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A NONSMOOTH NEWTON'S METHOD FOR DISCRETIZED OPTIMAL CONTROL PROBLEMS WITH STATE AND CONTROL CONSTRAINTS

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Abstract. We investigate a nonsmooth Newton's method for the numerical solution of discretized optimal control problems subject to pure state constraints and mixed control-state constraints. The infinite dimensional problem is discretized by application of a general one-step method to the differential equation. By use of the Fischer-Burmeister function the first order necessary conditions for the discretized problem are transformed into an equivalent nonlinear and nonsmooth equation. This nonlinear and nonsmooth equation is solved by a globally convergent nonsmooth Newton's method. Numerical examples for the optimal control of a robot conclude the article.

1. **Introduction.** We consider the following optimal control problem subject to pure state constraints $s(x(t)) \leq 0$ and mixed control-state constraints $c(x(t), u(t)) \leq 0$:

Problem (Optimal Control Problem (OCP))**.** *Minimize*

$$J(x(0), x(1))$$

w.r.t. $x \in W^{1,\infty}([0,1], \mathbb{R}^{n_x})$ *and* $u \in L^\infty([0,1], \mathbb{R}^{n_u})$ *subject to the constraints*

$$\begin{aligned} x'(t) &= f(x(t), u(t)) \text{ a.e. in } [0,1], \\ \psi(x(0), x(1)) &= 0, \\ c(x(t), u(t)) &\leq 0 \text{ a.e. in } [0,1], \\ s(x(t)) &\leq 0 \text{ in } [0,1]. \end{aligned}$$

Without loss of generality the discussion is restricted to autonomous problems on the fixed time interval $[0,1]$. The functions $J : \mathbb{R}^{n_x} \times \mathbb{R}^{n_x} \to \mathbb{R}$, $f : \mathbb{R}^{n_x} \times \mathbb{R}^{n_u} \to \mathbb{R}^{n_x}$, $\psi : \mathbb{R}^{n_x} \times \mathbb{R}^{n_x} \to \mathbb{R}^{n_\psi}$, $c : \mathbb{R}^{n_x} \times \mathbb{R}^{n_u} \to \mathbb{R}^{n_c}$, and $s : \mathbb{R}^{n_x} \to \mathbb{R}^{n_s}$, are supposed to be at least twice continuously differentiable w.r.t. to all arguments. Furthermore, we assume that the mixed control-state constraint c satisfies the rank condition $\operatorname{rank}(c'_u(t)) = n_c$ for a.e. $t \in [0,1]$. As usual, the Banach space $L^\infty([0,1], \mathbb{R}^n)$ consists of all measurable functions $h : [0,1] \to \mathbb{R}^n$ with

$$\|h\|_\infty := \operatorname*{ess\,sup}_{0 \leq t \leq 1} \|h(t)\| < \infty,$$

where $\|\cdot\|$ denotes the Euclidean norm on $\mathbb{R}^n$. The Banach space $W^{1,\infty}([0,1], \mathbb{R}^n)$ consists of all absolutely continuous functions $h : [0,1] \to \mathbb{R}^n$ with

$$\|h\|_{1,\infty} := \max\{\|h\|_\infty, \|h'\|_\infty\} < \infty.$$

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Several approaches towards the numerical solution of OCP have been investigated in the literature. The so-called indirect method for optimal control problems attempts to satisfy the first order necessary conditions that are provided by the well-known minimum principle numerically, cf., e.g. Oberle and Grimm [OG01]. The exploitation of the minimum principle leads to a nonlinear multi-point boundary value problem that has to be solved. Although the indirect method usually leads to the most accurate solutions, it suffers from the drawback that it requires a good initial guess in order to converge. One crucial task is to estimate the sequence of active and inactive intervals of the control-state constraints and the pure state constraints.

A related approach was analyzed in Gerdts [Ger06] for optimal control problems subject to mixed control-state constraints. Herein, the minimum principle was transformed into a nonlinear and nonsmooth equation in appropriate Banach spaces by use of a so-called NCP function, i.e. the Fischer-Burmeister function. A nonsmooth version of Newton's method was applied to this nonsmooth equation and global and locally superlinear convergence of the method was established under suitable regularity assumptions. This methodology was used successfully earlier in the context of optimal control problems governed by partial differential equations, cf. Ulbrich [Ulb02, Ulb03, HU04]. However, problems with pure state constraints have not been investigated rigorously by now. The presence of pure state constraints complicates the structure of the minimum principle considerably since the multiplier for the pure state constraint is a measure and the adjoint equation is an integral equation with a Riemann-Stieltjes integral, cf. Girsanov [Gir72]. Though it is possible to reformulate at least a weakened version of the minimum principle as a nonsmooth equation, the analysis of the resulting equation is very difficult and actually we did not succeed by now.

In this paper we leave the infinite setting and favor the so-called direct discretization method, which is based on a discretization of the infinite dimensional optimal control problem and leads to a finite dimensional nonlinear program, cf., e.g., Gerdts [Ger03]. The direct discretization method turns out to be very robust in practice. Nevertheless, the computational effort grows at a nonlinear rate with the number of grid points used for discretization.

One approach to solve the discretized problem numerically is to use a suitable optimization routine like sequential quadratic programming.

Another approach, which will be discussed in this article and which is very close to the methodology in the infinite setting, leads to a nonsmooth Newton's method for discretized optimal control problems. Our intention is to analyze the local and global convergence properties of the method and to discuss implementational details. Like in the infinite setting, the method is based on a nonsmooth reformulation of the first order necessary optimality conditions for the discretized problem. A brief outline of the essential ideas of the algorithm is as follows. The reformulation of the necessary conditions leads to the nonsmooth equation

$$F(z) = 0, \qquad F : \mathbb{R}^n \to \mathbb{R}^n. \tag{1}$$

Application of the globalized nonsmooth Newton's method generates sequences $\{z^k\}$, $\{d^k\}$ and $\{\alpha_k\}$ related by the iteration

$$z^{k+1} = z^k + \alpha_k d^k, \qquad k = 0, 1, 2, \ldots.$$

Herein, the search direction d^k is the solution of the linear equation $V_k d^k = -F(z^k)$ and the step length $\alpha_k > 0$ is determined by a line-search procedure of Armijo's type for a suitably defined merit function. The matrix V_k is chosen from Clarke's generalized Jacobian $\partial F(z^k)$.

The nonsmooth Newton's method was investigated in finite dimensions amongst others by Qi [Qi93], Qi and Sun [QS93], Xu and Glover [XG97], Xu and Chang [XC97], Han et al. [HPR92], Ralph [Ral94], and Dingguo and Weiwen [DW02]. Similar ideas were also used to

solve nonlinear complementarity problems, cf. Fischer [Fis97], Facchinei and Kanzow [FK97], Yamashita and Fukushima [YF97], Billups and Ferris [BF97], and Jiang [Jia99]. Extensions to infinite spaces can be found in Kummer [Kum88, Kum91], Chen et al. [CNQ00], and Ulbrich [Ulb02, Ulb03]. Fischer [Fis92] applies the nonsmooth Newton's method to the first order necessary optimality conditions of general nonlinear programs and analyzes the convergence behavior of the approach.

The paper is organized as follows. Section 2 introduces the nonsmooth Newton's method for nonlinear programs and summarizes convergence properties. Section 3 addresses the discretization of the optimal control problem, the evaluation of necessary conditions, and the application of the nonsmooth Newton's method. The special structure of the discretized optimal control problem is exploited. Implementational details are discussed in Section 4. Finally, numerical illustrations are presented in Section 5.

2. Nonsmooth Newton Methods for Nonlinear Programs.

We consider a nonlinear program of type

Problem (Nonlinear Program (NLP)). *Minimize $\tilde{f}(y)$ subject to the constraints*

$$\begin{aligned} h_j(y) &= 0, \qquad j = 1, \dots, p, \\ g_i(y) &\leq 0, \qquad i = 1, \dots, m. \end{aligned}$$

Herein, $\tilde{f} : \mathbb{R}^n \to \mathbb{R}$, $g = (g_1, \dots, g_m)^\top : \mathbb{R}^n \to \mathbb{R}^m$, and $h = (h_1, \dots, h_p)^\top : \mathbb{R}^n \to \mathbb{R}^p$ are assumed to be at least twice continuously differentiable functions. Furthermore, we assume that NLP satisfies some constraint qualification, e.g. the linear independence constraint qualification or the Mangasarian-Fromowitz constraint qualification. Then, given a local minimum y^* of NLP, there exist multipliers $v^* = (v_1^*, \dots, v_p^*)^\top \in \mathbb{R}^p$ and $w^* = (w_1^*, \dots, w_m^*)^\top \in \mathbb{R}^m$ satisfying the first order necessary KKT conditions

$$\nabla_y L(y^*, v^*, w^*) = 0, \tag{2}$$

$$h(y^*) = 0, \tag{3}$$

$$w_i^* \geq 0,\ g_i(y^*) \leq 0,\ w_i^* g_i(y^*) = 0, \quad i = 1, \dots, m, \tag{4}$$

where $L(y, v, w) = \tilde{f}(y) + v^\top h(y) + w^\top g(y)$ denotes the Lagrange function of NLP. If the inequality constraints $g(y) \leq 0$ were not present in NLP, the classical Newton's method could be applied to the remaining nonlinear equations (2) and (3) in order to solve them numerically. This approach is just the well-known Lagrange-Newton method. In the presence of the inequality constraints we are focused with a coupled system of equalities (2)-(3) and complementarity conditions (4) and the numerical solution becomes more intricate. The sequential quadratic programming (SQP) method and the trust region method are based on quadratic approximations of NLP and they require to solve a quadratic program within each iteration. Other approaches work more or less directly with the optimality conditions (2)-(4). For example, the most basic interior point method applies Newton's method to a perturbed KKT system with an additional strategy for letting the perturbation tend to zero. We will concentrate on a closely related method which was suggested by Fischer [Fis92]. The idea is to apply a so-called NCP function to the complementarity system (4) and transform the KKT system into an equivalent system of equations. This can be achieved by application of the Fischer-Burmeister function $\varphi : \mathbb{R}^2 \to \mathbb{R}$ defined by

$$\varphi(a, b) := \sqrt{a^2 + b^2} - a - b.$$

The Fischer-Burmeister function has the nice property that

$$\varphi(a, b) = 0 \qquad \Leftrightarrow \qquad a \geq 0,\ b \geq 0,\ ab = 0. \tag{5}$$

Notice, that there exist other NCP functions with this property, e.g. $\min\{a,b\}$. However, we prefer the Fischer-Burmeister function as it has additional properties which are particularly useful in view of the globalization strategy below. More precisely, we will exploit the fact that the squared function $\varphi(a,b)^2$ is continuously differentiable. Notice, that other NCP functions may not have this property, e.g. $\min\{a,b\}^2$ is not differentiable.

Exploitation of (5) immediately allows us to restate the KKT conditions equivalently as the nonlinear equation

$$F(z^*) = 0, \qquad z^* = (y^*, v^*, w^*)^\top,$$

where $F : \mathbb{R}^{n+p+m} \to \mathbb{R}^{n+p+m}$ is given by

$$F(z) = \begin{pmatrix} \nabla_y L(y,v,w) \\ h(y) \\ \varphi(-g_1(y), w_1) \\ \vdots \\ \varphi(-g_m(y), w_m) \end{pmatrix}, \qquad z = (y,v,w)^\top. \tag{6}$$

Unfortunately, this nonlinear equation can not be solved numerically by classical Newton's method as the Fischer-Burmeister function φ is not differentiable at the origin and thus F is not differentiable, whenever $(g_i(y), w_i) = (0,0)$ holds for some index $i \in \{1,\ldots,m\}$. In particular, F is not differentiable in a zero z^* if the strict complementarity condition $w_i^* - g_i(y^*) > 0$ is not satisfied for some i. However, F is continuously differentiable for every

$$z \in D_F := \{z = (y,v,w)^\top \in \mathbb{R}^{n+p+m} \mid |g_i(y)| + |w_i| > 0,\ i = 1,\ldots,m\},$$

since $\tilde{f}, g, h$ are assumed to be twice continuously differentiable. Furthermore, the Fischer-Burmeister function φ is convex and thus locally Lipschitz continuous. This in turn implies that F is locally Lipschitz continuous as well since the composition of a locally Lipschitz continuous function and a continuously differentiable function is again locally Lipschitz continuous.

Hence, according to Rademacher's theorem, F is differentiable almost everywhere and the B(ouligand)-differential

$$\partial_B F(z) := \left\{ V \;\middle|\; V = \lim_{\substack{z_i \in D_F \\ z_i \to z}} F'(z_i) \right\}$$

is well-defined. Taking the convex hull of the B-differential leads immediately to Clarke's [Cla83] generalized Jacobian

$$\partial F(z) := \operatorname{co}(\partial_B F(z)),$$

which is a non-empty, convex, and compact set, cf. Proposition 2.6.2 on page 70 in Clarke [Cla83].

The existence of the generalized Jacobian gives rise to the following nonsmooth Newton's method. The nonsmooth Newton's method is identical to the classical Newton's method for smooth equations except that the possibly non-existing Jacobian is replaced by some element of the B-differential.

Algorithm 1 (Local Nonsmooth Newton's Method)**.**

(0) Choose z^0 and set $k = 0$.
(1) If some stopping criterion is satisfied, stop.
(2) Choose $V_k \in \partial_B F(z^k)$ and compute the search direction d^k as the solution of the linear equation
$$V_k d = -F(z^k).$$
(3) Set $z^{k+1} = z^k + d^k$, $k = k+1$, and goto (1).

The locally superlinear convergence of the sequence $\{z^k\}$ to z^* with $F(z^*) = 0$ was established for more general functions F by Qi [Qi93] in Theorem 3.1 under the following assumptions:

(i) $\partial_B F(z^*)$ is non-singular, i.e. every $V \in \partial_B F(z^*)$ is non-singular.
(ii) F is locally Lipschitz continuous and semismooth at z^*.

Moreover, Qi [Qi93] showed that the order of convergence is two if in addition F is 1-order semismooth in a neighborhood of z^*.

Herein, F is called semismooth at z, if the limit

$$\lim_{\substack{V \in \partial F(z+th') \\ h' \to h, t \downarrow 0}} Vh'$$

exists for every h. F is called semismooth, if F is semismooth at all z. Another characterization of semismoothness for locally Lipschitz continuous functions was given by Ulbrich [Ulb02]. He showed in Proposition 2.7 on page 19 that a locally Lipschitz continuous function F is semismooth at z if and only if F is directionally differentiable at z and satisfies

$$\sup_{V \in \partial F(z+h)} \|F(z+h) - F(z) - Vh\| = o(\|h\|) \quad \text{as} \quad \|h\| \to 0. \tag{7}$$

F is called 1-order semismooth at z, if F is directionally differentiable at z and

$$\sup_{V \in \partial F(z+h)} \|Vh - F'(z;h)\| = \mathcal{O}(\|h\|^2) \quad \text{as} \quad \|h\| \to 0,$$

where $F'(z;h)$ denotes the directional derivative of F at z in direction h. For a locally Lipschitz continuous function F it was shown in Ulbrich [Ulb02], Proposition 2.14, page 22, that F is 1-order semismooth at z if and only if F is 1-order B-differentiable, i.e.

$$\|F(z+h) - F(z) - F'(z;h)\| = \mathcal{O}(\|h\|^2) \quad \text{as} \quad \|h\| \to 0,$$

and

$$\sup_{V \in \partial F(z+h)} \|F(z+h) - F(z) - Vh\| = O(\|h\|^2) \quad \text{as} \quad \|h\| \to 0. \tag{8}$$

It remains to establish the semismoothness and the 1-order semismoothness for our particular function F in (6). Therefore, let us summarize some well-known results. The Fischer-Burmeister function φ is 1-order semismooth (and thus semismooth) according to Fischer [Fis97], Lemma 20, and particularly satisfies conditions (10) and (7). Furthermore, due to a result of Mifflin, the composition $g = g_1 \circ g_2$ of semismooth functions g_1, g_2 is again semismooth, cf. Fischer [Fis97], page 527. Similarly, the composition of 1-order semismooth functions is again 1-order semismooth, cf. Fischer [Fis97], Theorem 19. In particular, continuously differentiable functions are semismooth and functions having a locally Lipschitz continuous first derivative are 1-order semismooth. By exploitation of these results we find the following convergence result. The proof is identical to the proof of Theorem 3.1 in Qi [Qi93].

Theorem 1 (Local Convergence)**.**
Let z^* satisfy $F(z^*) = 0$. Let $\tilde{f}$, g, and h be twice continuously differentiable. Let $\partial_B F(z^*)$ be nonsingular. Then, F is semismooth and there exists some $r > 0$ such that for any z^0, $\|z^0 - z^*\| < r$, Algorithm 1 is well-defined and the sequence $\{z^k\}$ converges superlinearly to z^*. If $F(z^k) \neq 0$ for all k, then

$$\lim_{k \to \infty} \frac{\|F(z^{k+1})\|}{\|F(z^k)\|} = 0.$$

If in addition the second derivatives of $\tilde{f}$, g, and h are locally Lipschitz continuous in a neighborhood of z^*, then F is 1-order semismooth and the order of convergence is 2.

Qi and Sun [QS93], Theorem 3.2 proved a similar result, if V_k is chosen from $\partial F(z^k)$ in step (2) of Algorithm 1.

2.1. **Global Convergence.** In practice, the local nonsmooth Newton's method has to be globalized in order to obtain global convergence for arbitrary starting points z^0. This is achieved by introducing the merit function

$$\Theta(z) := \frac{1}{2}\|F(z)\|^2 = \frac{1}{2}\left(\|\nabla_y L(y,v,w)\|^2 + \|h(y)\|^2 + \sum_{i=1}^{m} \varphi(-g_i(y), w_i)^2\right).$$

It is easy to check that the squared Fischer-Burmeister function φ^2 is continuously differentiable and thus Θ is continuously differentiable and it holds

$$\nabla\Theta(z) = V^\top F(z),$$

where V is an arbitrary element of $\partial F(z)$. Then, any search direction with $Vd = -F(z)$ with V being non-singular yields the directional derivative

$$\nabla\Theta(z)^\top d = -F(z)^\top F(z) = -\|F(z)\|^2 = -2\Theta(z). \tag{9}$$

Hence, d is a direction of descent unless $F(z) = 0$ and Armijo's line search is well-defined. A globalized version of Algorithm 1 reads as follows:

Algorithm 2 (Globalized Nonsmooth Newton's Method)**.**

(0) Choose z^0, $\beta \in (0,1)$, $\sigma \in (0, 1/2)$ and set $k = 0$.
(1) If some stopping criterion is satisfied, stop.
(2) Compute the search direction d^k as the solution of the linear equation

$$V_k d = -F(z^k), \qquad V_k \in \partial_B F(z^k).$$

(3) Find the smallest $i_k \in \mathbb{N}_0$ with

$$\Theta(z^k + \beta^{i_k} d^k) \le \Theta(z^k) + \sigma\beta^{i_k}\nabla\Theta(z^k)^\top d^k$$

and set $\alpha_k = \beta^{i_k}$.
(4) Set $z^{k+1} = z^k + \alpha_k d^k$, $k = k+1$, and goto (1).

The following global convergence result can be found to some extend in Theorem 4.1 in Jiang [JQ97].

Theorem 2. *Let $\tilde{f}$, g, and h be twice continuously differentiable. Let the inverse operators V_k^{-1} exist for all k and let $C > 0$ be a constant such that $\|V_k^{-1}\| \le C$ holds for all k. Let z^* be an accumulation point of the sequence $\{z^k\}$ generated by Algorithm 2.*

Then, z^* is a zero of F.

Furthermore, the step size $\alpha_k = 1$ is accepted for all k sufficiently large and the globalized method eventually turns into the local method.

Proof. Let $\{z^k\}$ be a (sub)sequence with $z^k \to z^*$ and $F(z^k) \neq 0$. According to (9) it holds $\nabla\Theta(z^k)^\top d^k = -2\Theta(z^k) < 0$. We have to investigate two cases.

(i) Assume $\alpha := \liminf_{k\to\infty} \alpha_k > 0$. Then

$$0 \le \Theta(z^{k+1}) \le \Theta(z^k) + \sigma\alpha_k\nabla\Theta(z^k)^\top d^k = \Theta(z^k)\left(1 - 2\sigma\alpha_k\right).$$

With $\sigma \in (0, 1/2)$ and $\alpha \le \alpha_k \le 1$ it follows inductively

$$0 \le \Theta(z^k) \le \Theta(z^0)\left(1 - 2\sigma\alpha\right)^k \to 0.$$

(ii) Assume that there is a subsequence with $\alpha_k \to 0$, $k \in J \subset \mathbb{N}$. The sequence $\{d^k\}$ is bounded since $\{V_k^{-1}\}$ is bounded and

$$0 \le \|d^k\| = \|V_k^{-1}F(z^k)\| \le C\|F(z^k)\| \le C\|F(z^0)\|.$$

Hence, there exists a convergent subsequence $\{d^k\}_{k\in\hat{J}}$, $\hat{J} \subseteq J$, with $d^k \to d^*$.

The line search in step (3) of the algorithm yields

$$\frac{\Theta(z^k + \alpha_k d^k) - \Theta(z^k)}{\alpha_k} \le \sigma \nabla\Theta(z^k)^\top d^k, \qquad k \in \hat{J},$$
$$\frac{\Theta(z^k + \frac{\alpha_k}{\beta} d^k) - \Theta(z^k)}{\frac{\alpha_k}{\beta}} > \sigma \nabla\Theta(z^k)^\top d^k, \qquad k \in \hat{J}.$$

Passing to the limits yields

$$\nabla\Theta(z^*)^\top d^* = \sigma \nabla\Theta(z^*)^\top d^*.$$

Since $\sigma \in (0, 1/2)$ this implies that $\nabla\Theta(z^*)^\top d^* = 0$. Multiplication by $F(z^k)^\top$ of the linear equation in step (2) yields

$$0 = \|F(z^k)\|^2 + \nabla\Theta(z^k)^\top d^k \to \|F(z^*)\|^2.$$

(i) and (ii) showed that z^* is a zero of F. Now, we will show that $\alpha_k = 1$ satisfies Armijo's rule for k sufficiently large. As in Corollary 3.2 in Qi [Qi93] we can show that for any $\varepsilon > 0$ there is a $\delta > 0$ such that for all $\|z^k - z^*\| < \delta$ it holds

$$\|z^k + d^k - z^*\| \le \varepsilon\|z^k - z^*\|, \qquad \|F(z^k + d^k)\| \le \varepsilon\|F(z^k)\|,$$

where $d^k = -V_k^{-1}F(z^k)$. Hence, for $\varepsilon = \sqrt{1-2\sigma} < 1$ there exists $\delta > 0$ such that for all $\|z^k - z^*\| \le \delta$ it holds

$$\|z^k + d^k - z^*\| \le \sqrt{1-2\sigma}\|z^k - z^*\|, \qquad \|F(z^k + d^k)\| \le \sqrt{1-2\sigma}\|F(z^k)\|.$$

Then,

$$\Theta(z^k + d^k) = \frac{1}{2}\|F(z^k + d^k)\|^2 \le \frac{1-2\sigma}{2}\|F(z^k)\|^2 = (1-2\sigma)\Theta(z^k)$$

resp.

$$\Theta(z^k + d^k) \le \Theta(z^k) - 2\sigma\Theta(z^k) = \Theta(z^k) + \sigma\nabla\Theta(z^k)^\top d^k.$$

Hence, Armijo's rule is satisfied for $\alpha_k = 1$ and $z^{k+1} = z^k + d^k$. Furthermore, $\|z^{k+1} - z^*\| \le \sqrt{1-2\sigma}\|z^k - z^*\| \le \delta$ and we are in the same situation as above and the argument can be repeated. □

2.2. **Computing one Element from the B-Differential.** It remains to compute at least one element of the B-differential of F in (6). For every $z \in D_F$, F is continuously differentiable in a neighborhood of z and it holds $\partial_B F(z) = \{F'(z)\}$ with

$$F'(z) = \begin{pmatrix} \nabla^2_{yy} L(y, v, w) & h'(y)^\top & g'(y)^\top \\ h'(y) & 0 & 0 \\ -R(z)g'(y) & 0 & T(z) \end{pmatrix},$$

where $R := \operatorname{diag}(R_1, \ldots, R_m)$, $T := \operatorname{diag}(T_1, \ldots, T_m)$, and

$$(R_i(z), T_i(z)) = \left(\frac{-g_i(y)}{\sqrt{g_i(y)^2 + w_i^2}} - 1, \frac{w_i}{\sqrt{g_i(y)^2 + w_i^2}} - 1 \right) = \varphi'(-g_i(y), w_i).$$

For $z \notin D_F$ we define the non-empty index set

$$I(y, w) = \{i \in \{1, \ldots, m\} \mid (g_i(y), w_i) = (0, 0)\}$$

and the sequence $z^\ell = (y, v, w^\ell)^\top$ with $w_i^\ell = w_i$ for $i \notin I(y,w)$ and $w_i^\ell = 1/\ell > 0$ for $i \in I(y,w)$. Then, $z^\ell \to z$, $z^\ell \in D_F$, and

$$\lim_{\ell\to\infty} F'(z^\ell) = \begin{pmatrix} \nabla^2_{yy} L(y,v,w) & h'(y)^\top & g'(y)^\top \\ h'(y) & 0 & 0 \\ -\hat{R}(z)g'(y) & 0 & \hat{T}(z) \end{pmatrix} =: \hat{V}(z) \tag{10}$$

with $\hat{R} := \operatorname{diag}(\hat{R}_1, \ldots, \hat{R}_m)$, $\hat{T} := \operatorname{diag}(\hat{T}_1, \ldots, \hat{T}_m)$, and

$$\begin{aligned} (\hat{R}_i(z), \hat{T}_i(z)) &= \lim_{\ell\to\infty} \big(R_i(z^\ell), T_i(z^\ell)\big) \\ &= \begin{cases} \left(\frac{-g_i(y)}{\sqrt{g_i(y)^2+w_i^2}} - 1, \frac{w_i}{\sqrt{g_i(y)^2+w_i^2}} - 1\right), & \text{if } i \notin I(y,w), \\ (-1, 0), & \text{if } i \in I(y,w). \end{cases} \end{aligned}$$

Hence, we have constructed one particular element $\hat{V}(z) \in \partial_B F(z)$ for any $z \notin D_F$. We proved

Lemma 1. *The matrix*

$$V = \begin{cases} F'(z), & \text{if } z \in D_F, \\ \hat{V}(z), & \text{otherwise} \end{cases}$$

with $\hat{V}$ from (10) is an element of $\partial_B F(z)$ and may be chosen in step (2) of Algorithms 1 and 2.

2.3. **A More General Generalized Jacobian.** While it is comparatively simple to compute just one element of the B-differential of F, in general it is not possible to compute the B-differential in total. But, the following considerations will provide a superset $\partial_* F(z)$ of the generalized Jacobian $\partial F(z)$ whose elements can be used in Algorithms 1 and 2 instead of $\partial_B F(z)$ resp. $\partial F(z)$. First, we compute the generalized Jacobian of the Fischer-Burmeister function.

Lemma 2. *The generalized Jacobian of φ is given by*

$$\partial\varphi(a,b) = \begin{cases} \left\{\left(\frac{a}{\sqrt{a^2+b^2}} - 1, \frac{b}{\sqrt{a^2+b^2}} - 1\right)\right\}, & \text{if } (a,b) \neq (0,0), \\ \big\{(r,t) \;\big|\; (r+1)^2 + (t+1)^2 \le 1\big\}, & \text{if } (a,b) = (0,0). \end{cases}$$

Proof. The B-differential contains all limits of $\varphi'(a,b)$ for $(a,b) \to (0,0)$, $(a,b) \neq (0,0)$. Obviously, it holds

$$\varphi'(a,b) \in M := \{(r,t) \mid (r+1)^2 + (t+1)^2 \le 1\} \qquad \forall (a,b) \neq (0,0).$$

Consequently, $\partial_B\varphi(0,0) \subseteq \partial\varphi(0,0) \subseteq M$. On the other hand, using the sequences $(a_i, b_i) = \frac{1}{i}(\cos\alpha, \sin\alpha)$ with arbitrary $\alpha \in [0, 2\pi)$ it follows

$$\lim_{i\to\infty} \varphi'(a_i, b_i) = (\cos\alpha - 1, \sin\alpha - 1)$$

and hence $\partial\varphi(0,0) = M$. □

The generalized chain rule in Theorem 2.6.6 and Proposition 2.6.2 in Clarke [Cla83] and the fact that a convex set times a matrix is again convex yield the relation

$$\partial_B F(z) \subseteq \partial F(z) \subseteq \begin{pmatrix} \nabla^2_{yy} L(y,v,w) & h'(y)^\top & g'(y)^\top \\ h'(y) & 0 & 0 \\ -R(z)g'(y) & 0 & T(z) \end{pmatrix} =: \partial_* F(z), \tag{11}$$

where $R = \operatorname{diag}(R_1, \ldots, R_m)$, $T = \operatorname{diag}(T_1, \ldots, T_m)$, and

$$(R_i(z), T_i(z)) \in \partial\varphi(-g_i(y), w_i).$$

In the sequel we will show that the convergence results in Theorems 1 and 2 still hold, if the B-differential $\partial_B F$ in Algorithms 1 and 2 is replaced by the larger set $\partial_* F$. We need an auxiliary result.

Lemma 3. *Let $\eta : \mathbb{R}^m \to \mathbb{R}^n$ be twice continuously differentiable. Let $\gamma : \mathbb{R}^n \to \mathbb{R}$ be locally Lipschitz continuous and let for all $z \in \mathbb{R}^n$,*

$$\sup_{V \in \partial\gamma(z+h)} \|\gamma(z+h) - \gamma(z) - Vh\| = O(\|h\|^2), \quad as \quad \|h\| \to 0.$$

Then the composite function $\zeta = \gamma \circ \eta$ satisfies

$$\sup_{V \in \partial\gamma|_{\eta(x+h)}} \|\zeta(x+h) - \zeta(x) - V \cdot \eta'(x+h)h\| = O(\|h\|^2) \quad as \quad \|h\| \to 0$$

for all $x \in \mathbb{R}^m$.

Proof. The differentiability assumption for η yields

$$\eta(x) - \eta(x+h) = -\eta'(x+h)h + O(\|h\|^2).$$

By the upper semicontinuity of $\partial\gamma(\cdot)$, cf. Proposotion 2.6.2 in Clarke [Cla83], and the boundedness of $\partial\gamma(z)$ for every z it holds

$$\begin{aligned}
& \sup_{V \in \partial\gamma|_{\eta(x+h)}} \|\zeta(x+h) - \zeta(x) - V \cdot \eta'(x+h)h\| \\
= & \sup_{V \in \partial\gamma|_{\eta(x+h)}} \|\gamma(\eta(x+h)) - \gamma(\eta(x)) - V \cdot \big(\eta(x+h) - \eta(x) + O(\|h\|^2)\big)\| \\
\leq & \sup_{V \in \partial\gamma|_{\eta(x+h)}} \|\gamma(\eta(x+h)) - \gamma(\eta(x)) - V \cdot (\eta(x+h) - \eta(x))\| \\
& \quad + \sup_{V \in \partial\gamma|_{\eta(x+h)}} \|V\| \cdot O(\|h\|^2) \\
= & \; O(\|h\|^2).
\end{aligned}$$

□

The following lemma states that the semismoothness condition (7) and the 1-order semismoothness condition (8) even hold w.r.t. the set $\partial_* F$.

Lemma 4. *Let $\tilde{f}$, g, and h be twice continuously differentiable. Then,*

$$\sup_{V \in \partial_* F(z+h)} \|F(z+h) - F(z) - Vh\| = o(\|h\|) \quad as \quad \|h\| \to 0. \tag{12}$$

If in addition the second derivatives of $\tilde{f}$, g, and h are locally Lipschitz continuous, then

$$\sup_{V \in \partial_* F(z+h)} \|F(z+h) - F(z) - Vh\| = O(\|h\|^2), \quad as \quad \|h\| \to 0. \tag{13}$$

Proof. If $\tilde{f}, g, h$ are twice continuously differentiable, the first $n+p$ components of F are continuously differentiable and thus satisfy the corresponding condition (12). Moreover, if $\tilde{f}, g, h$ possess Lipschitz continuous second derivatives, it is straightforward to verify (13) for these components. It remains to analyze the components $F_{n+p+i}(z) = \varphi(-g_i(y), w_i)$, $1 \leq i \leq m$. The mapping $(y, v, w) \mapsto (-g_i(y), w_i)$ is twice continuously differentiable according to our assumptions. The function φ is locally Lipschitz continuous, 1-order semismooth, cf. Fischer [Fis97], Lemma 20, and satisfies (8). Hence, we may apply Lemma 3 and immediately obtain (13) (and particularly (12)) for the components F_{n+p+i}, $i = 1, \ldots, m$. □

Lemma 4 provides the tool needed for a local convergence analysis of Algorithm 1 if $\partial_* F(z)$ is used instead of $\partial_B F(z)$. So, let $V_k d^k = -F(z^k)$ hold with $V_k \in \partial_* F(z^k)$ and let V_k^{-1} exist. We derive

$$\begin{aligned}\|z^k + d^k - z^*\| &= \|z^k - V_k^{-1}F(z^k) - z^*\| \\ &= \|V_k^{-1}\left(F(z^k) - F(z^*) - V_k(z^k - z^*)\right)\| \\ &\leq \|V_k^{-1}\| \cdot \sup_{V_k \in \partial_* F(z^k)} \|F(z^k) - F(z^*) - V_k(z^k - z^*)\|.\end{aligned}$$

Application of Lemma 4 yields superlinear resp. quadratic convergence of $\{z^k\}$ for the local nonsmooth Newton's method under the assumptions of Theorem 1 (with $\partial_B F$ replaced by $\partial_* F$). Similarly, the proof of Theorem 2 can be repeated for $\partial_* F$ as well, as it can be verified that $\nabla\Theta(z) = V^\top F(z)$ even holds for every $V \in \partial_* F(z)$.

Summarizing, Theorems 1 and 2 remain valid, if $\partial_B F$ is replaced by $\partial_* F$.

3. **Discretization of the Optimal Control Problem.** Direct discretization methods for the optimal control problem OCP are based on a discretization of the infinite dimensional optimal control problem. The resulting discretized problem will be a finite dimensional nonlinear program as in NLP but with a special structure of the objective function and the constraints. The subsequently discussed method works on the grid

$$\mathbb{G}_N := \{0 = t_0 < t_1 < \ldots < t_N = 1\}$$

with step sizes $h_j = t_{j+1} - t_j,\ j = 0, \ldots, N-1$ and mesh-size $h := \max_{j=0,\ldots,N-1} h_j$. Often, $\mathbb{G}_N$ will be an equidistant partition of the interval $[0,1]$ with constant step size $h = 1/N$ and grid points $t_i = ih,\ i = 0, \ldots, N$.

In the sequel we illustrate the direct discretization method for a generic one-step method with increment function Φ which is supposed to be appropriate for the ODE $x'(t) = f(x(t), u(t))$. We replace the control $u : [0,1] \to \mathbb{R}^{n_u}$ by a grid function $u_h : \mathbb{G}_N \to \mathbb{R}^{n_u}$ with values $u_i := u_h(t_i),\ i = 0, \ldots, N$. Usually, we associate with u_h a piecewise constant approximation of u on the interval $[0,1]$. Notice, that $u_h(\cdot)$ is completely determined by the vector $(u_0, \ldots, u_N)^\top \in \mathbb{R}^{n_u(N+1)}$.

For a given initial value x_0 and a given control approximation u_h the one-step method generates a grid function $x_h : \mathbb{G}_N \to \mathbb{R}^{n_x}$ with values $x_i := x_h(t_i),\ i = 0, \ldots, N$, by the recursion

$$x_{i+1} = x_i + h_i \Phi(x_i, u_i, h_i), \qquad i = 0, 1, \ldots, N-1.$$

Most often, the one-step method is given by an s-staged Runge-Kutta method defined by

$$\begin{aligned}x_{i+1} &= x_i + h_i \sum_{j=1}^{s} b_j k_j(x_i, u_i, h_i), \\ k_j(x,u,h) &= f\left(x + h\sum_{\ell=1}^{s} a_{j\ell} k_\ell(x,u,h), u\right), \qquad j = 1, \ldots, s,\end{aligned}$$

where b_j and $a_{j\ell}$ are appropriate coefficients. For brevity we identify x with $(x_0, \ldots, x_N)^\top$ and u with $(u_0, \ldots, u_N)^\top$. We obtain a discretization of the optimal control problem by replacing the ODE by the one-step method and discretizing the constraints on the grid $\mathbb{G}_N$:

Problem (Discretized Optimal Control Problem (DOCP))**.** *Find vectors*

$$x = (x_0, \ldots, x_N)^\top \in \mathbb{R}^{n_x(N+1)} \quad \textit{and} \quad u = (u_0, \ldots, u_N)^\top \in \mathbb{R}^{n_u(N+1)}$$

such that the objective function

$$J(x_0, x_N)$$

is minimized subject to

$$\begin{aligned} x_{i+1} - x_i - h_i\Phi(x_i, u_i, h_i) &= 0, & i = 0, 1, \ldots, N-1, \\ \psi(x_0, x_N) &= 0, & \\ c(x_i, u_i) &\le 0, & i = 0, 1, \ldots, N, \\ s(x_i) &\le 0, & i = 0, 1, \ldots, N. \end{aligned}$$

Remark 1. If the mixed control-state constraint c is not present in OCP and DOCP, respectively, the variable u_N is obsolete in DOCP and will be canceled from the formulation.

The discretized optimal control problem is a nonlinear programming problem of type NLP in Section 2 with the optimization variable

$$y := (x_0, x_1, \ldots, x_N, u_0, \ldots, u_N)^\top \in \mathbb{R}^{(n_x+n_u)(N+1)},$$

and the functions

$$\begin{aligned} \tilde{f}(y) &:= J(x_0, x_N), \\ g(y) &:= \begin{pmatrix} c(x_0, u_0) \\ \vdots \\ c(x_N, u_N) \\ s(x_0) \\ \vdots \\ s(x_N) \end{pmatrix} \in \mathbb{R}^{(n_c+n_s)(N+1)}, \\ h(y) &:= \begin{pmatrix} x_1 - x_0 - h_0\Phi(x_0, u_0, h_0) \\ \vdots \\ x_N - x_{N-1} - h_{N-1}\Phi(x_{N-1}, u_{N-1}, h_{N-1}) \\ \psi(x_0, x_N) \end{pmatrix} \in \mathbb{R}^{n_xN+n_\psi}. \end{aligned}$$

The size of the programming problem can become very large. In practice, dimensions up to a million of optimization variables or even more are not unrealistic. In order to handle these dimensions it is essential to exploit the sparse structure of the problem.

We state first order necessary conditions. The Lagrange function is given by

$$\begin{aligned} L(x, u, \lambda, \sigma, \eta, \mu) &:= J(x_0, x_N) + \sum_{i=0}^{N} \eta_i^\top c(x_i, u_i) + \sum_{i=0}^{N} \mu_i^\top s(x_i) \\ &\quad + \sum_{i=0}^{N-1} \lambda_i^\top \left(x_{i+1} - x_i - h_i\Phi(x_i, u_i, h_i)\right) + \sigma^\top \psi(x_0, x_N) \end{aligned}$$

with multipliers $\lambda = (\lambda_0, \ldots, \lambda_{N-1})^\top \in \mathbb{R}^{n_xN}$, $\eta = (\eta_0, \ldots, \eta_N)^\top \in \mathbb{R}^{n_c(N+1)}$, $\sigma \in \mathbb{R}^{n_\psi}$, $\mu = (\mu_0, \ldots, \mu_N)^\top \in \mathbb{R}^{n_s(N+1)}$. Define

$$\begin{aligned} H(x_i, u_i, \lambda_i, \eta_i, \mu_i) &:= -h_i\lambda_i^\top\Phi(x_i, u_i, h_i) + \eta_i^\top c(x_i, u_i) + \mu_i^\top s(x_i), \\ \gamma(x_0, x_N, u_N, \sigma, \eta_N, \mu_N) &:= J(x_0, x_N) + \eta_N^\top c(x_N, u_N) + \mu_N^\top s(x_N) + \sigma^\top \psi(x_0, x_N). \end{aligned}$$

Then, using the abbreviation $[t_i]$ for $H(x_i, u_i, \lambda_i, \eta_i, \mu_i)$, we obtain a simpler representation of the Lagrange function:

$$L(x, u, \lambda, \sigma, \eta, \mu) = \gamma(x_0, x_N, u_N, \sigma, \eta_N, \mu_N) + \sum_{i=0}^{N-1} \left(H[t_i] + \lambda_i^\top (x_{i+1} - x_i)\right).$$

The first order necessary KKT conditions read as

$$\begin{aligned}
\nabla_x L(x,u,\lambda,\sigma,\eta,\mu) &= 0,\\
\nabla_u L(x,u,\lambda,\sigma,\eta,\mu) &= 0,\\
h(x,u) &= 0,\\
c(x_i,u_i)\le 0,\ \eta_i\ge 0,\ \eta_i^\top c(x_i,u_i) &= 0, \quad i=0,\ldots,N,\\
s(x_i)\le 0,\ \mu_i\ge 0,\ \mu_i^\top s(x_i) &= 0, \quad i=0,\ldots,N.
\end{aligned}$$

Application of the Fischer-Burmeister function leads to the nonsmooth equation

$$F(z) := \begin{pmatrix}
\nabla_x L(x,u,\lambda,\sigma,\eta,\mu)\\
\nabla_u L(x,u,\lambda,\sigma,\eta,\mu)\\
h(x,u)\\
\varphi(-c(x_0,u_0),\eta_0)\\
\vdots\\
\varphi(-c(x_N,u_N),\eta_N)\\
\varphi(-s(x_0),\mu_0)\\
\vdots\\
\varphi(-s(x_N),\mu_N)
\end{pmatrix} = 0, \qquad z=(x,u,\lambda,\sigma,\eta,\mu)^\top,$$

cf. (6). For brevity we use the notation

$$\varphi(-s(x_i),\mu_i) := \begin{pmatrix}
\varphi(-s_1(x_i),\mu_{i,1})\\
\vdots\\
\varphi(-s_{n_s}(x_i),\mu_{i,n_s})
\end{pmatrix}, \qquad i=0,\ldots,N,$$

and likewise for $\varphi(-c(x_i,u_i),\eta_i)$. The relation in (11) reads as

$$\partial_B F(z) \subseteq \partial F(z) \subseteq \partial_* F(z) = \begin{pmatrix}
L''_{xx} & L''_{xu} & (h'_x)^\top & C_x^\top & S^\top\\
L''_{ux} & L''_{uu} & (h'_u)^\top & C_u^\top & 0\\
h'_x & h'_u & 0 & 0 & 0\\
-R_cC_x & -R_cC_u & 0 & T_c & 0\\
-R_sS & 0 & 0 & 0 & T_s
\end{pmatrix} \tag{14}$$

where

$$\begin{aligned}
C_x &= \operatorname{diag}(c'_x[t_0],\ldots,c'_x[t_N]),\\
C_u &= \operatorname{diag}(c'_u[t_0],\ldots,c'_u[t_N]),\\
S &= \operatorname{diag}(s'_x(x_0),\ldots,s'_x(x_N)),\\
R_c &= \operatorname{diag}(R_c^0,\ldots,R_c^N),\\
T_c &= \operatorname{diag}(T_c^0,\ldots,T_c^N),\\
R_s &= \operatorname{diag}(R_s^0,\ldots,R_s^N),\\
T_s &= \operatorname{diag}(T_s^0,\ldots,T_s^N).
\end{aligned}$$

Herein, $R_c^j, T_c^j \in \mathbb{R}^{n_c\times n_c}$ and $R_s^j, T_s^j \in \mathbb{R}^{n_s\times n_s}$, $j=0,\ldots,N$, are diagonal matrices. A specific element of the B-differential of F can be computed according to Lemma 1 in Section 2:

$$\begin{pmatrix} (R_c^j)_{ii}\\ (T_c^j)_{ii}\end{pmatrix} = \begin{cases}
\begin{pmatrix} \frac{-c_i[t_j]}{\sqrt{c_i[t_j]^2+\eta_{j,i}^2}}-1\\ \frac{\eta_{i,j}}{\sqrt{c_i[t_j]^2+\eta_{j,i}^2}}-1\end{pmatrix} & \text{if } (c_i[t_j],\eta_{j,i})\neq(0,0),\\
\begin{pmatrix}-1\\0\end{pmatrix}, & \text{otherwise,}
\end{cases}$$

for $i = 1, \ldots, n_c$, $j = 0, \ldots, N$, and

$$\begin{pmatrix} (R_s^j)_{ii} \\ (T_s^j)_{ii} \end{pmatrix} = \begin{cases} \begin{pmatrix} \frac{-s_i(x_j)}{\sqrt{s_i(x_j)^2+\mu_{j,i}^2}} - 1 \\ \frac{\mu_{i,j}}{\sqrt{s_i(x_j)^2+\mu_{j,i}^2}} - 1 \end{pmatrix} & \text{if } (s_i(x_j), \mu_{j,i}) \neq (0,0), \\ \begin{pmatrix} -1 \\ 0 \end{pmatrix}, & \text{otherwise,} \end{cases}$$

for $i = 1, \ldots, n_s$, $j = 0, \ldots, N$. Furthermore, we find

$$h'_x = \left(\begin{array}{cccc} -M_0 & I & & \\ & \ddots & & \\ & & -M_{N-1} & I \\ \hline \psi'_{x(0)} & & & \psi'_{x(1)} \end{array}\right),$$

$$h'_u = \left(\begin{array}{cccc} -h_0\Phi'_u[t_0] & & & \\ & \ddots & & \\ & & -h_{N-1}\Phi'_u[t_{N-1}] & 0 \\ \hline & & & \end{array}\right),$$

where $M_j := I + h_j\Phi'_x(x_j, u_j, h_j)$, $j = 0, \ldots, N-1$, and

$$L''_{xx} = \begin{pmatrix} \gamma''_{x_0x_0} + H''_{xx}[t_0] & & & \gamma''_{x_0x_N} \\ & H''_{xx}[t_1] & & \\ & & \ddots & \\ & & H''_{xx}[t_{N-1}] & \\ \gamma''_{x_Nx_0} & & & \gamma''_{x_Nx_N} \end{pmatrix},$$

$$L''_{xu} = (L''_{ux})^\top = \begin{pmatrix} H''_{xu}[t_0] & & & \\ & \ddots & & \\ & & H''_{xu}[t_{N-1}] & \\ & & & \gamma''_{x_Nu_N} \end{pmatrix},$$

$$L''_{uu} = \begin{pmatrix} H''_{uu}[t_0] & & & \\ & \ddots & & \\ & & H''_{uu}[t_{N-1}] & \\ & & & \gamma''_{u_Nu_N} \end{pmatrix}.$$

The convergence results of Theorems 1 and 2 hold accordingly for DOCP. It is without the scope of this paper to provide sufficient conditions that guarantee the non-singularity of the matrices V_k in (14) resp. (11). Results in this direction can be found in Fischer [Fis92], Lemma 4.2. These results assume linear independence of the linearized constraints and strong second order sufficient conditions.

4. **Implementation.** The globalized nonsmooth Newton's method was implemented in C++. The Jacobians and the Hessian of the Lagrange function were computed by the algorithmic differentiation code ADOL-C by Griewank et al. [GJU96]. In each iteration of the nonsmooth Newton's method we have to solve the linear equation $V_k d = -F(z^k)$. The matrix V_k is large scale and sparse and has the same structure as in (14). We used the

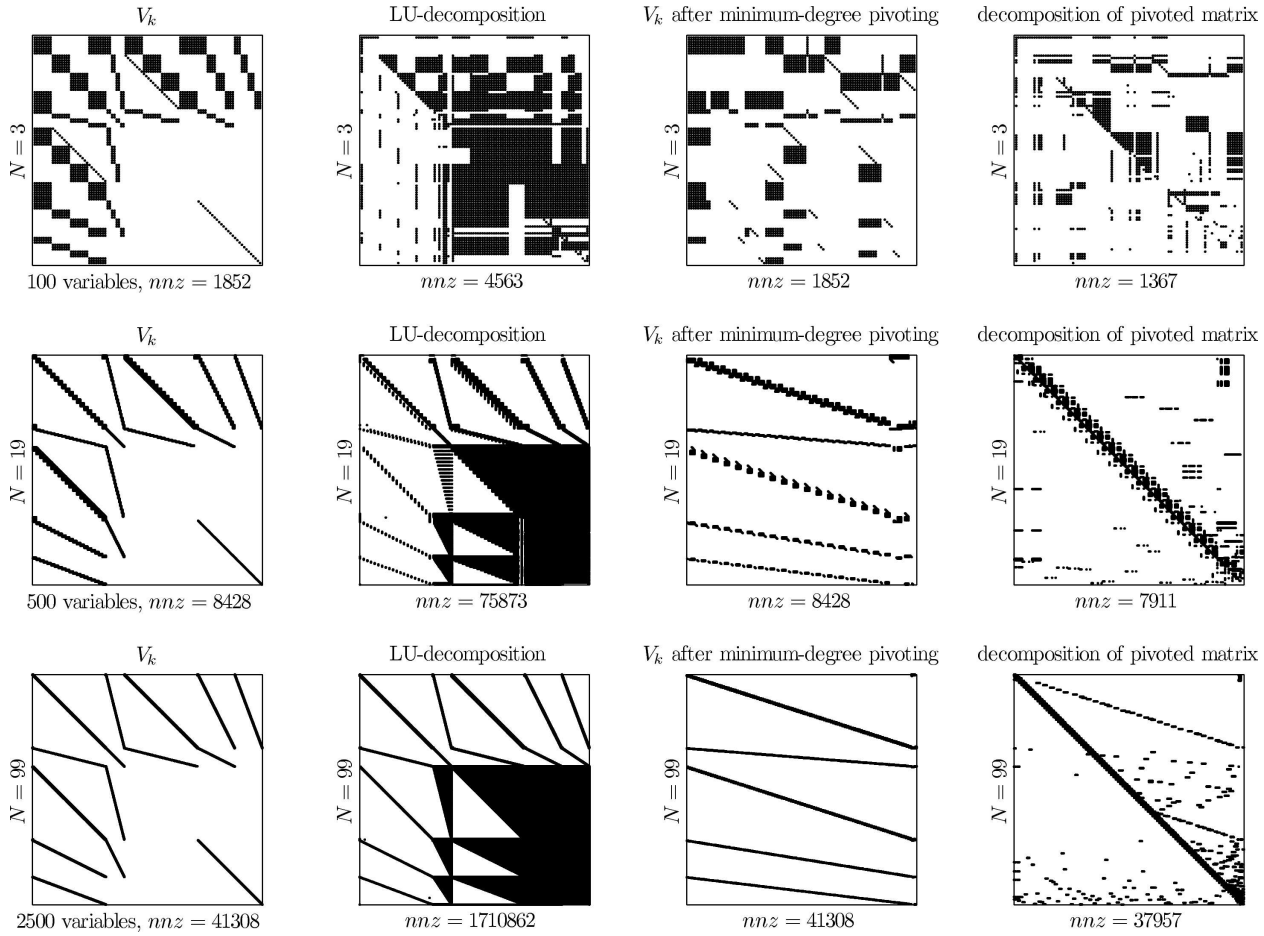

FIGURE 1. LU-decomposition (e.g. $L + U - I$) of $V_k \in \partial_B F(z^k)$ before and after minimum-degree pivoting. Dimensions: $n_x = 8$, $n_u = 2$, $n_\psi = 8$, $n_c = 4$, $n_s = 3$.

software package SUPERLU by Demmel et al. [DEG+99] for numerical computations. SUPERLU in combination with the minimum degree heuristic as a pivoting strategy computes a sparse LU decomposition of V_k. Figure 1 illustrates LU decompositions of V_k with or without minimum-degree pivoting. The example shows that the resulting factors L and U without pivoting are dense even for a sparse matrix V_k. The pivoting strategy produces sparse factors L and U which allow to solve the linear equation efficiently by forward-backward elimination.

5. **Numerical Results.** In this section the established globalized nonsmooth Newton's method will be used to solve two sample optimal control problems subject to pure state constraints and control constraints. All computations were performed on a personal computer with 2.26 GHz. For all computations, the initial guess for x was computed by forward integration of the differential equation for a given initial value and a constant control u. The initial guess for the multipliers was chosen in such a way that the initial V_0 is non-singular. Moreover, we used the parameters $\beta = 0.9$ and $\sigma = 0.1$ in Armijo's rule in step (3) of the globalized Newton's method. The algorithm terminates if $\|F(z^k)\| \leq 10^{-10}$.

5.1. **Minimum Energy Problem.** The following minimum energy problem was investigated earlier in Bryson and Ho [BH75], sec. 3.11, ex. 2.

Problem (Minimum Energy Problem)**.** *Minimize* $x_3(1)$ *subject to the constraints*

$$\begin{aligned} x_1'(t) &= x_2(t), & x_1(0) = x_1(1) &= 0, \\ x_2'(t) &= u(t), & x_2(0) = -x_2(1) &= 1, \\ x_3'(t) &= \tfrac{1}{2}u(t)^2, & x_3(0) &= 0, \\ x_1(t) &\leq \tfrac{1}{9}. \end{aligned}$$

The problem is an ideal test problem because an analytical solution to the problem is known and can be found in Bryson and Ho [BH75], sec. 3.11, ex. 2. Hence, we can calculate the absolute error of the numerical approximation. The minimum energy problem is solved on equidistant grids with $N \in \{100, 200, 400, 800, 1600\}$ grid points. For the discretization of the differential equations the well-known Euler's method, Heun's method and the classical RK method of order 4 are used.

integrator	N	$\|F(z)\|_2$	iterations	runtime (sec)
Euler	100	9.4e-015	26	0.18
	200	1.8e-011	37	0.57
	400	5.2e-015	57	1.80
	800	3.6e-014	109	7.53
	1600	1.0e-011	183	27.84
Heun	100	3.2e-012	33	0.38
	200	5.5e-013	84	2.32
	400	6.2e-013	76	3.44
	800	5.6e-013	164	17.77
	1600	1.5e-012	380	78.49
RK4	100	3.2e-012	33	0.63
	200	5.5e-013	84	3.95
	400	6.2e-013	76	5.82
	800	1.0e-012	166	31.75
	1600	5.6e-014	226	80.91

TABLE 1. Numerical results for the minimum energy problem

Table 1 shows for the different discretization methods the value of the residuum $\|F(z^k)\|$ at last iteration, the number of iterations needed and the overall runtime of the algorithm. Notice, that the algorithm terminates successfully in all cases. The number of iterations grows approximately linear in N. The consequence is a quadratically growing runtime. The calculated solution is plotted in Figure 2. It is important to point out that the multiplier μ associated with the discretized state constraint perfectly resembles the behavior of the derivative of the corresponding multiplier function of the pure state constraint of the original optimal control problem. From optimal control theory it is well-known, that the multiplier for a pure state constraint is a non-decreasing function of bounded variation. For the minimum energy problem it can be shown that the multiplier is constant on the intervals $[0, t_1)$, (t_1, t_2), and $(t_2, 1]$, where $t_1 = 1/3$ and $t_2 = 2/3$ denote the switching points, i.e. those points at which the state constraint becomes active resp. inactive. The multiplier jumps at the points t_1 and t_2. The discrete solution shows exactly the same behavior, if the discrete multiplier μ is interpreted as an approximation of the derivative of the corresponding multiplier function for OCP.

The errors of the numerical solution w.r.t. the exact solution are given in Table 2. The errors in state and control, measured in the norm $\|\cdot\|_\infty$, as well as the error in the switching points t_1, t_2 show a linear rate of convergence.

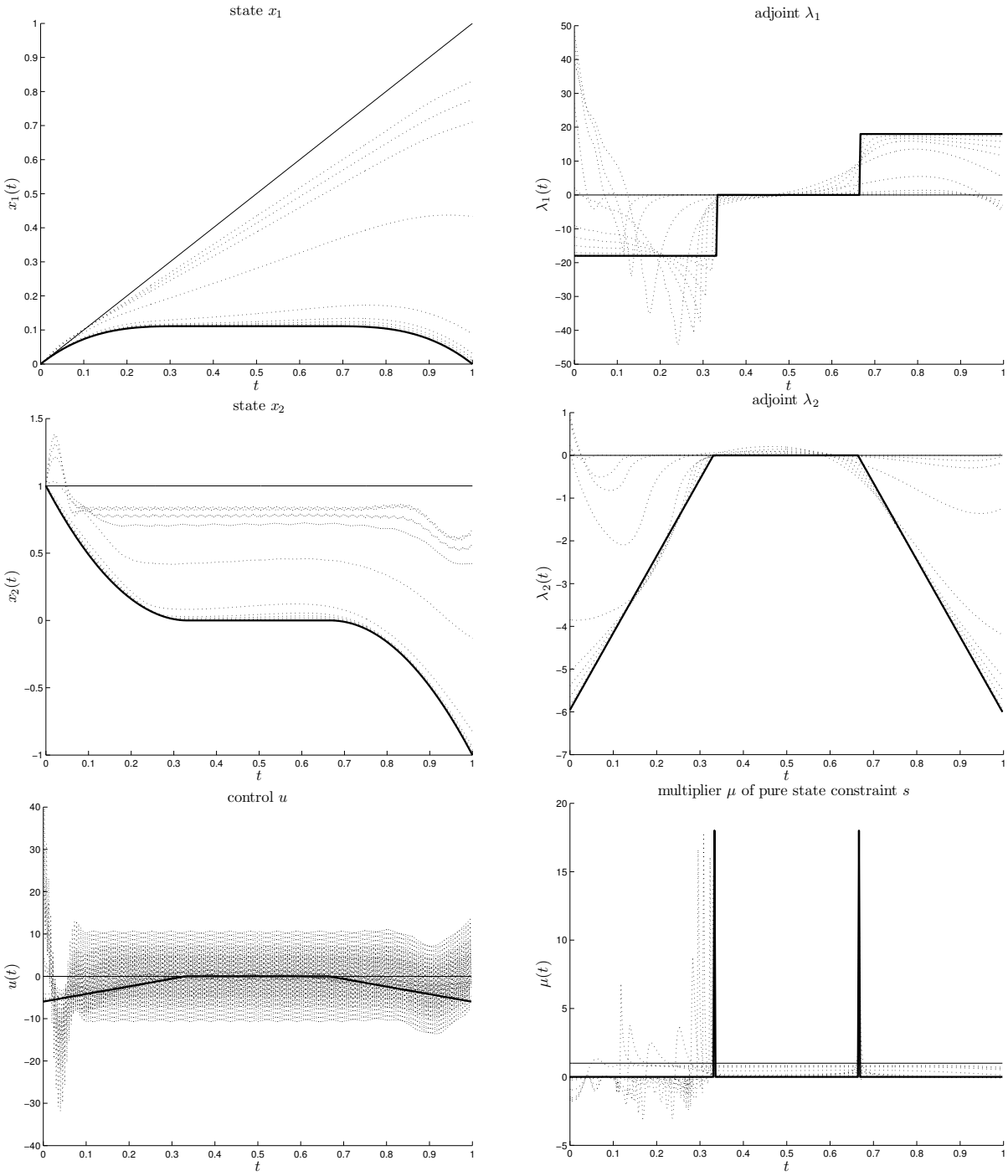

FIGURE 2. Numerical solution of the minimum energy problem with Heun's method and $N = 400$ grid points: converged solution (bold curves), initial guess (solid curve), and intermediate iterates (dashed curves)

There is no need to calculate the errors for the RK4 method, due to the fact that the differential equation of the minimum energy problem is already integrated exactly by Heun's method. There would be no further improvement if we would use a 4th-order integration method.

	max. error state $x = (x_1, x_2)$		max. error control u		max. error switching points	
N	Euler	Heun	Euler	Heun	Euler	Heun
100	2.3e-02	2.0e-04	3.6e-01	9.3e-02	1.0e-02	0.0e-00
200	1.1e-02	6.5e-05	1.8e-01	4.6e-02	5.1e-03	3.4e-05
400	5.7e-03	1.3e-05	9.0e-02	2.3e-02	2.5e-03	0.0e-00
800	2.8e-03	3.7e-06	4.5e-02	1.1e-02	1.3e-03	2.1e-06
1600	1.4e-03	7.8e-07	2.3e-02	5.6e-03	6.3e-04	0.0e-00

TABLE 2. Comparison between exact and numerical solution: errors $\|x_h - x^*\|_\infty$, $\|u_h - u^*\|_\infty$, and error in switching points where the state constraint becomes active and inactive.

The iterations of the globalized nonsmooth Newton's method are summarized in Table 3 and indicate the fast quadratic convergence for the last three iterations. Notice, that the step size $\alpha_k = 1$ finally is accepted as it was predicted by Theorem 2.

iteration k	$\|F(z^{k+1})\|_2$	$\|z^{k+1} - z^k\|_2$	α_k
1	1.5e+001	3.0e+001	6.4e-003
2	1.5e+001	2.1e+001	3.0e-003
3	1.5e+001	3.1e+001	1.6e-002
4	1.4e+001	4.4e+001	8.0e-002
5	1.4e+001	1.0e+001	6.4e-003
...	...	...	...
28	5.7e-004	2.4e+000	1.0e+000
29	1.3e-005	2.3e-002	1.0e+000
30	1.3e-008	4.7e-004	1.0e+000
31	2.7e-014	3.8e-007	1.0e+000

TABLE 3. Output of program for the minimum energy problem with $N = 150$ grid points and Heun's discretization method.

5.2. **Optimal Control of a Robot.** We investigate an optimal control problem for a planar two-linked robot which is depicted in Figure 3. The robot can be controlled by two torques u_1 and u_2 which apply at the joints M_1 and M_2, respectively.

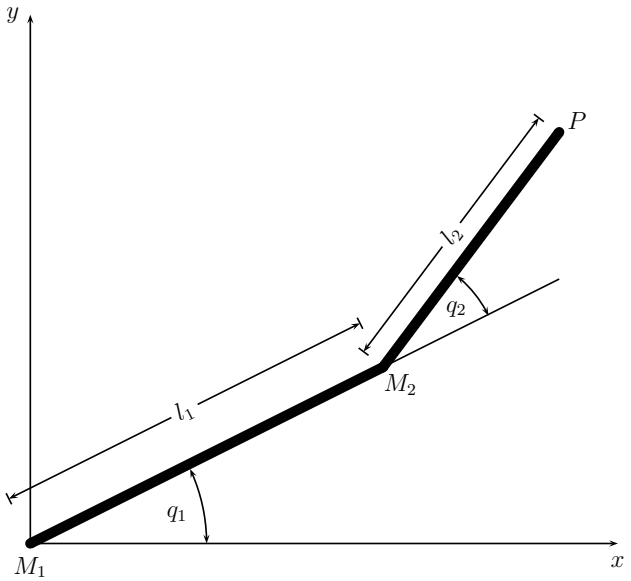

FIGURE 3. 2D industrial robot

The task is to determine an optimal control $u = (u_1, u_2)^\top$ for the transport of a payload (mounted in P) from a specified starting position to the prescribed position (x_f, y_f). The objective function consists of the free final time t_f and a regularization term for minimal control effort. The equations of motion of the robot are given by the Lagrangian equations for mechanical multibody systems. In addition, box-constraints for the angles q_1 and q_2, the controls u_1 and u_2, and the accelerations w_1 and w_2 are imposed. This leads to the following optimal control problem, which can be transformed by standard techniques to a Mayer-problem on the fixed time interval $[0, 1]$ as in OCP.

Problem (Robot Problem)**.** *Minimize*

$$t_f + \frac{\delta}{2}\int_0^{t_f} u(t)^\top u(t)\,dt$$

subject to the differential equations

$$\begin{aligned}
\dot{q_1} &= w_1,\\
\dot{q_2} &= w_1 + w_2,\\
\dot{w_1} &= \frac{J_{22}(u_1 - u_2 + J_{12}\sin q_2 w_2^2) - J_{12}\cos q_2(u_2 - J_{12}\sin q_2 w_1^2)}{J_{11}J_{22} - J_{12}^2\cos^2 q_2},\\
\dot{w_2} &= \frac{J_{11}(u_2 - J_{12}\sin q_2 w_1^2) - J_{12}\cos q_2(u_1 - u_2 + J_{12}\sin q_2 w_2^2)}{J_{11}J_{22} - J_{12}^2\cos^2 q_2},
\end{aligned}$$

the boundary conditions $q_1(0) = q_2(0) = w_1(0) = w_2(0) = w_1(t_f) = w_2(t_f) = 0$ *and*

$$\begin{aligned}
x_f &= l_1\cos(q_1(t_f)) + l_2\cos(q_1(t_f) + q_2(t_f)),\\
y_f &= l_1\sin(q_1(t_f)) + l_2\sin(q_1(t_f) + q_2(t_f)),
\end{aligned}$$

and the control and state constraints

$$|u_i(t)| \le 25, \quad |q_i(t)| \le 3, \quad |w_i(t)| \le 5, \quad i = 1, 2.$$

The following parameters represent the IBM 7535 B 04 industrial robot and were used for numerical computations:

$$\begin{array}{rclrrclrrcl} m_1 &=& 24 & [kg], & m_2 &=& 15 & [kg], & m &=& 6 & [kg], \\ J_1 &=& 1.6 & [kgm^2], & J_2 &=& 0.43 & [kgm^2], & J_3 &=& 0.01 & [kgm^2], \\ l_1 &=& 0.4 & [m], & l_2 &=& 0.25 & [m], & a_1 &=& 0.2 & [m], \\ a_2 &=& 0.125 & [m], & & & & & & & & \end{array}$$

and

$$J_{11} = J_1 + (m_2 + m)l_1^2, \quad J_{12} = m_2 a_2 l_1 + m l_1 l_2, \quad J_{22} = J_2 + J_3 + m l_2^2.$$

Our first attempts towards the numerical solution of the robot problem were not successful. We encountered problems due to bad scaling which resulted in breakdowns of the line search procedure in the globalized nonsmooth Newton's method. To avoid these breakdowns we experimented with a modification of Armijo's line search in step (3) of the globalized nonsmooth Newton's method. It is based on the so-called Armijo rule with expansion and works as follows. If the step-width $\alpha = 1$ fulfills the Armijo condition we increase α in discrete steps until the Armijo-condition is violated. Then, we choose that $\alpha \geq 1$ as step length which returned the smallest value of the merit function Θ. A drawback of this method is the loss of the superlinear convergence as we can not guarantee that the step length $\alpha_k = 1$ is accepted for sufficiently large k. In our numerical tests we observed only a linear convergence rate. Figure 4 shows the converged solution and intermediate iterates of the nonsmooth Newton's method for $N = 150$ and Euler's method. Notice, that the state constraint for the angular velocity w_2 and the control constraints for u_1 and u_2 become active. More intuitive snapshots of the motion of the optimally controlled robot are depicted in Figure 5. It is interesting to mention, that the iterates for the control functions behave much 'wilder' than the iterates for the state functions.

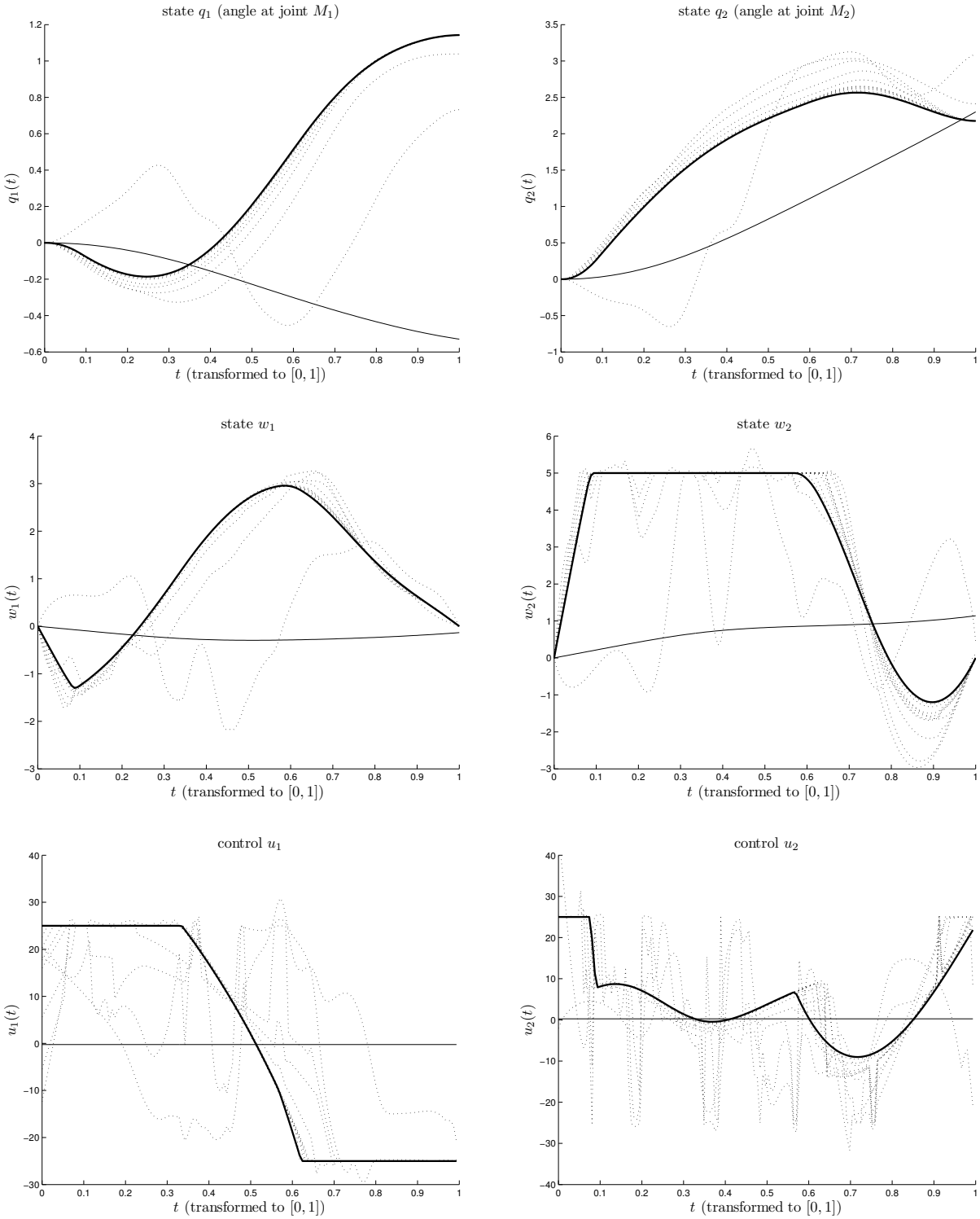

FIGURE 4. Numerical solution of the robot problem with Euler's method and $N = 150$ grid points: converged solution (bold curves), initial guess (solid curve), and intermediate iterates (dashed curves)

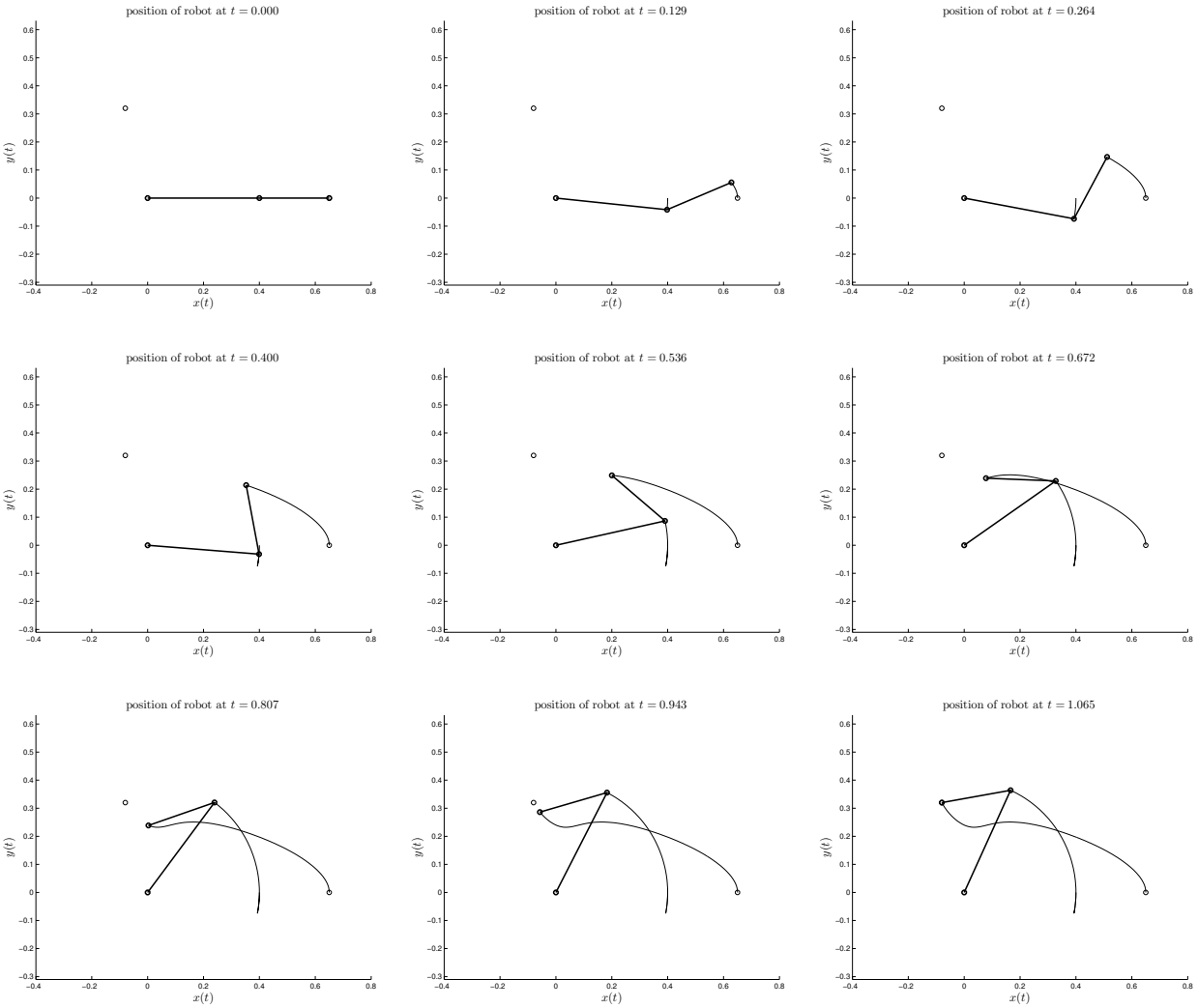

FIGURE 5. Snapshots of the robot's motion at different time points.

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