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Convergence of finite-dimensional approximations for mixed-integer optimization with differential equations*

by

Falk M. Hante[1] and Martin Schmidt[2]

[1]Friedrich-Alexander-Universität Erlangen-Nürnberg, Angewandte Mathematik 2, Cauerstr. 11, 91058 Erlangen, Germany
falk.hante@fau.de;
[2]Trier University, Department of Mathematics, Universitätsring 15, 54296 Trier, Germany
martin.schmidt@uni-trier.de

Dedicated to Günter Leugering on the occasion of His 65th birthday

Abstract: We consider a direct approach to solving the mixed-integer nonlinear optimization problems with constraints depending on initial and terminal conditions of an ordinary differential equation. In order to obtain a finite-dimensional problem, the dynamics are approximated using discretization methods. In the framework of general one-step methods, we provide sufficient conditions for the convergence of this approach in the sense of the corresponding optimal values. The results are obtained by considering the discretized problem as a parametric mixed-integer nonlinear optimization problem in finite dimensions, where the step size for discretization of the dynamics is the parameter. In this setting, we prove the continuity of the optimal value function under a stability assumption for the integer feasible set and second-order conditions from nonlinear optimization. We address the necessity of the conditions on the example of pipe sizing problems for gas networks.

Keywords: optimization with differential equations, optimal value function, Lipschitz continuity, parametric optimization, mixed-integer nonlinear programming

1. Introduction

Optimization with integer and dynamic constraints needs to deal with the complexity of combinatorics and infinite-dimensional variables simultaneously. Such problems appear naturally, for example, in gas network optimization problems, where the infinite-dimensional variables are subject to partial differential equations and mixed-integer aspects model the choice of opening or closing a

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valve or the decision of turning on or off a compressor; see Fügenschuh et al. (2015). Similar problems also appear in other critical infrastructure systems, such as the control of water flow in networks of canals, considered in Hante et al. (2017), Leugering and Schmidt (2002), in resource- and energy-efficient building, appearing in Bachmann et al. (2017), Kufner et al. (2018), and in many control problems in chemical engineering, such as optimization of column switching in simulated moving bed chromatography; see Kawajiri and Biegler (2006), Sager(2012).

In order to tackle this particular class of problems, we consider in this paper a direct approach, where a discretization of the dynamic constraints—for example, performed with the help of a Runge–Kutta scheme—yields a finite-dimensional approximation. More precisely, we consider nonlinear optimization problems, in which mixed-integer nonlinear constraints are imposed on the initial and terminal states of the solution of an ordinary differential equation (ODE) and approximate the ODE using a one-step method. This yields a mixed-integer nonlinear program (MINLP), parameterized by the step size used for the discretization. A natural question is the convergence of these approximations for a sequence of step sizes tending to zero. We consider problems, in which the terminal states enter linearly into the otherwise nonlinear problem. This particular structure is given in a natural manner for stationary considerations of the network problems mentioned above. We will explicitly discuss here the example of gas networks.

A canonical concept of convergence for the approximations is given by the topology of the underlying spaces. However, for integer constraints, the discrete topology is too fine as to provide a useful notion of limits. We therefore focus on establishing convergence of the corresponding optimal values as the essential measure for the quality of a solution. This approach is in line with the early investigations concerning the convergence of Euler discretization of optimal control problems without integer constraints (Polak, 1973).

For the particular problem class under consideration here, this path leads to the study of parametric MINLPs. Necessary and sufficient conditions for the continuity of the optimal value function for parametric linear problems are given in Williams (1989). The optimal value function of parametric convex problems has been studied in Gugat (1994) as well as Gugat and Hante (2016). In these cases, a constraint qualification of Slater type is sufficient to establish both the stability of the integer feasible set and the regularity of the constraints for a sufficiently small perturbation of the parameter. For parametric mixed-integer quadratic optimization problems, the continuity of the optimal value function is guaranteed by assuming stability of the integer feasible set and additional regularity conditions on the constraints; see Chen and Han (2012) or Han and Chen (2015). We later discuss these conditions and highlight the relation to the conditions that we use for general nonlinear problems (instead of quadratic) problems. Conditions imposing the stability of the integer feasible set have been investigated in Bank and Hansel (1984).

Our contribution here is to provide sufficient conditions for the continuity of the optimal value function for parametric mixed-integer nonlinear optimization problems with perturbations of the right-hand sides of the equality and inequality constraints. We show that stability of the integer feasible set, combined with standard second-order sufficient conditions, known from nonlinear optimization, ensures the continuous dependence of the optimal value on parameters entering the nonlinear constraints linearly. This result, combined with convergence results for general one-step methods, yields sufficient conditions for the convergence of the optimal value of the approximations to the limit problem for the general problem class, described above. We show by an example that the stability assumption on the integer feasible set is a necessary condition.

The impetus for this research came from a conversation with Günter Leugering during a seminar in Hirschegg in the Kleinwalsertal (Austria) in 2017. Motivated by gas network optimization problems, Günter posed the question of whether one can say something about the convergence of solutions of a sequence of parametric MINLPs as, for example, obtained from direct discretizations of differential equations. Here, we answer the question for a special type of MINLPs with ODEs. The case of PDEs is still open and a topic of future research. In addition, the questions considered in this paper are also highly related to a lot of work that both authors carried out together with Günter and in which both dynamic and integer aspects have been combined; see Elbinger et al. (2016), Gugat et al. (2018a,b), Hante and Leugering (2009), Hante et al. (2017), Hante, Leugering and Seidman (2009, 2010), or Leugering et al. (2017).

The remainder of the paper is organized as follows. In Section 2 we present the problem formulation and details concerning the direct approach as a finite-dimensional approximation to the considered problems. In Section 3 we provide auxiliary results concerning the regularity of the optimal value function for general parametric MINLPs. In Section 4 we apply these results to obtain sufficient conditions for the convergence of the direct approach. In Section 5 we illustrate our results on the example of optimal sizing of gas pipeline networks. Finally, in Section 6 we present conclusions and discuss future working directions.

2. Problem statement

We consider problems of the following type

$$\min_{x,y,z} \quad f(x, y, z(0), z(1)) \tag{1a}$$

$$\text{s.t.} \quad g(x, y, z(0), z(1)) \le 0, \quad h(x, y, z(0), z(1)) = 0, \tag{1b}$$

$$\frac{\mathrm{d}}{\mathrm{d}t} z(t) = \psi(t, z(t), x, y), \quad t \in (0, 1), \tag{1c}$$

$$z(0) = \psi_0(x, y), \tag{1d}$$

$$x \in \mathbb{R}^n, \quad y \in \mathcal{Z} \subseteq \mathbb{Z}^k, \quad z \in C([0, 1]; \mathbb{R}^\ell). \tag{1e}$$

Here, $x \in \mathbb{R}^n$ is the vector of continuous variables and $y \in \mathbb{Z}^k$ is the vector of discrete variables, which is part of the finite (and thus bounded) set $\mathcal{Z} \subseteq \mathbb{Z}^k$. Moreover, z is the trajectory of the Cauchy problem (1c) and (1d) with states $z(t) \in \mathbb{R}^\ell$ for $t \in (0, 1)$ and given maps $\psi_0 \colon \mathbb{R}^n \times \mathbb{Z}^k \to \mathbb{R}^\ell$ as well as $\psi \colon [0, 1] \times \mathbb{R}^\ell \times \mathbb{R}^n \times \mathbb{Z}^k \to \mathbb{R}^\ell$. The initial and terminal values of the trajectory z are coupled with the other variables, x, y, by the algebraic constraints (1b). We consider constraint functions $g \colon \mathbb{R}^n \times \mathbb{Z}^k \times \mathbb{R}^\ell \times \mathbb{R}^\ell \to \mathbb{R}^{\ell_g}$ and $h \colon \mathbb{R}^n \times \mathbb{Z}^k \times \mathbb{R}^\ell \times \mathbb{R}^\ell \to \mathbb{R}^{\ell_h}$, which may be both nonlinear with respect to the first three components (x, y and $z(0)$) and linear with respect to the fourth component for the final state $z(1)$. The latter assumption is required in the proof of our main theorem. Furthermore, the objective function $f \colon \mathbb{R}^n \times \mathbb{Z}^k \times \mathbb{R}^\ell \times \mathbb{R}^\ell \to \mathbb{R}$ can also be nonlinear.

Note that problems with any finite number of intermediate states of the trajectory z in the constraints g and h can be equivalently written in this form. Moreover, the formulation of Problem (1) also contains algebraic constraints that do not act on the initial and terminal values of the Cauchy problem if the respective rows of the constraint vectors g and h do not depend on the entries of $z(0)$ or $z(1)$.

In order to solve problems of the form (1) numerically, we consider a direct approach by approximating the solution of the Cauchy problem (1c) and (1d) using a discretization method. For a sequence of discretization grids, this yields a sequence of corresponding mixed-integer nonlinear optimization problems (MINLPs). More specifically, we consider an equidistant grid, $\{t_n\}_{n=0}^N$, with $t_0 = 0$, $t_{n+1} > t_n$, for $n = 0, \dots, N-1$, and $t_N = 1$, on which we approximate (1) using a general one-step method. This yields the finite-dimensional MINLP

$$\min_{x,y,z_0,\dots,z_N} \quad f(x, y, z_0, z_N) \tag{2a}$$

$$\text{s.t.} \quad g(x, y, z_0, z_N) \le 0, \quad h(x, y, z_0, z_N) = 0, \tag{2b}$$

$$z_{n+1} = z_n + \tau\, \Theta(t_n, z_n, x, y, \tau), \quad n = 0, \dots, N-1, \tag{2c}$$

$$z_0 = \psi_0(x, y), \tag{2d}$$

$$x \in \mathbb{R}^n, \quad y \in \mathcal{Z} \subseteq \mathbb{Z}^k, \quad z_n \in \mathbb{R}^\ell, \quad n = 0, \dots, N, \tag{2e}$$

with $\tau = t_{n+1} - t_n$ for $n = 0, \dots, N-1$, and some increment function $\Theta\colon [0,1] \times \mathbb{R}^\ell \times \mathbb{R}^n \times \mathbb{Z}^k \times [0,1] \to \mathbb{R}^\ell$. For a detailed discussion of general one-step methods we refer to Hairer, Norsett and Wanner (1993, Chapter III.8) and Quarteroni, Sacco and Saleri (2007, Chapter 11.2).

Let $\varphi(\tau)$ be the optimal value of (2) as a function of the step size τ. In the following, we develop theory to obtain conditions that ensure the convergence of $\varphi(\tau)$ to the optimal value of Problem (1) for $\tau \to 0$. The practical relevance can be seen from the following examples.

Example 1 *In the context of resource- and energy-efficient building the decisions on the inner warmth isolation for external walls is an important step in planning processes for constructions of facades; see also Kufner et al. (2018). Based on Bachmann et al. (2017), we consider here as a prototypical problem the heat distribution on a sectional area of a single room modeled in a simplified manner as*

$$\xi_t - \kappa \Delta \xi = \chi, \quad -\kappa_0 \xi_s|_{s=0} = y, \quad \kappa_1 \xi_s|_{s=1} = u$$

on $\Omega = (0,1)$ where ξ is the room temperature, $\kappa, \kappa_0, \kappa_1 > 0$ are given diffusion coefficients, χ is a known distributed heat source, u is a continuous parameter for a wall heater at $s = 1$ within bounds $u^- \le u \le u^+$, and $y \in \{1, \dots, M\}$ is a discrete parameter, corresponding to available isolation material products to be used at $s = 0$. The goal is to choose u and y so as to bring ξ as close as possible to a desired temperature distribution ξ_d on $(0,1)$, subject to costs αu^2 for heating and βy for material, with suitable coefficients $\alpha, \beta \ge 0$. With $z = (z_1, z_2, z_3)^\top$ and $x = (x_1, x_2)^\top$, setting $z_1 = \xi$, $z_2 = \xi_s$, and $x_1 = u$ and auxiliary variables z_3 and x_2, the stationary case for the above scenario then yields a problem of the form (1) with

$$\begin{aligned}
\min_{x,y,z} \quad & f(x, y, z(0), z(1)) := z_3(1) + \alpha x_1^2 + \beta y \\
\text{s.t.} \quad & g(x, y, z(0), z(1)) := (x_1 - u^+, u^- - x_1)^\top \le 0, \\
& h(x, y, z(0), z(1)) := \kappa_1 z_2 - x_1 = 0, \\
& \frac{\mathrm{d}}{\mathrm{d}s} z(s) = \psi(t, z(s), x, y) := \begin{pmatrix} z_2(s) \\ -\kappa^{-1} \chi(s) \\ (z_1(s) - \xi_d(s))^2 \end{pmatrix}, \quad s \in (0,1), \\
& z(0) = \psi_0(x, y) := (x_2, -\kappa_0^{-1} y, 0)^\top, \\
& x = (x_1, x_2)^\top \in \mathbb{R}^2, \quad y \in \mathcal{Z} := \{1, \dots, M\} \subset \mathbb{Z}, \\
& z = (z_1, z_2, z_3)^\top \in C([0,1]; \mathbb{R}^3).
\end{aligned}$$

Later, in Section 5, we consider another example that is defined on a graph which models a transport network. Our framework as given in Problem (1) is perfectly suited for the special case, in which a differential equation is defined on every arc of a graph, but in which only the initial and terminal values of the solution of this differential equation are of interest (and no intermediate solution values). This is, e.g., the case in gas transport network optimization, where the initial and terminal values correspond to gas pressures on nodes and no intermediate nodes (in the pipe) are used in other constraints or the objective function. The details are given in Section 5 and we refer to Habec, Pfetsch and Ulbrich (2017), where this mathematical structure is used to design a global optimization algorithm for mixed-integer gas transport problems with differential equations on the arcs.

3. Continuity of optimal value functions of parametric MINLPs

In this section we study the finite-dimensional MINLP

$$\varphi(e_G, e_H) := \min_{x,y} \quad f(x,y) \tag{3a}$$

$$\text{s.t.} \quad G(x,y) \le e_G, \tag{3b}$$

$$H(x,y) = e_H, \tag{3c}$$

$$x \in \mathbb{R}^n, \quad y \in \mathcal{Z} \subseteq \mathbb{Z}^k, \tag{3d}$$

which we consider as a parameterized optimization problem, having parameters $e_G \in \mathbb{R}^{\ell_G}$ and $e_H \in \mathbb{R}^{\ell_H}$. Here, $f : \mathbb{R}^n \times \mathbb{Z}^k \to \mathbb{R}$, $G : \mathbb{R}^n \times \mathbb{Z}^k \to \mathbb{R}^{\ell_G}$, and $H : \mathbb{R}^n \times \mathbb{Z}^k \to \mathbb{R}^{\ell_H}$. As before, we assume that $\mathcal{Z}$ is finite and thus bounded.

Our goal is to derive a continuity result for the optimal value function $\varphi(e)$, $e = (e_G^\top, e_H^\top)^\top$. To this end, we first consider the case, in which we fix the discrete variables y to some feasible values $\bar{y} \in \mathcal{Z} \subseteq \mathbb{Z}^k$. Thus, we consider the continuous problem

$$\varphi(e;\bar{y}) := \min_{x \in \mathbb{R}^n} \quad f(x,\bar{y}) \tag{4a}$$

$$\text{s.t.} \quad G(x,\bar{y}) \le e_G, \tag{4b}$$

$$H(x,\bar{y}) = e_H. \tag{4c}$$

In what follows, we make use of the Lagrangian function of Problem (4), which is defined as

$$L(x,\lambda,\mu;\bar{y}) = f(x,\bar{y}) + \lambda^\top (G(x,\bar{y}) - e_G) + \mu^\top (H(x,\bar{y}) - e_H),$$

where $0 \le \lambda \in \mathbb{R}^{\ell_G}$ and $\mu \in \mathbb{R}^{\ell_H}$ are the Lagrange multipliers of the constraints in (4). Moreover, we need to introduce some notation. For any fixed parameter e, let $\mathcal{F}(e_G, e_H)$ denote the feasible set of Problem (3), i.e.,

$$\mathcal{F}(e_G,e_H) = \{(x,y) \in \mathbb{R}^n \times \mathcal{Z} \colon G(x,y) \le e_G,\ H(x,y) = e_H\}$$

and let $\mathcal{F}_y(e_G, e_H)$ be the projection onto the space of the feasible discrete variables, i.e.,

$$\mathcal{F}_y(e_G,e_H) = \left\{ y \in \mathbb{Z}^k \colon \exists x \text{ with } (x,y) \in \mathcal{F}(e_G,e_H) \right\}.$$

With that, we can state a sensitivity result for the mixed-integer nonlinear optimization problem (3) w.r.t. e in a neighborhood of the origin.

THEOREM 1 *Suppose that the following conditions hold for all fixed $\bar{y} \in \mathcal{F}_y(0)$:*

(a) The functions $f(\cdot, \bar{y})$, $G(\cdot, \bar{y})$, and $H(\cdot, \bar{y})$ are twice continuously differentiable and

(b) for any global minimum $x^* = x^*(\bar{y})$ of Problem (4) with $e = 0$ and $\lambda^* = \lambda^*(\bar{y})$, $\mu^* = \mu^*(\bar{y})$ being the corresponding Lagrange multipliers, it holds that

$$\begin{aligned} \nabla_x L(x^*, \lambda^*, \mu^*; \bar{y}) &= 0, \\ G(x^*, \bar{y}) &\leq 0, \\ H(x^*, \bar{y}) &= 0, \\ \lambda^* &\geq 0, \\ \lambda_i^* &= 0 \quad \text{for all} \quad i \text{ with } G(x^*, \bar{y}) < 0, \end{aligned}$$

and

$$w^\top \nabla^2_{xx} L(x^*, \lambda^*, \mu^*; \bar{y}) w > 0$$

for all $w \neq 0$ with

$$\begin{aligned} \nabla_x G_i(x^*, \bar{y})^\top w &= 0 \quad \text{for all} \quad i \in \{1, \dots, \ell_G\} \text{ with } G_i(x^*, \bar{y}) = 0, \\ \nabla_x H_i(x^*, \bar{y})^\top w &= 0 \quad \text{for all} \quad i \in \{1, \dots, \ell_H\}. \end{aligned}$$

Moreover, suppose that the linear independence constraint qualification (LICQ) is fulfilled in x^* and that the strict complementarity slackness condition, i.e.,

$$\lambda_i^* > 0 \quad \text{for all} \quad i \in \{1, \dots, \ell_G\} \text{ with } G_i(x^*, \bar{y}) = 0$$

holds.

Further, assume that

$$\mathcal{F}_y(e) = \mathcal{F}_y(0) \quad \text{for } e \text{ sufficiently small.} \tag{5}$$

Then, the optimal value function $\varphi(e)$ of the parametric mixed-integer nonlinear optimization problem (3) is Lipschitz continuous in a neighborhood of $e = 0$.

PROOF Let $\varphi(e; \bar{y})$ be the optimal value function of the parametric problem (4) for fixed $\bar{y}$. Under the assumption (5) we have

$$\varphi(e) = \min_{\bar{y} \in \mathcal{F}_y(e)} \varphi(e; \bar{y}) = \min_{\bar{y} \in \mathcal{F}_y(0)} \varphi(e; \bar{y}) \tag{6}$$

if e is sufficiently small. Moreover, under Assumptions (a) and (b), it follows that $\varphi(e; \bar{y})$ is continuously differentiable with respect to e in an open sphere centered at $e = 0$; see, e.g., Bertsekas (1999, Proposition 3.2.2). In particular, $\varphi(e;\bar{y})$ is locally Lipschitz continuous for all $\bar{y} \in \mathcal{F}_y(e)$. Using that the pointwise minimum of finitely many locally Lipschitz continuous functions is locally Lipschitz, the result then follows from the boundedness of $\mathcal{F}_y(0) \subseteq \mathcal{Z}$ and (6). □

One of the main assumptions of Theorem 1 is the stability condition (5) for the integer components of the feasible sets. In order to discuss its necessity, we consider the case of Problem (3) without inequality constraints. The problem then reads

$$\varphi(e_H) := \min_{x,y} \quad f(x,y) \tag{7a}$$

$$\text{s.t.} \quad H(x,y) = e_H, \tag{7b}$$

$$x \in \mathbb{R}^n, \quad y \in \mathcal{Z} \subseteq \mathbb{Z}^k \tag{7c}$$

and Theorem 1 also holds with a smaller set of assumptions:

Corollary 1 *Suppose that the following conditions hold for all fixed $\bar{y} \in \mathcal{F}_y(0)$:*

(a) The functions $f(\cdot,\bar{y})$ and $H(\cdot,\bar{y})$ are twice continuously differentiable and

(b) for any global minimum $x^* = x^*(\bar{y})$ of Problem (7) with $e_H = 0$ and $\mu^* = \mu^*(\bar{y})$ being the corresponding Lagrange multiplier, it holds that

$$\nabla_x L(x^*,\mu^*;\bar{y}) = 0,$$
$$H(x^*,\bar{y}) = 0,$$

and

$$w^\top \nabla^2_{xx} L(x^*,\mu^*;\bar{y}) w > 0$$

for all $w \neq 0$ with

$$\nabla_x H_i(x^*,\bar{y})^\top w = 0 \quad \text{for all} \quad i \in \{1,\dots,\ell_H\}.$$

Moreover, suppose the LICQ is fulfilled in x^*.

Further, assume that

$$\mathcal{F}_y(e) = \mathcal{F}_y(0) \quad \text{for } e \text{ sufficiently small.} \tag{8}$$

Then, the optimal value function $\varphi(e)$ of the parametric mixed-integer nonlinear optimization problem (7) is Lipschitz continuous in a neighborhood of $e = 0$.

The following example now shows that the stability condition (8) is necessary.

Example 2 *Consider the parametric MINLP*

$$\begin{aligned} \min_{x,y} \quad & f(x,y) = -y(\exp(x)+1) \\ s.t. \quad & H(x,y) = (1-y)x + y\exp(x) = \xi, \\ & x \in \mathbb{R}, \quad y \in \{0,1\}. \end{aligned}$$

For the unperturbed problem ($\xi = 0$), there are no feasible points other than $x^* = y^* = 0$ with the optimal value $f^* = f(x^*, y^*) = 0$. However, for small perturbations $\xi > 0$, the feasible set consists of the points $x^{(1)} = \xi,\ y^{(1)} = 0$ and $x^{(2)} = \ln(\xi),\ y^{(2)} = 1$ with $f(x^{(1)}, y^{(1)}) = 0$ and $f(x^{(2)}, y^{(2)}) = -(\xi + 1) < 0$. Hence, the optimal value function $\varphi(\xi)$ satisfies

$$\varphi(\xi) \to -1 \neq f^* \quad \text{for } \xi \searrow 0,$$

showing that it is not continuous in $\xi = 0$. The reason is that

$$\mathcal{F}_y(\xi) = \{0, 1\} \neq \{0\} = \mathcal{F}_y(0)$$

holds for sufficiently small $\xi > 0$, i.e., the stability condition (8) is violated. At the same time, for all $\bar{y} \in \mathcal{F}_y(0) = \{0\}$, we have $f(x, \bar{y}) = 0$ and $H(x, \bar{y}) = x$, so that the conditions (a) and (b) of Corollary 1 are satisfied.

Of course, the above example can be easily extended to include inequality constraints in order illustrate the necessity of the stability condition for the integer components of the respective feasible set for the general case in Theorem 1.

The next example shows that there are also problems, for which all conditions are satisfied. For simplicity, we again consider the conditions of Corollary 1.

Example 3 *Consider the parametric MINLP*

$$\begin{aligned} \min_{x_1, x_2, y_1} \quad & f(x, y) = \frac{1}{2}\left[\left(x_1 - \frac{1}{2}\right)^2 + \left(x_2 - \frac{1}{2}\right)^2 + \left(y_1 - \frac{1}{2}\right)^2\right] \\ s.t. \quad & H(x, y) = x_1 + x_2 - y_1 = e, \\ & x_1, x_2 \in \mathbb{R}, \quad y_1 \in \{0, 1, 2\}. \end{aligned}$$

For the unperturbed problem, i.e., $e = 0$, one can easily verify that

$$x^* = \begin{pmatrix} 1/2 \\ 1/2 \end{pmatrix}, \quad y_1^* = 1, \quad f^* = \frac{1}{8}$$

are the global optimal solution and the global optimal objective function value, respectively. Moreover, it is easy to see that $\mathcal{F}_y(0) = \{0, 1, 2\} = \mathcal{F}_y(e)$ for all e, i.e., the stability condition (8) is fulfilled. Obviously, also condition (a) of Corollary 1 is satisfied. For the conditions in (b) we first consider the case $\bar{y} = y_1^* = 1$ and the resulting continuous problem

$$\begin{aligned} \min_{x_1, x_2} \quad & \frac{1}{2}\left[\left(x_1 - \frac{1}{2}\right)^2 + \left(x_2 - \frac{1}{2}\right)^2 + \frac{1}{4}\right] \\ s.t. \quad & x_1 + x_2 - 1 = 0. \end{aligned}$$

The KKT conditions are given by

$$x_1 - \frac{1}{2} + \lambda = 0,$$
$$x_2 - \frac{1}{2} + \lambda = 0,$$
$$x_1 + x_2 - 1 = 0,$$

and we thus obtain the unique primal-dual solution $x = (1/2, 1/2)^\top$, $\lambda = 0$. *The constraint gradient is* $(1,1)^\top$ *and LICQ is thus obviously satisfied. The Hessian of the Lagrangian is the* 2×2 *identity matrix and the second-order condition needs to be checked for all vectors* $w = (\alpha, -\alpha)$, $0 \neq \alpha \in \mathbb{R}$.

Since the first- and second-order conditions are the same for $\bar{y} = 0$ *and* $\bar{y} = 2$, *they are also satisfied in these cases. Hence, all conditions of Theorem 1 are satisfied and the optimal value function of the parametric MINLP is Lipschitz continuous in a neighborhood of* $e = 0$.

Remark 1 *We note that the stability condition (5) for general mixed-integer nonlinear problems coincides with the one used in Chen and Han (2012) or Han and Chen (2015) for the special case of mixed-integer quadratic problems. For convex problems, constraint regularity conditions and stability of the integer component can be combined in a Slater-type condition; see Gugat (1997), Gugat and Hante (2016), and Williams (1989). In the linear case, these conditions are also necessary (Williams, 1989). In the latter work, the author uses the classical complementarity slackness theorem of linear optimization (Chvatal, 1983) to obtain the required sensitivity result for linear optimization; see also Mills (1956) and Williams (1963) for the original publications. Necessity in Theorem 1 is not given, because these conditions are not necessary even with a fixed integer component, i.e., in the purely continuous case.*

Remark 2 *Theorem 1 also extends to problems of the form*

$$\varphi(e_F, e_G, e_H) := \min_{x,y} \quad F(x, y, e_F) \tag{9a}$$
$$\text{s.t.} \quad G(x, y) \leq e_G, \tag{9b}$$
$$H(x, y) = e_H, \tag{9c}$$
$$x \in \mathbb{R}^n, \quad y \in \mathcal{Z} \subseteq \mathbb{Z}^k, \tag{9d}$$

for parametric cost functions $F \colon \mathbb{R}^n \times \mathbb{Z}^k \times \mathbb{R} \to \mathbb{R}$ *if the assumptions on* f *are replaced with the assumption that for all* $y \in \mathcal{F}_y$, F *is twice continuously differentiable in the first component and continuous in the third component. For fixed* e_F, *the continuity of* φ *with respect to* e_G *and* e_H *then follows from Theorem 1 as before. The continuity with respect to* e_F, *hence joint continuity of* φ *with respect to* (e_F, e_G, e_H), *is then implied by continuity of* F *with respect to* e_F. *Analogously, the remark applies to Corollary 1.*

4. Continuity of MINLPs with discretized ODEs

In this section we apply the results on parametric MINLPs, obtained in the previous section, to obtain sufficient conditions for the continuity of the optimal value when we pass to the limit in finite-dimensional approximations, obtained from one-step methods for ODEs. To this end, we make the following assumptions concerning the regularity of the nonlinearities in the limit problem (1) and of the increment function used in the discretization scheme to obtain the approximation (2).

ASSUMPTION 1 *We assume that the Cauchy problem* (1c) *and* (1d) *has a unique solution* $z(\cdot;x,y) \in C([0,1];\mathbb{R}^\ell)$ *in the sense that*

$$z(t;x,y) = \psi_0(x,y) + \int_0^t \psi(s, z(s;x,y), x, y)\,\mathrm{d}s, \quad t \in [0,1],$$

for all feasible $x \in \mathbb{R}^n$ *and* $y \in \mathcal{Z}$. *We further assume that, for all fixed* $y \in \mathcal{Z}$, *the functions* $f(\cdot,y,\cdot,\cdot)$, $g(\cdot,y,\cdot,\cdot)$, $h(\cdot,y,\cdot,\cdot)$, *and* $z(1;\cdot,y)$ *in Problem* (1) *are twice continuously differentiable.*

A sufficient condition for the properties of the solution z, required by Assumption 1, is that φ be continuous in s, globally Lipschitz continuous with respect to z and twice continuously differentiable with respect to z and x; see, e.g., Teschl (2012).

ASSUMPTION 2 *We assume that the increment function* Θ *is consistent, i.e.,*

$$\Theta(t,z,x,y,0) = \psi(t,z,x,y) \quad \textit{for all} \quad t \in [0,1],\ x \in \mathbb{R}^n,\ z \in \mathbb{R}^\ell,\ y \in \mathbb{Z}^k$$

and stable, i.e.,

$$\|\Theta(t,z,x,y,\tau) - \Theta(t,\tilde{z},x,y,\tau)\| \le L_\Theta \|z - \tilde{z}\|$$
$$\textit{for all} \quad t \in [0,1],\ z,\tilde{z} \in \mathbb{R}^\ell,\ x \in \mathbb{R}^n,\ y \in \mathbb{Z}^k,\ \tau \in [0,\bar{\tau}]$$

and some $L_\Theta > 0$ *as well as* $\bar{\tau} > 0$. *Moreover, we assume that*

$$\lim_{\tau \to 0} \Theta(t,z,x,y,\tau) = \psi(t,z,x,y)$$

holds for all $t \in [0,1]$.

For the statement of our main result, let $\mathcal{F}$ and $\mathcal{F}(\tau)$ denote the feasible sets of Problem (1) and Problem (2), respectively, and let $\mathcal{F}_y$ and $\mathcal{F}_y(\tau)$ be the corresponding projections onto the discrete variables, i.e.,

$$\mathcal{F}_y = \left\{ y \in \mathbb{Z}^k \colon \exists x \text{ with } (x,y) \in \mathcal{F} \right\},$$
$$\mathcal{F}_y(\tau) = \left\{ y \in \mathbb{Z}^k \colon \exists x \text{ with } (x,y) \in \mathcal{F}(\tau) \right\}.$$

Moreover, we use the shorthand notation

$$\hat{z}(x,y) := (z(0;x,y), z(1;x,y)).$$

Theorem 2 *Suppose that Assumptions 1 and 2 hold. Suppose further that the following conditions hold for all* $\bar{y} \in \mathcal{F}_y$. *For the global optimal solution* $x^* = x^*(\bar{y})$ *of Problem* (1) *with* $y = \bar{y}$ *let Lagrange multipliers* $\lambda^* = \lambda^*(\bar{y})$, $\mu^* = \mu^*(\bar{y})$ *exist such that*

$$\begin{aligned}
&\nabla_x \left(f(x^*, \bar{y}) + (\lambda^*)^\top g(x^*, \bar{y}, \hat{z}(x^*, \bar{y})) + (\mu^*)^\top h(x^*, \bar{y}, \hat{z}(x^*, \bar{y})) \right) = 0, \\
&g(x^*, \bar{y}, \hat{z}(x^*, \bar{y})) \le 0, \\
&h(x^*, \bar{y}, \hat{z}(x^*, \bar{y})) = 0, \\
&\lambda^* \ge 0, \\
&\lambda_i^* = 0 \quad \textit{for all} \quad i \in \{1, \dots, \ell_g\} \textit{ with } g(x^*, \bar{y}, \hat{z}(x^*, \bar{y})) < 0
\end{aligned}$$

and

$$w^\top \nabla_{xx}^2 \left(f(x^*, \bar{y}) + (\lambda^*)^\top g(x^*, \bar{y}, \hat{z}(x^*, \bar{y})) + (\mu^*)^\top h(x^*, \bar{y}, \hat{z}(x^*, \bar{y})) \right) w > 0$$

for all $w \neq 0$ *with*

$$\begin{aligned}
&\nabla_x [g_i(x^*, \bar{y}, \hat{z}(x^*, \bar{y}))]^\top w = 0, \quad i \in \{1, \dots, \ell_g\} \textit{ with } g_i(x^*, \bar{y}, \hat{z}(x^*, \bar{y})) = 0, \\
&\nabla_x [h_i(x^*, \bar{y}, \hat{z}(x^*, \bar{y}))]^\top w = 0, \quad i \in \{1, \dots, \ell_h\}
\end{aligned}$$

holds. Furthermore, assume that the LICQ is satisfied in x^* *and that*

$$\lambda_i^* > 0 \quad \textit{for all} \quad i \in \{1, \dots, \ell_g\} \textit{ with } g_i(x^*, \bar{y}, \hat{z}(x^*, \bar{y})) = 0$$

holds. Finally, suppose that

$$\mathcal{F}_y(\tau) = \mathcal{F}_y \quad \textit{for } \tau \textit{ sufficiently small.}$$

Then

$$\lim_{\tau \to 0} \varphi(\tau) = \varphi, \tag{10}$$

where φ *is the optimal value of Problem* (1).

Proof Let $\mathcal{S} \colon \mathbb{R}^n \times \mathcal{Z} \to \mathbb{R}^\ell$ denote the associated shooting operator

$$\mathcal{S} \colon (x, y) \mapsto z(1; x, y).$$

With

$$\begin{aligned}
&e(\tau) := S(x, y) - z_N, \\
&e_g(\tau) := g(x, y, \psi_0(x, y), e(\tau)), \quad e_h(\tau) := h(x, y, \psi_0(x, y), e(\tau)), \\
&G(x, y) := g(x, y, \psi_0(x, y), S(x, y)), \quad H(x, y) := h(x, y, \psi_0(x, y), S(x, y)), \\
&F(x, y, e(\tau)) := f(x, y, \psi_0(x, y), S(x, y) - e(\tau)),
\end{aligned}$$

and using the linearity of g and h with respect to the fourth component, Problem (2) admits the following reduced form

$$\min_{x,y} \quad F(x,y,e(\tau)) \tag{11a}$$
$$\text{s.t.} \quad G(x,y) \le e_g(\tau), \tag{11b}$$
$$H(x,y) = e_h(\tau), \tag{11c}$$
$$x \in \mathbb{R}^n, \quad y \in \mathcal{Z} \subseteq \mathbb{Z}^k, \tag{11d}$$

i.e., we obtain a parametric mixed-integer nonlinear problem of the form of (9). Consistency and stability of Θ from Assumption 2 implies that $\lim_{\tau\to 0} e(\tau) = 0$; see, e.g., Quarteroni, Sacco and Saleri (2007, Chapter 11.2). Using the continuity of the constraint functions g and h this yields

$$\lim_{\tau\to 0} e_g(\tau) = 0 \quad \text{and} \quad \lim_{\tau\to 0} e_h(\tau) = 0.$$

Moreover, $e(\tau) = 0$ yields the reduced form of the original problem (1). Further, under the stated assumptions, Problem (11) satisfies the conditions imposed in Remark 2 and Theorem 1. Using the continuity of φ in $\tau = 0$ hence yields (10). □

The assumptions of Theorem 2 of course simplify if the problem does not have inequality constraints. We can then use the conditions given in Corollary 1 on the reduced problem (11).

Finally, we note that Assumption 2 on the one-step method is satisfied for many numerical discretization schemes.

Remark 3 *For Lipschitz continuous vector fields $\psi(t,z,y)$, in the sense that*

$$\|\psi(t,z,x,y) - \psi(t,\tilde{z},x,y)\| \le L_\varphi \|z-\tilde{z}\|, \quad t\in[0,1],\ z,\tilde{z}\in\mathbb{R}^\ell,\ x\in\mathbb{R}^n,\ y\in\mathbb{Z}^k,$$

s-stage Runge–Kutta methods of the form

$$z_{n+1} = z_n + \tau \sum_{i=1}^{s} b_i \psi(t_n + c_i\tau, z_{n+1}^{(i)}),$$
$$z_{n+1}^{(i)} = z_n + \tau \sum_{j=1}^{s} a_{ij} \psi(t_n + c_j\tau, z_{n+1}^{(j)}), \quad i = 1,\dots,s,$$

with coefficients $c = (c_1,\dots,c_s)$, $A = (a_{ij})_{i,j=1}^s$, and $b = (b_1,\dots,b_s)$ are stable and consistent if and only if $\sum_{i=1}^s b_i = 1$. In particular, this condition is satisfied for the explicit and the implicit Euler method. For details see, e.g., Strehmel and Weiner (1995).

5. Case study: optimal sizing of gas pipeline networks

In order to illustrate the theoretical results of the previous sections we now present a case study. To this end, we consider the problem of optimal sizing of gas pipeline networks. This problem can be described as follows. We are given a finite and directed graph $G = (V, A)$ with node set V and arc set A, which models a gas transport network topology. The nodes $v \in V$ are split into the set V_+ of entry nodes, where gas is supplied, the set V_- of exit nodes, where gas is withdrawn, and the set V_0 of remaining nodes. A related problem is also considered in Bragalli et al. (2006, 2012), where the authors consider the optimal sizing of water transport networks. In the cited papers, however, the authors do not consider discretized ordinary differential equations for the change of hydraulic heads in water pipes in their MINLP, but consider an algebraic approximation.

At all nodes $v \in V$, minimum and maximum gas pressure levels $0 < p_v^- \leq p_v^+$ are specified. Additionally, the amount of gas q_v is prescribed for every entry and exit node such that all of the entry flows and exit flows are balanced, i.e.,

$$\sum_{v \in V_+} q_v + \sum_{v \in V_-} q_v = 0.$$

Here, we fix the notational convention that entry flows are non-negative and exit flows are non-positive.

The arcs $a = (u, v) \in A$ of the graph represent gas pipes, for which we need to choose cost-optimal diameters that influence the pressure loss that appears if gas flows through the pipes. Since we only consider the stationary situation, gas flow through a cylindrically shaped and horizontal pipe is described by the Euler momentum equation

$$\frac{\partial p}{\partial s}\left(1 - \frac{q^2}{A^2}\frac{c^2}{p^2}\right) = -\frac{\lambda c^2}{2A^2 D p}|q|q, \quad s \in [0, L]. \tag{12}$$

Here, A, D, and L are, respectively, the cross-sectional area, the diameter, and the length of the pipe, p is again the gas pressure, and q represents mass flow. Moreover, g describes the gravitational acceleration, c is the speed of sound, and λ models friction at the rough inner pipe walls. Note that, in practice, many formulas for λ exist. For simplicity, we choose here a flow-independent model like the formula of Nikuradse; see Fügenschuh et al. (2015), Hante et al. (2017), Schmidt, Steinbach and Willert (2015a,b, 2016).

Finally, s denotes the spatial coordinate. Note that we omitted the index a here for better reading. We refer to, for instance, Fügenschuh et al. (2015), Schmidt, Steinbach and Willert (2015a) for more details.

In addition, we are given lower and upper bounds $q_a^- \leq q_a^+$ for the mass flow q_a through a pipe $a \in A$ and we couple the flows on the arcs via Kirchhoff's first law

$$\sum_{a \in \delta_v^{\text{out}}} q_a - \sum_{a \in \delta_v^{\text{in}}} q_a = q_v \quad \text{for all } v \in V.$$

Here, we use the standard δ-notation,

$$\delta_v^{\text{in}} := \{a \in A\colon \exists u \in V \text{ with } a = (u, v)\},$$
$$\delta_v^{\text{out}} := \{a \in A\colon \exists u \in V \text{ with } a = (v, u)\},$$

and assume that $q_v = 0$ holds for all inner nodes V_0.

The problem now is to choose for every pipe $a \in A$ a diameter D_a out of a discrete and finite set $\mathcal{D} = \{D_1, \dots, D_k\}$ of commercially available diameters with $D_1 < D_2 < \cdots < D_k$. In what follows we denote with C_i the costs per meter of diameter D_i. Typically, the costs are increasing w.r.t. the diameter magnitude, i.e., $C_1 < C_2 < \cdots < C_k$. Thus, we want to determine a cost-optimal diameter per pipe such that

(i) the given supplied and withdrawn flows can be transported,
(ii) all pressure and flow bounds are satisfied, and
(iii) the gas flow is feasible w.r.t. the Euler equation (12).

We model the discrete diameter choice by a set $b_{a,i} \in \{0, 1\}$, $i = 1, \dots, k$, of binary variables such that diameter D_i is chosen for arc a if and only if $b_{a,i} = 1$. Hence, we impose the constraints

$$D_a = \sum_{i=1}^{k} b_{a,i} D_i, \quad 1 = \sum_{i=1}^{k} b_{a,i} \quad \text{for all } a \in A.$$

More formally, the problem under consideration reads

$$\min \quad \sum_{a \in A} L_a \sum_{i=1}^{k} C_i b_{a,i} \tag{13a}$$

$$\text{s.t.} \quad \sum_{a \in \delta_v^{\text{out}}} q_a - \sum_{a \in \delta_v^{\text{in}}} q_a = q_v \quad \text{for all } v \in V, \tag{13b}$$

$$q_a \in \left[q_a^-, q_a^+\right] \quad \text{for all } a \in A, \tag{13c}$$

$$p_v \in \left[p_v^-, p_v^+\right] \quad \text{for all } v \in V, \tag{13d}$$

$$D_a = \sum_{i=1}^{k} b_{a,i} D_i, \quad 1 = \sum_{i=1}^{k} b_{a,i} \quad \text{for all } a \in A, \tag{13e}$$

$$b_{a,i} \in \{0, 1\} \quad \text{for all } a \in A,\ i = 1, \dots, k, \tag{13f}$$

$$\frac{\partial p_a}{\partial s} \left(1 - \frac{q_a^2}{A_a^2} \frac{c^2}{p_a^2}\right) = -\frac{\lambda c^2}{2 A_a^2 D_a p_a} |q_a| q_a \quad \text{for all} \quad s \in (0, L_a),\ a \in A, \tag{13g}$$

$$p_v = p_a(0) \quad \text{for all } a \in \delta_v^{\text{out}},\ v \in V, \tag{13h}$$

$$p_v = p_a(L_a) \quad \text{for all } a \in \delta_v^{\text{in}},\ v \in V. \tag{13i}$$

Note that we can also replace the area A_a with the diameter D_a using the formula $A_a = \pi D_a^2/4$. It can be verified that Problem (13) is of the form (1).

As continuous variables we have

$$x = \left((q_a)_{a\in A}^\top, (p_v)_{v\in V}^\top, (D_a)_{a\in A}^\top\right)^\top$$

and the discrete variables of the problem are

$$y = (b_{a,i})_{a\in A, i=1,\dots,k} \in \mathcal{Z} = \{0,1\}^{A\times\{1,\dots,k\}}.$$

Furthermore, the states are given by

$$z = (p_a)_{a\in A} \quad \text{with} \quad p_a : [0, L_a] \to \mathbb{R},$$

i.e., we have

$$z(0) = (p_a(0))_{a\in A} \in \mathbb{R}^{|A|} \quad \text{and} \quad z(L_a) = (p_a(L_a))_{a\in A} \in \mathbb{R}^{|A|}.$$

This, in particular, means that we scaled the interval $[0,1]$ to $[0, L_a]$ for every pipe $a \in A$. The objective function, which only depends on discrete variables in this case, is given by

$$f(y) = \sum_{a\in A} L_a \sum_{i=1}^{k} C_i b_{a,i}$$

and the algebraic constraints read

$$h(x, y, z(0), z(1)) = \begin{pmatrix} \left(\sum_{a\in\delta_v^{\text{out}}} q_a - \sum_{a\in\delta_v^{\text{in}}} q_a - q_v\right)_{v\in V} \\ \left(D_a - \sum_{i=1}^k b_{a,i} D_i\right)_{a\in A} \\ \left(1 - \sum_{i=1}^k b_{a,i}\right)_{a\in A} \\ (p_v - p_a(0))_{v\in V, a\in\delta_v^{\text{out}}} \\ (p_v - p_a(L_a))_{v\in V, a\in\delta_v^{\text{in}}} \end{pmatrix},$$

$$g(x) = \begin{pmatrix} (q_a - q_a^+)_{a\in A} \\ (q_a^- - q_a)_{a\in A} \\ (p_v - p_v^+)_{v\in V} \\ (p_v^- - p_v)_{v\in V} \end{pmatrix}.$$

Finally, the ODE's right-hand side is given by

$$\psi = (\psi_a)_{a\in A} \quad \text{with} \quad \psi_a = \psi_a(s, p_a(s), (q_a, D_a)) = \frac{-\frac{\lambda c^2}{2A_a^2 D_a p_a}|q_a|q_a}{1 - \frac{q_a^2}{A_a^2}\frac{c^2}{p_a^2}}.$$

In addition to these identifications, a family of finite-dimensional MINLPs like in (2) can be obtained by, e.g., discretizing the ODE in Constraint (13g) with an implicit Euler scheme, which yields

$$\frac{p_{a,n+1} - p_{a,n}}{\tau_{a,n}} \left(1 - \frac{q_a^2}{A_a^2}\frac{c^2}{p_{a,n+1}^2}\right) = -\frac{\lambda c^2}{2A_a^2 D_a p_{a,n+1}}|q_a|q_a, \quad n = 0, \dots, N-1,$$

on the grid $0 = x_{a,0} < x_{a,1} < \cdots < x_{a,N} = L_a$ with $\tau_{a,n} = x_{a,n+1} - x_{a,n}$ for $n = 0, \ldots, N-1$.

We now also discuss the crucial stability condition (5) for this real-world problem. To this end, we show that there might be situations, in which this assumption does not hold. Consider, for example, an instance of Problem (13) on a network with two nodes $u, v \in V$ and a single pipe $a = (u, v) \in A$, connecting these two nodes. Assume further a fixed inflow pressure p_u and a fixed inflow $q_u = q_a$ that leads—for a given diameter D_i, $i \in \{1, \ldots, k\}$—to the uniquely determined outflow pressure p_v. If $p_v = p_v^-$ for $D_a = D_i$, $i > 1$ (with costs C_i), it also holds $p_v < p_v^-$ for $D_a = D_j$ with $1 \leq j < i$. The binary variables would thus take the values $b_{a,j} = 0$ for all $j \neq i$ and $b_{a,i} = 1$. Hence, the exact solution has the objective function value $L_a C_i$. We now compare this solution with a solution $p_v(\tau)$ for all $\tau > 0$. It is shown in Habeck, Pfetsch and Ulbrich (2017) that an Euler discretization leads to a lower bound $p_v(\tau) < p_v$ for all τ. As a consequence, for a series of discretized and finite-dimensional MINLPs we always obtain objective function values $L_a C_{i+1} \neq L_a C_i$ for all sufficiently small $\tau > 0$.

Thus, we have shown that the stability condition (5) is also a necessary condition for Theorem 1 in this real-world setting. We note that the violation of this condition is, at least in the above situation, rather pathological and could be recovered by arbitrary small perturbations of the sizes of the pipe diameters or of the outflow pressure bound. It might therefore appear to be of low practical relevance. However, there are many situations, in which one needs to be very careful regarding this viewpoint. One example is robust optimization: If we, e.g., assume that the supplied flow and the inflow pressure are allowed to vary in given uncertainty sets, these sets may contain values such that the "pathological" situation arises quite naturally.

The bottom line of this discussion is that one should not carelessly expect convergence of a direct approach for problems of this kind. If convergence is needed, one should then check the provided or similar conditions. To this end, further research may for example aim to exploit the network structure for conditions in a decoupled fashion in order to avoid the requirement of knowing the exact solution of the fully coupled problem. Alternatively, one may investigate regularization techniques that foster stability of the integer feasible set.

6. Conclusion

We showed that the convergence of direct approximations for mixed-integer nonlinear optimization problems with constraints depending on initial and terminal conditions of an ordinary differential equation can be guaranteed under certain regularity assumptions for the limit problem. Such problems appear naturally in many applications—we specifically considered the example of gas networks.

The conditions provided in this paper ensure convergence of the optimal value. While this is an important achievement, we note that, in general, the convergence of the variables and states is not guaranteed under the conditions found here.

The results are obtained by considering the discretized problem as a parametric mixed-integer nonlinear optimization problem with parameters in the right-hand sides of the equality and inequality constraints. For this class of problems, we could find sufficient conditions for the continuity of the optimal value function by combining stability assumptions for the integer feasible set and second-order sufficient conditions from nonlinear optimization.

The theory can be extended to problems involving partial differential equations. For linear-quadratic problems, one may consider a combination of error estimates for finite-element approximations with Slater-type constraint qualifications. For mixed-integer nonlinear problems with constraints involving a coupling, for example, through boundary values, similar results as those found here may be obtained by combining stability assumptions for the integer feasible set and results on parametric infinite-dimensional optimization problems. This is left for future work.

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