. \tag{62}$$

Again the sensitivity derivative coincides with a direct differentiation of the first ten arguments of $\bar{z}$ in (52) with respect to (m^0, g^0, s^0).

6 Conclusions

In this article parametric differential–algebraic systems are considered. Due to the parameter dependency of the DAE system, in general the solution and in particular consistent initial values depend on these parameters. Therefore the concept of consistency functions is introduced. A consistency function maps a given parameter to a consistent initial value for the DAE system. This consistent initial value need not to be unique, such that the resulting degrees of freedom in the choice of the consistent value can be exploited to optimize a given performance index. This leads to optimal consistent initial values, which play an important role in conjunction with direct shooting methods for the numerical solution of optimal control problems with DAE systems of higher index and free initial values, see Refs. 8,12. One type of such consistency functions is given in Section 2. Of particular importance, e.g. for DAE optimal control problems, is the investigation, under which conditions consistency functions are differentiable functions with respect to the parameters. Therefore necessary and sufficient conditions are stated. It turns out that these conditions are too restrictive in some cases. An example is given in Section 3. Another class of consistency functions given in Section 4 is based on the idea to extract only relevant information and allows to formulate weaker conditions to obtain the desired differentiability properties. The discussion of several illustrative examples shows the capability of our investigations.

Because the required derivatives of the DAE system can not be provided nor computed analytically, in realistic technical applications it is often not possible to construct a consistency function in the depicted way. Therefore, methods for the *numerical approximation* of consistency functions are needed. A first approach can be found in Büskens and Gerdts (Ref. 8). As mentioned before, differentiable consistency functions can be incorporated in direct shooting techniques for the numerical solution of DAE optimal control problems. The sensitivities, i.e. the differentials of the consistency function w.r.t. parameters, play an import role in the calculation of gradients and Jacobians, e.g. by means of the so called sensitivity DAE system, see Gerdts (Ref. 12).

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