

A DERIVATIVE-FREE ALGORITHM FOR INEQUALITY CONSTRAINED NONLINEAR PROGRAMMING VIA SMOOTHING OF AN ℓ_∞ PENALTY FUNCTION*

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Abstract. In this paper we consider inequality constrained nonlinear optimization problems where the first order derivatives of the objective function and the constraints cannot be used. Our starting point is the possibility to transform the original constrained problem into an unconstrained or linearly constrained minimization of a nonsmooth exact penalty function. This approach shows two main difficulties: the first one is the nonsmoothness of this class of exact penalty functions which may cause derivative-free codes to converge to nonstationary points of the problem; the second one is the fact that the equivalence between stationary points of the constrained problem and those of the exact penalty function can only be stated when the penalty parameter is smaller than a threshold value which is not known a priori. In this paper we propose a derivative-free algorithm which overcomes the preceding difficulties and produces a sequence of points that admits a subsequence converging to a Karush–Kuhn–Tucker point of the constrained problem. In particular the proposed algorithm is based on a smoothing of the nondifferentiable exact penalty function and includes an updating rule which, after at most a finite number of updates, is able to determine a “right value” for the penalty parameter. Furthermore we present the results obtained on a real world problem concerning the estimation of parameters in an insulin-glucose model of the human body.

Key words. derivative-free optimization, constrained optimization, nonlinear programming, nondifferentiable exact penalty functions

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1. Introduction. We consider the following problem:

$$(1) \quad \begin{array}{ll} \min & f(x) \\ \text{s.t.} & g(x) \leq 0, \\ & Ax \leq b, \end{array}$$

where $x \in R^n$, $f : R^n \rightarrow R$, $g : R^n \rightarrow R^m$, $A \in R^{p \times n}$, $b \in R^p$, and we assume that f and g are twice continuously differentiable on R^n . We denote by a_j^\top , $j = 1, \dots, p$, the rows of matrix A and by

$$\mathcal{F} = \{x \in R^n : Ax \leq b, g(x) \leq 0\}$$

the feasible set of problem (1). We assume that the derivatives of the objective and nonlinear constraint functions can be neither calculated nor explicitly approximated. Indeed, in many engineering problems the analytic expressions of the functions defining the objective and constraints of the problem are not available and their values

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are computed by means of complex simulation computer programs. For further motivations on the necessity of using derivative-free methods we refer the reader to the survey paper [14].

In the literature, some globally convergent derivative-free methods for the solution of problem (1) have been proposed. In [20] a pattern search algorithm is used within a sequential augmented Lagrangian approach. Essentially, the method embeds the pattern search algorithm proposed in [18], within the augmented Lagrangian method [6], which is the basis for the subroutine AUGLG in the LANCELOT optimization package. More recently, in [15] a generating set direct search augmented Lagrangian algorithm is proposed which explicitly handles the linear constraints.

In [1] the filter method proposed in [10] is adapted to include a pattern search minimization strategy. Basically, the method employs a “filter” for acceptance of the points produced by the pattern search local optimizer.

In [2] a so-called *extreme barrier* approach is employed. Namely the constrained problem is converted to an unconstrained one by setting the objective function value to infinity for infeasible points. To minimize this extreme barrier function, the authors propose an extension of the generalized pattern search class of algorithms which allows local exploration in an asymptotically dense set of directions. More recently, in [3] Audet and Dennis propose a mesh adaptive direct search algorithm which uses a progressive barrier strategy and allows infeasible starting points.

Similarly to [20, 15, 2] and [3], in this paper we propose an algorithm which is based on the idea of employing a derivative-free method to solve a linearly constrained reformulation of problem (1). Our approach differs from the preceding ones in that we use the fact that one can solve problem (1) by minimizing a nonsmooth exact penalty function over a set defined by the linear constraints of problem (1). However, nonsmooth exact penalty functions cannot be straightforwardly combined to a globally convergent derivative-free algorithm. Indeed, the following theoretical and computational aspects should be carefully taken into account.

- Ill-conditioning of merit functions. This aspect makes the minimization of such functions a difficult task, especially for derivative-free codes which use only evaluations of the objective function.
- Nondifferentiability of the penalty function. The lack of differentiability may have negative effects on the convergence of derivative-free methods to stationary points of the penalty function. Indeed, most of the unconstrained derivative-free methods require the objective function to be at least continuously differentiable.
- Equivalence between stationary points of the penalty function and KKT pairs of problem (1). An exact penalty function enjoys its exactness properties only if the penalty parameter is below a certain threshold value which is not known a priori. This aspect is crucial also in the case where derivatives are available.

As regards the first point, we introduce a new exact penalty function which penalizes only the nonlinear constraints and does this penalization in such a way to reduce as much as possible the ill-conditioning.

The nondifferentiability of the new penalty function is tackled by employing the smoothing technique proposed in [4, 31]. In particular, in order to find a stationary point of the penalty function by minimizing the smooth approximation, we adapted the method proposed in [21] to solve linearly constrained finite minimax problems.

As for the last point, the properties of the smooth approximation allow us to define a suitable updating rule for the penalty parameter ϵ . This rule, after a finite

number of reductions, is able to find a right value for ϵ so as to convey the desirable exactness properties to the penalty function.

To conclude, we propose a globally convergent algorithm which is based on the derivative-free minimization of a smooth approximation of a nondifferentiable exact penalty function which does an ℓ_∞ penalization of the constraints. Moreover, this new algorithm exploits the structure of the problem by allowing an explicit handling of the linear constraints.

In regards to a possible practical interest of the proposed approach, we recall the encouraging results described in [12]. In fact, [12] reports an extensive numerical testing and comparison which point out significant computational advantages in using a smooth approximation of an exact ℓ_∞ penalty function in the field of derivative-free methods.

Even though the main aim of this paper is the definition of a new algorithm and the study of its theoretical properties, we also show that a rough implementation of the method is able to solve successfully a real world problem concerning the estimation of parameters in an insulin-glucose model of the human body. This result seems to confirm further the conclusion of [12].

This paper is organized as follows. In section 2, the exact penalty function approach is introduced and discussed. Section 3 is devoted to the description of a smooth approximation technique along with some preliminary properties. In section 4, the derivative-free method is presented and its global convergence is studied. Section 5 is devoted to the solution of the constrained parameter estimation problem. Finally, in section 6, we draw some conclusions.

We end this section by introducing some notations which will be used in the rest of this paper. Given a set \mathcal{S} , we denote by $\overset{\circ}{\mathcal{S}}$ and $\bar{\mathcal{S}}$, respectively, the interior and the closure of \mathcal{S} . By $\|\cdot\|$ we indicate the Euclidean norm. The following index sets will be used in this paper:

$$\begin{aligned} I_0(x) &:= \{i : g_i(x) = 0\}, & I_\pi(x) &:= \{i : g_i(x) \geq 0\}, & I_\nu(x) &:= \{i : g_i(x) < 0\}, \\ J(x) &:= \{j : a_j^\top x = b_j\}. \end{aligned}$$

2. An exact penalty function approach. As already said in the introduction, the first step of our approach is that of defining and using a penalty function which will be more tractable from a computational point of view. Namely, a penalty function which

- (i) has a structure that presents fewer nonlinearities than previous exact penalty functions [9];
- (ii) allows direct handling of linear and bound constraints thus penalizing only the nonlinear ones.

As regards point (i), nondifferentiable globally exact penalty functions were introduced in [9] for nonlinear programming problems of the form

$$(2) \quad \begin{aligned} \min & \quad f(x) \\ \text{s.t.} & \quad g(x) \leq 0. \end{aligned}$$

In order to prove the relevant exactness properties, it is necessary to introduce a compact relaxation of the feasible set \mathcal{F} .

Thus, following [9], given a vector $\alpha \in R^m$ such that $\alpha_i > 0$, $i = 1, \dots, m$, the set

$$\mathcal{D}_\alpha = \{x \in R^n : g(x) \leq \alpha\}$$

is considered. Then, on the interior of set \mathcal{D}_α , the penalty function

$$Q(x; \epsilon) = f(x) + \frac{1}{\epsilon} \max \left\{ 0, \frac{g_1(x)}{\alpha_1 - g_1(x)}, \dots, \frac{g_m(x)}{\alpha_m - g_m(x)} \right\}$$

can be defined, where the terms $\alpha_i - g_i(x)$ make $Q(x; \epsilon)$ go to infinity when x approaches the boundary of \mathcal{D}_α , thus guaranteeing the compactness of its level sets.

In [9], it is shown that $Q(x; \epsilon)$ is a globally exact penalty function for problem (2); that is, a value $\epsilon^* > 0$ for the penalty parameter exists such that for every $\epsilon \in (0, \epsilon^*]$ the solution of problem (2) is equivalent to the solution of

$$(3) \quad \min Q(x; \epsilon) \quad \text{s.t.} \quad x \in \overset{\circ}{\mathcal{D}}_\alpha,$$

which, essentially, amounts to an unconstrained minimization of $Q(x; \epsilon)$, due to the fact that $\overset{\circ}{\mathcal{D}}_\alpha$ is an open set. More precisely, a value $\epsilon^* > 0$ for the penalty parameter exists such that for every $\epsilon \in (0, \epsilon^*]$, every local (global, stationary) point of problem (3) is a local (global Karush–Kuhn–Tucker (KKT)) point of problem (2) and conversely.

However, we note that the structure of $Q(x; \epsilon)$ is such that two contrasting effects, tied with the choice of parameters α and ϵ , may arise. Indeed, rewriting

$$Q(x; \epsilon) = f(x) + \max \left\{ 0, \frac{g_1(x)}{\epsilon(\alpha_1 - g_1(x))}, \dots, \frac{g_m(x)}{\epsilon(\alpha_m - g_m(x))} \right\},$$

two conflicting requirements become apparent. On the one hand, in order to limit the ill-conditioning of the penalty function near the boundary of the compact set \mathcal{D}_α , sufficiently large α_i 's should be chosen. On the other hand, the exactness properties follow only when the constraints are sufficiently penalized, that is, when the terms $\epsilon(\alpha_i - g_i(x))$ are sufficiently small on all \mathcal{D}_α . Hence, choosing large α_i 's requires very small values of ϵ thus increasing the ill-conditioning of the penalty function whenever at least one term $(\alpha_i - g_i(x))$ exists which is not excessively large. Besides, reasonable values for ϵ preclude the possibility of choosing large values for the α_i 's, that is, the possibility of choosing sets \mathcal{D}_α having the boundary sufficiently away from the feasible region.

In order to overcome the preceding difficulties, we introduce the following new penalty function:

$$Z(x; \epsilon) = f(x) + \max \left\{ 0, \left(\frac{1}{\epsilon} + \frac{1}{\alpha_1 - g_1(x)} \right) g_1(x), \dots, \left(\frac{1}{\epsilon} + \frac{1}{\alpha_m - g_m(x)} \right) g_m(x) \right\},$$

where the terms $g_i(x)/\epsilon$ (needed to achieve the exactness properties) and $g_i(x)/(\alpha_i - g_i(x))$ (required to guarantee the compactness of the level sets) are split in such a way that they no longer interfere one another. Introducing the functions

$$\hat{g}_i(x; \epsilon) = \left(1 + \frac{\epsilon}{\alpha_i - g_i(x)} \right) g_i(x), \quad i = 1, \dots, m,$$

$\hat{g}_0(x; \epsilon) = 0$, $Z(x; \epsilon)$ can be rewritten in the compact form

$$Z(x; \epsilon) = f(x) + \frac{1}{\epsilon} \max_{i=0,1,\dots,m} \{ \hat{g}_i(x; \epsilon) \}.$$

As regards point (ii), the need for an “ad-hoc” handling of the constraints arises every time they can be partitioned into two subsets of “difficult” and “easy” constraints. A more traditional approach to problem (1) would be that of penalizing all

the constraints by adding to the objective function a penalty term for every constraint. However, every penalty term increases the nonlinearities and the ill-conditioning of the penalty function. This, in turn, would surely result in a difficult problem to solve especially for a derivative-free method. On the other hand, many efficient derivative-free methods exist which are able to solve linearly and bound constrained optimization problems by explicitly handling the linear and bound constraints [19, 22, 30]. For this reason, instead of problem (2), we consider problem (1) and penalize only the nonlinear constraints.

To this aim, we shall prove that a threshold value $\epsilon^* > 0$ exists such that, for all $\epsilon \in (0, \epsilon^*]$, problem (1) is equivalent to

$$(4) \quad \begin{aligned} \min \quad & Z(x; \epsilon) \\ \text{s.t.} \quad & Ax \leq b, \\ & x \in \overset{\circ}{\mathcal{D}}_\alpha. \end{aligned}$$

Note that the new structure of the penalty function along with the presence of the linear constraints and, hence, the fact that $Z(x; \epsilon)$ is to be minimized on the set $\{x \in R^n : Ax \leq b, x \in \overset{\circ}{\mathcal{D}}_\alpha\}$, makes the analysis of [7, 9] not readily applicable. Therefore, in the following subsections, we analyze the theoretical properties and connections between problems (4) and (1), by adapting the analysis carried out in [7, 9].

In what follows we denote

$$\mathcal{S}_\alpha = \overset{\circ}{\mathcal{D}}_\alpha \cap \{x \in R^n : Ax \leq b\}.$$

2.1. Definitions and assumptions. In order to state the equivalence between problems (1) and (4), we introduce the following assumptions which we require to hold true throughout this paper. They are standard assumptions in a constrained context.

Assumption 1. The set $\bar{\mathcal{S}}_\alpha$ is compact.

Assumption 2. At any point $x \in \bar{\mathcal{S}}_\alpha$, a vector $d \in T(x)$ exists such that

$$\nabla g_i(x)^\top d < 0 \quad \forall i \text{ s.t. } g_i(x) \geq 0,$$

where

$$(5) \quad T(x) = \{d \in R^n : a_j^\top d \leq 0 \forall j \in J(x)\}$$

is the *cone of feasible directions* with respect to the linear inequality constraints.

The first assumption is needed to guarantee that the penalty function has compact level sets while the second one guarantees that the feasible region of problem (1) is not empty with a nonempty interior.

As concerns problem (1), the presence of the linear inequality constraints allows us to define necessary optimality conditions under somewhat weaker assumptions than usual. In particular, under Assumption 2 it is possible to state the following (KKT) necessary conditions for local optimality of problem (1).

PROPOSITION 1. *Let $\bar{x} \in \mathcal{F}$ be a local solution of problem (1). Then,*

$$(6) \quad \begin{aligned} \nabla f(\bar{x}) + \nabla g(\bar{x})\bar{\lambda} + A^\top \bar{\mu} &= 0, \\ \bar{\lambda}^\top g(\bar{x}) &= 0, \quad \bar{\lambda} \geq 0, \\ \bar{\mu}^\top (Ax - b) &= 0, \quad \bar{\mu} \geq 0, \end{aligned}$$

for some vectors $\bar{\lambda} \in R^m$ and $\bar{\mu} \in R^p$.

Proof. The proof follows by considering Propositions 3.3.11 and 3.3.12 in [5] along with the Motzkin theorem of the alternative [23]. \square

As regards problem (4), we recall that the directional derivative $DZ(x, d; \epsilon)$ of $Z(x; \epsilon)$ at $x \in \mathcal{S}_\alpha$ along direction $d \in R^n$ exists and is given by (see, for instance, [4])

$$DZ(x, d; \epsilon) = \nabla f(x)^\top d + \frac{1}{\epsilon} \max_{i \in B(x; \epsilon)} \{ \nabla \hat{g}_i(x; \epsilon)^\top d \},$$

where

$$B(x; \epsilon) = \left\{ i \in \{0, 1, \dots, m\} : \hat{g}_i(x; \epsilon) = \max_{j=0, 1, \dots, m} \{ \hat{g}_j(x; \epsilon) \} \right\}$$

and

$$\nabla \hat{g}_i(x; \epsilon) = \left(1 + \frac{\epsilon \alpha_i}{(\alpha_i - g_i(x))^2} \right) \nabla g_i(x), \quad i = 1, \dots, m.$$

Therefore, the usual definition of stationarity for problem (4) can be given as follows.

DEFINITION 1. *A point $\bar{x} \in \mathcal{S}_\alpha$ is a stationary point of problem (4) if*

$$DZ(\bar{x}, d; \epsilon) \geq 0 \quad \forall d \in T(\bar{x}).$$

By exploiting the particular structure of problem (4), that is, the expression of the penalty function $Z(x; \epsilon)$, it is possible to state a different characterization of its stationary points.

PROPOSITION 2. *For any given $\epsilon > 0$, a point $\bar{x} \in \mathcal{S}_\alpha$ is a stationary point of problem (4) if and only if for each $i \in B(\bar{x}; \epsilon)$ there exists λ_i satisfying*

$$(7) \quad \lambda_i \geq 0, \quad \sum_{i \in B(\bar{x}; \epsilon)} \lambda_i = 1,$$

$$(8) \quad \left(\nabla f(\bar{x}) + \frac{1}{\epsilon} \sum_{i \in B(\bar{x}; \epsilon)} \lambda_i \nabla \hat{g}_i(\bar{x}; \epsilon) \right)^\top d \geq 0 \quad \forall d \in T(\bar{x}).$$

Proof. First let us assume that $\bar{x} \in \mathcal{S}_\alpha$ is a stationary point of problem (4). Then (7) and (8) follows by considering Propositions 3.3.10 and 3.3.11 of [5].

On the contrary, let $\bar{x} \in \mathcal{S}_\alpha$ be a point which satisfies conditions (7) and (8); then we can write

$$\begin{aligned} 0 &\leq \left(\nabla f(\bar{x}) + \frac{1}{\epsilon} \sum_{i \in B(\bar{x}; \epsilon)} \lambda_i \nabla \hat{g}_i(\bar{x}; \epsilon) \right)^\top d \\ &\leq \left(\nabla f(\bar{x})^\top d + \frac{1}{\epsilon} \max_{i \in B(\bar{x}; \epsilon)} \{ \nabla \hat{g}_i(\bar{x}; \epsilon)^\top d \} \sum_{i \in B(\bar{x}; \epsilon)} \lambda_i \right) \\ &= \left(\nabla f(\bar{x})^\top d + \frac{1}{\epsilon} \max_{i \in B(\bar{x}; \epsilon)} \{ \nabla \hat{g}_i(\bar{x}; \epsilon)^\top d \} \right) \end{aligned}$$

for all $d \in T(\bar{x})$, which shows that \bar{x} is a stationary point of problem (4). \square

2.2. Exactness properties. The exactness properties of the penalty function $Z(x; \epsilon)$ heavily hinge on the following lemma, which is a slight modification of Theorem 2.2 of [13].

LEMMA 1. *Let $\hat{x} \in \{x \in R^n : Ax \leq b\}$. Then, an open neighborhood $\mathcal{B}(\hat{x}; \rho)$ of \hat{x} and a direction $d \in T(\hat{x})$ exist such that, for all $i \in I_\pi(\hat{x})$, we have*

$$(9) \quad \nabla g_i(x)^\top d \leq -1 \quad \forall x \in \mathcal{B}(\hat{x}; \rho) \cap \{x \in R^n : Ax \leq b\},$$

$$(10) \quad \nabla \hat{g}_i(x; \epsilon)^\top d \leq -1 \quad \forall x \in \mathcal{B}(\hat{x}; \rho) \cap \mathcal{S}_\alpha, \forall \epsilon > 0.$$

Proof. By Assumption 2, a vector $\hat{z} \in T(\hat{x})$ exists such that $\nabla g_i(\hat{x})^\top \hat{z} < 0$ for all $i \in I_\pi(\hat{x})$. Hence, by continuity, a $\rho > 0$ exists such that

$$\nabla g_i(x)^\top \hat{z} \leq -\gamma/2$$

for all $x \in \mathcal{B}(\hat{x}; \rho) \cap \{x \in R^n : Ax \leq b\}$ and $i \in I_\pi(\hat{x})$, where

$$-\gamma = \max_{i \in I_\pi(\hat{x})} \{\nabla g_i(\hat{x})^\top \hat{z}\} < 0.$$

Thus (9) follows by choosing $d = 2\hat{z}/\gamma$.

For $x \in \mathcal{B}(\hat{x}; \rho) \cap \mathcal{S}_\alpha$ we can write

$$\nabla g_i(x)^\top d = \frac{(\alpha_i - g_i(x))^2}{(\alpha_i - g_i(x))^2 + \epsilon \alpha_i} \nabla \hat{g}_i(x; \epsilon)^\top d \leq -1 \quad \forall i \in I_\pi(\hat{x}),$$

so that, considering

$$\frac{(\alpha_i - g_i(x))^2 + \epsilon \alpha_i}{(\alpha_i - g_i(x))^2} > 1 \quad \forall i \in I_\pi(\hat{x}), \forall \epsilon > 0$$

we have

$$(11) \quad \nabla \hat{g}_i(x; \epsilon)^\top d \leq -1 \quad \forall i \in I_\pi(\hat{x}), \forall \epsilon > 0$$

which proves (10). \square

The analysis of the exactness properties of $Z(x; \epsilon)$ follows the same reasonings used in [7] and [9]. For the sake of clarity, here we report only the statement of the main results and refer the interested reader to the appendix for a thorough development and analysis of the exactness properties.

The following propositions establish a connection between stationary points of the exact penalty function $Z(x; \epsilon)$ which are feasible and KKT pairs of problem (1).

PROPOSITION 3. *Let $\bar{x} \in \mathcal{F}$. Then, for any $\epsilon > 0$, if \bar{x} is a critical point of $Z(x; \epsilon)$, there exist multipliers $\bar{\lambda} \in R^m$ and $\bar{\mu} \in R^p$ such that $(\bar{x}, \bar{\lambda}, \bar{\mu})$ is a KKT triple for problem (1).*

For sufficiently small values of the penalty parameter ϵ , a one-to-one correspondence between KKT pairs of problem (1) and critical points of the penalty function $Z(x; \epsilon)$ exist.

PROPOSITION 4. *There exists an $\epsilon^* > 0$ such that, for all $\epsilon \in (0, \epsilon^*]$, if $\bar{x} \in \mathcal{S}_\alpha$ is a critical point of $Z(x; \epsilon)$, there exist multipliers $\bar{\lambda} \in R^m$ and $\bar{\mu} \in R^p$ such that $(\bar{x}, \bar{\lambda}, \bar{\mu})$ is a KKT triple for problem (1) and conversely.*

Finally, the last proposition describes a connection between local and global minimum points of the penalty function and problem (1).

PROPOSITION 5. *There exists an $\epsilon^* > 0$ such that, for all $\epsilon \in (0, \epsilon^*]$,*

- (a) if $x_\epsilon \in \mathcal{S}_\alpha$ is a (strict) local unconstrained minimum point of $Z(x; \epsilon)$, then x_ϵ is a (strict) local constrained minimum point of problem (1);
- (b) if $x^* \in \mathcal{S}_\alpha$ is a global unconstrained minimum point of $Z(x; \epsilon)$ on \mathcal{S}_α , then x^* is a global solution to problem (1) and conversely.

3. Smooth approximation and preliminary results. In this section we concentrate on the derivative-free approach to the solution of problem (1). As already argued, in order to solve this problem we resort to a reformulation of problem (1) by means of the exact penalty function $Z(x; \epsilon)$, so that, on the basis of the exactness properties studied in the preceding section, we can concentrate on the solution of the linearly constrained problem (4).

To tackle the nondifferentiability of function $Z(x; \epsilon)$, we adopt a smoothing technique [4, 31] which consists of solving a sequence of smooth problems approximating the nonsmooth one in the limit. Let $\mu > 0$ be a smoothing parameter, and define

$$Z(x; \mu, \epsilon) = f(x) + \mu \ln \left(\sum_{i=0}^m \exp \left(\frac{\hat{g}_i(x; \epsilon)}{\mu \epsilon} \right) \right) = f(x) + \mu \ln \left(1 + \sum_{i=1}^m \exp \left(\frac{\hat{g}_i(x; \epsilon)}{\mu \epsilon} \right) \right).$$

We report some properties of $Z(x; \mu, \epsilon)$ [31] that exploit the fact that $\nabla \hat{g}_0(x; \epsilon) = 0$.

PROPOSITION 6.

- (i) For any given $x \in R^n$ and $\epsilon > 0$, $Z(x; \mu, \epsilon)$ is increasing with respect to μ and

$$(12) \quad Z(x; \epsilon) \leq Z(x; \mu, \epsilon) \leq Z(x; \epsilon) + \mu \ln m.$$

- (ii) $Z(x; \mu, \epsilon)$ is twice continuously differentiable for all $\mu > 0$, $\epsilon > 0$, and

$$(13) \quad \begin{aligned} \nabla_x Z(x; \mu, \epsilon) &= \nabla f(x) + \frac{1}{\epsilon} \sum_{i=0}^m \lambda_i(x; \mu, \epsilon) \nabla \hat{g}_i(x; \epsilon) \\ &= \nabla f(x) + \frac{1}{\epsilon} \sum_{i=1}^m \lambda_i(x; \mu, \epsilon) \nabla \hat{g}_i(x; \epsilon), \end{aligned}$$

$$(14) \quad \begin{aligned} \nabla_x^2 Z(x; \mu, \epsilon) &= \nabla^2 f(x) + \frac{1}{\epsilon} \sum_{i=1}^m (\lambda_i(x; \mu, \epsilon) \nabla^2 \hat{g}_i(x; \epsilon)) \\ &\quad + \frac{1}{\mu \epsilon^2} \sum_{i=1}^m (\lambda_i(x; \mu, \epsilon) \nabla \hat{g}_i(x; \epsilon) \nabla \hat{g}_i(x; \epsilon)^\top) \\ &\quad - \frac{1}{\mu \epsilon^2} \left(\sum_{i=1}^m \lambda_i(x; \mu, \epsilon) \nabla \hat{g}_i(x; \epsilon) \right) \left(\sum_{i=1}^m \lambda_i(x; \mu, \epsilon) \nabla \hat{g}_i(x; \epsilon) \right)^\top, \end{aligned}$$

where

$$(15) \quad \lambda_i(x; \mu, \epsilon) = \frac{\exp \left(\frac{\hat{g}_i(x; \epsilon)}{\mu \epsilon} \right)}{1 + \sum_{j=1}^m \exp \left(\frac{\hat{g}_j(x; \epsilon)}{\mu \epsilon} \right)} \in (0, 1), \quad i = 0, 1, \dots, m,$$

and $\sum_{i=0}^m \lambda_i(x; \mu, \epsilon) = 1$.

Thus, having introduced the smoothing function $Z(x; \mu, \epsilon)$, we consider the following smooth approximating problem:

$$(16) \quad \min_{x \in \mathcal{S}_\alpha} Z(x; \mu, \epsilon),$$

where the approximating parameter μ and the penalty parameter ϵ will be adaptively reduced during the optimization process.

Considering problem (16), it is important to study the connections that $Z(x; \mu, \epsilon)$ has with the original constrained problem. In particular, $Z(x; \mu, \epsilon)$ should be able, when minimized, to drive the algorithm away from infeasible points with respect to the nonlinear inequality constraints. Indeed, the following proposition states an important result needed to prove convergence of the algorithm. Namely, on every $\hat{x} \in \mathcal{S}_\alpha$ a sufficiently small neighborhood of \hat{x} exists such that in every infeasible point belonging to this neighborhood a direction $d \in T(\hat{x})$ exists such that the directional derivative of the smooth approximating function along direction d is negative and uniformly bounded away from zero, for ϵ sufficiently small.

PROPOSITION 7. *Let $\hat{x} \in \mathcal{S}_\alpha$ and $\mu_{MAX} > 0$ be any given scalar. Then, $\epsilon(\hat{x}) > 0$ and $\sigma(\hat{x}) > 0$ exist such that for all $x \in \mathcal{B}(\hat{x}; \sigma(\hat{x})) \cap \mathcal{S}_\alpha$ and satisfying $g(x) \not\leq 0$, and for all $\epsilon \in (0, \epsilon(\hat{x})]$ a direction $d \in T(\hat{x})$ exists such that*

$$\nabla Z(x; \mu, \epsilon)^\top d \leq -\frac{1}{2\epsilon(m+1)}$$

for all $\mu \in (0, \mu_{MAX}]$.

Proof. Let $\mathcal{B}(\hat{x}; \rho)$ and d be the neighborhood and the direction considered in Lemma 1. By continuity, we can find a neighborhood $\mathcal{B}(\hat{x}; \sigma(\hat{x})) \subseteq \mathcal{B}(\hat{x}; \rho)$ such that for $i \notin I_\pi(\hat{x})$ and $x \in \mathcal{B}(\hat{x}; \sigma(\hat{x}))$, we have $g_i(x) < 0$; it follows that $I_\pi(x) \subseteq I_\pi(\hat{x})$ and $I_\nu(\hat{x}) \subseteq I_\nu(x)$ for $x \in \mathcal{B}(\hat{x}; \sigma(\hat{x}))$.

Now let $x \in \mathcal{B}(\hat{x}; \sigma(\hat{x})) \cap \mathcal{S}_\alpha$ be an infeasible point with respect to the nonlinear inequality constraints. Then, there must exist at least an index $i \in I_\pi(x)$ such that $g_i(x) > 0$, which implies $I_\pi(x) \neq \phi$. By recalling expression (13), we can write

$$\begin{aligned} \nabla Z(x; \mu, \epsilon)^\top d &= \nabla f(x)^\top d \\ &+ \frac{1}{\epsilon} \left(\sum_{i \in I_\nu(\hat{x})} \lambda_i(x; \mu, \epsilon) \nabla \hat{g}_i(x; \epsilon)^\top d + \sum_{i \in I_\pi(\hat{x})} \lambda_i(x; \mu, \epsilon) \nabla \hat{g}_i(x; \epsilon)^\top d \right). \end{aligned}$$

By Lemma 1 we have that $\nabla \hat{g}_i(x; \epsilon)^\top d \leq -1$, $i \in I_\pi(\hat{x})$, so that we can write

$$(17) \quad \begin{aligned} \nabla Z(x; \mu, \epsilon)^\top d &\leq \nabla f(x)^\top d \\ &+ \frac{1}{\epsilon} \left(\sum_{i \in I_\nu(\hat{x})} \lambda_i(x; \mu, \epsilon) \nabla \hat{g}_i(x; \epsilon)^\top d - \sum_{i \in I_\pi(\hat{x})} \lambda_i(x; \mu, \epsilon) \right). \end{aligned}$$

Let $\bar{i} \in I_\pi(\hat{x})$ be an index such that $\hat{g}_{\bar{i}}(x; \epsilon) = \max_{i \in I_\pi(\hat{x})} \{\hat{g}_i(x; \epsilon)\}$. It is easily seen that $\sum_{i \in I_\pi(\hat{x})} \lambda_i(x; \mu, \epsilon) \geq \lambda_{\bar{i}}(x; \mu, \epsilon)$, and, since

$$\frac{\exp(\hat{g}_i(x; \epsilon)/\mu\epsilon)}{\exp(\hat{g}_{\bar{i}}(x; \epsilon)/\mu\epsilon)} \leq 1 \quad \forall i \in \{1, \dots, m\},$$

then

$$\lambda_{\bar{i}}(x; \mu, \epsilon) \geq \frac{1}{1 + 1 + \sum_{i=1, i \neq \bar{i}}^m \frac{\exp(\hat{g}_i(x; \epsilon)/\mu\epsilon)}{\exp(\hat{g}_{\bar{i}}(x; \epsilon)/\mu\epsilon)}} \geq \frac{1}{1 + m}.$$

Hence we get

$$(18) \quad \sum_{i \in I_\pi(\hat{x})} \lambda_i(x; \mu, \epsilon) \geq 1/(1 + m).$$

By considering (17) and (18), we get

$$(19) \quad \begin{aligned} \nabla Z(x; \mu, \epsilon)^\top d &\leq \nabla f(x)^\top d \\ &+ \frac{1}{\epsilon} \left(\sum_{i \in I_\nu(\hat{x})} \lambda_i(x; \mu, \epsilon) \nabla \hat{g}_i(x; \epsilon)^\top d - \frac{1}{1 + m} \right). \end{aligned}$$

Now, since $I_\nu(\hat{x}) \subseteq I_\nu(x)$, for $x \in \mathcal{B}(\hat{x}; \sigma(\hat{x}))$, by expression (15), it follows that, for any given $\mu > 0$ and $x \in \mathcal{B}(\hat{x}; \sigma(\hat{x})) \cap \mathcal{S}_\alpha$ not feasible,

$$\lim_{\epsilon \rightarrow 0^+} \lambda_i(x; \mu, \epsilon) = 0, \quad i \in I_\nu(\hat{x}).$$

Hence, by the boundedness of $\nabla \hat{g}_i(x; \epsilon)^\top d$ and $\nabla f(x)^\top d$, an $\epsilon(\hat{x}) > 0$ exists such that for all $\epsilon \in (0, \epsilon(\hat{x})]$ we have

$$(20) \quad \sum_{i \in I_\nu(\hat{x})} \lambda_i(x; \mu, \epsilon) \nabla \hat{g}_i(x; \epsilon)^\top d < \frac{1}{4(m+1)} \quad \forall \mu \in (0, \mu_{MAX}]$$

$$(21) \quad \nabla f(x)^\top d < \frac{1}{4\epsilon(m+1)}.$$

The result follows from (20), (21), and (19). \square

In order to guarantee the global convergence of the algorithm in the case where first derivatives are unavailable, it is necessary to get alternative information by sampling the objective function along a suitable set of search directions. Specifically, we follow the approach proposed in [22], which uses a set of search directions that positively span a “ ν -approximation” of the cone of feasible directions; or in other words, the cone of feasible directions with respect to the ν -active linear constraints.

Formally, for any $\nu > 0$ and $x \in \mathcal{S}_\alpha$, we define the set of indices of ν -active linear constraints by

$$J(x; \nu) = \{j : a_j^\top x \geq b_j - \nu\},$$

and the ν -approximation of the cone of feasible directions by

$$T(x; \nu) = \{d \in R^n : a_j^\top d \leq 0 \forall j \in J(x; \nu)\}.$$

The following proposition (see [22]) describes some properties of sets $J(x; \nu)$ and $T(x; \nu)$.

PROPOSITION 8. *Let $\{x_k\}$ be a sequence of iterates converging towards a point $\bar{x} \in \mathcal{S}_\alpha$. Then, there exists a value $\nu^* > 0$ (depending on \bar{x} only) such that for every $\nu \in (0, \nu^*]$ there exists \bar{k}_ν such that*

$$(22) \quad J(x_k; \nu) = J(\bar{x}),$$

$$(23) \quad T(x_k; \nu) = T(\bar{x})$$

for all $k \geq \bar{k}_\nu$.

Proof. See the proof of Proposition 1 in [22]. \square

The first step toward defining a derivative-free method for the solution of problem (16) is to associate a suitable set of search directions with each point x_k produced by the algorithm. This set should have the property that the local behavior of the objective function in each direction in the set provides sufficient information to overcome the lack of the gradient. Formally, we introduce the following assumption.

Assumption 3. Let $\{x_k\}$ be sequence of points belonging to \mathcal{S}_α , $\{r_k\}$ a sequence of positive scalars, and $\{D_k\}$ a sequence of sets of search directions defined as

$$D_k = \{p_k^i : \|p_k^i\| = 1, \quad i = 1, \dots, r_k\} \quad \forall k.$$

Then, for some constant $\bar{\nu} > 0$,

$$\text{cone}\{D_k \cap T(x_k; \nu)\} = T(x_k; \nu) \quad \forall \nu \in [0, \bar{\nu}].$$

Moreover, $\bigcup_{k=0}^{\infty} D_k$ is a finite set and r_k is bounded.

Assumption 3 is quite a standard assumption in a derivative-free context and is needed to guarantee that the search directions are well defined and able to capture sufficiently well the local geometry of the feasible set. An example on how to compute a set of directions satisfying the above assumption can be found in the paper [19].

The proposition which follows is essential to prove convergence of the proposed algorithm to a KKT point. In particular, it points out the minimal requirements on the sampling of the smoothed penalty function $Z(x; \mu, \epsilon)$ along the directions p_k^i , $i = 1, \dots, r_k$, and on the updating of both the smoothing parameter μ and penalty parameter ϵ which are able to guarantee that feasibility of problem (1) is attained in a finite number of steps.

PROPOSITION 9. *Let $\{\mu_k\}$ be a sequence of smoothing parameters and $\{\epsilon_k\}$ a sequence of penalty parameters. Let $\{x_k\}$ be a sequence of points and \bar{x} be a limit point of a subsequence $\{x_k\}_K$, for some infinite set $K \subseteq \{0, 1, \dots\}$, such that $\bar{x} \in \mathcal{S}_\alpha$. Let $\{D_k\}$, with $D_k = \{p_k^1, \dots, p_k^{r_k}\}$, be a sequence of sets of directions which satisfy Assumption 3 and $J_k = \{i \in \{1, \dots, r_k\} : p_k^i \in T(x_k; \nu)\}$ with $\nu \in (0, \min\{\bar{\nu}, \nu^*\})$, where ν^* and $\bar{\nu}$ are defined in Proposition 8 and Assumption 3, respectively. Suppose that the following conditions hold:*

(i) *for each $k \in K$ and $i \in J_k$, there exist y_k^i and scalars $\xi_k^i > 0$ such that*

$$(24) \quad y_k^i + \xi_k^i p_k^i \in \mathcal{S}_\alpha, \quad Z(y_k^i + \xi_k^i p_k^i; \mu_k, \epsilon_k) \geq Z(y_k^i; \mu_k, \epsilon_k) - o(\xi_k^i);$$

(ii) *and, furthermore, $\{\mu_k\}_K$ is a bounded sequence and*

$$(25) \quad \lim_{k \rightarrow \infty, k \in K} \epsilon_k = 0, \quad \lim_{k \rightarrow \infty, k \in K} \frac{\max_{i \in J_k} \{\xi_k^i, \|x_k - y_k^i\|\}}{\mu_k \epsilon_k} = 0.$$

It results that a $\bar{k} \geq 0$ exists such that, for all $k \in K$ and k satisfying $k \geq \bar{k}$, x_k is feasible for problem (1).

Proof. As a first step, we show that for every bounded sequence $\{d_k\} \subset T(x_k; \nu)$ of directions, an infinite set $\bar{K} \subseteq K$ exists such that

$$\lim_{k \rightarrow \infty, k \in \bar{K}} \epsilon_k \nabla Z(x_k; \mu_k, \epsilon_k)^\top d_k \geq 0.$$

By assumption the limit point \bar{x} belongs to \mathcal{S}_α , thus an open neighborhood $\mathcal{B}(\bar{x})$ of \bar{x} exists which is strictly contained within \mathcal{S}_α . Therefore, by points (i) and (ii), we have that, for $k \in K$ sufficiently large and for all $i \in J_k$, x_k , y_k^i , and $y_k^i + \xi_k^i p_k^i$ belong to $\mathcal{B}(\bar{x})$.

By applying the mean-value theorem to (24), we can write

$$(26) \quad -o(\xi_k^i) \leq Z(y_k^i + \xi_k^i p_k^i; \mu_k, \epsilon_k) - Z(y_k^i; \mu_k, \epsilon_k) = \xi_k^i \nabla Z(u_k^i; \mu_k, \epsilon_k)^\top p_k^i, \quad i \in J_k,$$

where $u_k^i = y_k^i + t_k^i \xi_k^i p_k^i$, with $t_k^i \in (0, 1)$. By using the mean-value theorem again and the Cauchy–Schwarz inequality, we can write

$$\begin{aligned} \xi_k^i \nabla Z(u_k^i; \mu_k, \epsilon_k)^\top p_k^i &= \xi_k^i \nabla Z(x_k; \mu_k, \epsilon_k)^\top p_k^i + \xi_k^i (u_k^i - x_k)^\top \nabla^2 Z(\tilde{u}_k^i; \mu_k, \epsilon_k) p_k^i \\ &\leq \xi_k^i \nabla Z(x_k; \mu_k, \epsilon_k)^\top p_k^i + \xi_k^i \|u_k^i - x_k\| \|\nabla^2 Z(\tilde{u}_k^i; \mu_k, \epsilon_k) p_k^i\|, \end{aligned}$$

where $\tilde{u}_k^i = x_k + \tilde{t}_k^i (u_k^i - x_k)$, with $\tilde{t}_k^i \in (0, 1)$. By considering expression (14) of $\nabla^2 Z(\tilde{u}_k^i; \mu_k, \epsilon_k)$ and the triangle inequality, we get that

$$\begin{aligned} \xi_k^i \nabla Z(u_k^i; \mu_k, \epsilon_k)^\top p_k^i &\leq \xi_k^i \nabla Z(x_k; \mu_k, \epsilon_k)^\top p_k^i \\ &+ \xi_k^i \|u_k^i - x_k\| \left\{ \|\nabla^2 f(\tilde{u}_k^i) p_k^i\| + \frac{1}{\epsilon_k} \left\| \sum_{j=1}^m \lambda_j(\tilde{u}_k^i; \mu_k, \epsilon_k) \nabla^2 \hat{g}_j(\tilde{u}_k^i; \epsilon_k) p_k^i \right\| \right. \\ &+ \frac{1}{\mu_k \epsilon_k^2} \left\| \sum_{j=1}^m \lambda_j(\tilde{u}_k^i; \mu_k, \epsilon_k) \nabla \hat{g}_j(\tilde{u}_k^i; \epsilon_k) \nabla \hat{g}_j(\tilde{u}_k^i; \epsilon_k)^\top p_k^i - \left(\sum_{j=1}^m \lambda_j(\tilde{u}_k^i; \mu_k, \epsilon_k) \nabla \hat{g}_j(\tilde{u}_k^i; \epsilon_k) \right) \right. \\ &\cdot \left. \left. \left(\sum_{j=1}^m \lambda_j(\tilde{u}_k^i; \mu_k, \epsilon_k) \nabla \hat{g}_j(\tilde{u}_k^i; \epsilon_k) \right)^\top p_k^i \right\| \right\}. \end{aligned}$$

Since $\{x_k\}_K$ converges, it follows from Assumption 3 and (15) that, for all i and j , $\{x_k\}_K$, $\{\tilde{u}_k^i\}$, $\{\lambda_j(\tilde{u}_k^i; \mu_k, \epsilon_k)\}$, $\{p_k^i\}$ are bounded sequences. Therefore, by the continuity assumption on $f(x)$ and $g(x)$, we can find positive constants c_1 , c_2 , and c_3 such that

$$(27) \quad \xi_k^i \nabla Z(u_k^i; \mu_k, \epsilon_k)^\top p_k^i \leq \xi_k^i \nabla Z(x_k; \mu_k, \epsilon_k)^\top p_k^i + \xi_k^i \left(c_1 + \frac{1}{\epsilon_k} c_2 + \frac{1}{\mu_k \epsilon_k^2} c_3 \right) \|u_k^i - x_k\|.$$

By (24), (26), and (27), we obtain

$$\nabla Z(x_k; \mu_k, \epsilon_k)^\top p_k^i + \left(c_1 + \frac{1}{\epsilon_k} c_2 + \frac{1}{\mu_k \epsilon_k^2} c_3 \right) \|u_k^i - x_k\| \geq -\frac{o(\xi_k^i)}{\xi_k^i}$$

from which, taking into account (13), we can write

$$(28) \quad \left(\nabla f(x_k) + \frac{1}{\epsilon_k} \sum_{j=1}^m \lambda_j(x_k; \mu_k, \epsilon_k) \nabla \hat{g}_j(x_k; \epsilon_k) \right)^\top p_k^i + \left(c_1 + \frac{c_2}{\epsilon_k} + \frac{c_3}{\mu_k \epsilon_k^2} \right) \|u_k^i - x_k\| \geq -\frac{o(\xi_k^i)}{\xi_k^i}.$$

Since $u_k^i = y_k^i + t_k^i \xi_k^i p_k^i$, with $t_k^i \in (0, 1)$, and, by Assumption 3, p_k^i , $i \in J_k$, are bounded, we have that

$$\left(c_1 + \frac{1}{\epsilon_k} c_2 + \frac{1}{\mu_k \epsilon_k^2} c_3 \right) \|u_k^i - x_k\| \leq \left(c_1 + \frac{1}{\epsilon_k} c_2 + \frac{1}{\mu_k \epsilon_k^2} c_3 \right) (\|y_k^i - x_k\| + \xi_k^i) \quad \forall i \in J_k,$$

and from (28) we obtain

$$(29) \quad \left(\nabla f(x_k) + \frac{1}{\epsilon_k} \sum_{j=1}^m \lambda_j(x_k; \mu_k, \epsilon_k) \nabla \hat{g}_j(x_k; \epsilon_k) \right)^\top p_k^i + \left(c_1 + \frac{c_2}{\epsilon_k} + \frac{c_3}{\mu_k \epsilon_k^2} \right) (\|y_k^i - x_k\| + \xi_k^i) \geq -\frac{o(\xi_k^i)}{\xi_k^i}.$$

Now, let $\{d_k\}$ be the generic and bounded sequence of directions such that $\{d_k\} \subset T(x_k; \nu)$. By Assumption 3 and by Corollary 10.2 of [19], we know that, for every index $k \in \bar{K}$, $\beta_k^i \geq 0$, $i \in J_k$, and $\bar{c} > 0$ exist such that

$$(30) \quad d_k = \sum_{i \in J_k} \beta_k^i p_k^i \quad \text{and} \quad |\beta_k^i| \leq \bar{c} \|d_k\|.$$

By multiplying (29) by $\epsilon_k \beta_k^i$, $i \in J_k$, and summing up, we get, for every index $k \in \bar{K}$,

$$(31) \quad \left(\epsilon_k \nabla f(x_k) + \sum_{j=1}^m \lambda_j(x_k; \mu_k, \epsilon_k) \nabla \hat{g}_j(x_k; \epsilon_k) \right)^\top \sum_{i \in J_k} \beta_k^i p_k^i \geq - \sum_{i \in J_k} \epsilon_k \left(\left(c_1 + \frac{1}{\epsilon_k} c_2 + \frac{1}{\mu_k \epsilon_k^2} c_3 \right) (\|y_k^i - x_k\| + \xi_k^i) + \frac{o(\xi_k^i)}{\xi_k^i} \right) \beta_k^i.$$

Recalling the boundedness of sequences $\{x_k\}$, $\{\lambda_j(x_k; \mu_k, \epsilon_k)\}$, $j = 1, \dots, m$, an infinite set $\bar{K} \subseteq K$ exists such that

$$(32) \quad \lim_{\substack{k \rightarrow \infty \\ k \in \bar{K}}} x_k = \bar{x},$$

$$(33) \quad \lim_{\substack{k \rightarrow \infty \\ k \in \bar{K}}} \lambda_j(x_k; \mu_k, \epsilon_k) = \bar{\lambda}_j, \quad j = 1, \dots, m.$$

By Proposition 8, for all $k \in \bar{K}$ sufficiently large, we have that $T(x_k; \nu) = T(\bar{x})$, so that, considering the boundedness of sequence $\{d_k\}$, a direction $\bar{d} \in T(\bar{x})$ exists such that

$$(34) \quad \lim_{\substack{k \rightarrow \infty \\ k \in \bar{K}}} d_k = \bar{d}.$$

Furthermore, given the fact that r_k is bounded, a finite set $J \subseteq \{1, 2, \dots\}$ exists such that, for $k \in \bar{K}$ and sufficiently large, $J_k = J$.

Now, taking the limit for $k \rightarrow \infty$, $k \in \bar{K}$ in (31), and recalling assumption (ii), the boundedness of β_k^i , and the expression of $\nabla \hat{g}_j(x; \epsilon)$, we obtain

$$(35) \quad \lim_{k \rightarrow \infty, k \in \bar{K}} \epsilon_k \nabla Z(x_k; \mu_k, \epsilon_k)^\top d_k = \left(\sum_{j=1}^m \bar{\lambda}_j \nabla g_j(\bar{x}) \right)^\top \bar{d} \geq 0.$$

Let us now suppose by contradiction that an infinite set $\hat{K} \subseteq K$ exists such that $\lim_{k \rightarrow \infty, k \in \hat{K}} x_k = \bar{x}$ and $g(x_k) \not\leq 0$ for all $k \in \hat{K}$. By virtue of Proposition 7, given the fact that (25) holds and recalling that, by assumption, $\nu \in (0, \min\{\bar{\nu}, \nu^*\}]$ so that, by Proposition 8, $T(x_k; \nu) = T(\bar{x})$, we have that a $\hat{k} \in \hat{K}$ and a direction $\hat{d} \in T(\bar{x})$ exist such that

$$\epsilon_k \nabla Z(x_k; \mu_k, \epsilon_k)^\top \hat{d} \leq -\frac{1}{2(m+1)}.$$

By setting $d_k = \hat{d}$, for all $k \in \hat{K}$, the above relation constitutes a contradiction with (35) thus completing the proof. \square

4. A derivative-free method and global convergence result. In this section we define an algorithm for the solution of problem (1). The main tools are the nondifferentiable exact penalty function $Z(x; \epsilon)$ defined in section 2 along with its exactness properties and the smooth approximating function introduced in section 3. Hence, it would be plausible to employ the algorithm proposed in [21]. Roughly speaking, the latter algorithm inexactly solves a sequence of problems (16) when the smoothing parameter μ is driven to zero at a suitable rate. The convergence analysis carried out in [21] guarantees that a subsequence exists which converges towards a stationary point of problem (4). However, it should be noted that the mentioned result is unsatisfactory in that a proper value for the penalty parameter ϵ is not known a priori (namely, ϵ should be smaller than the threshold ϵ^* introduced in Propositions 4 and 5). This implies that a stationary point of problem (4) might have no connections with a solution of problem (1).

In this section, by exploiting Proposition 9, we define a derivative-free algorithm for problem (1) which hinges on a suitable automatic updating rule of the penalty parameter that in a finite number of steps is able to find a value below the mentioned threshold ϵ^* .

The method that we propose uses as a building block the algorithm proposed in [21]. For the sake of clarity, we report a single iteration of the method therein proposed and refer to it as iteration map \mathcal{M} .

Iteration map $\mathcal{M}(x, \mu, \tilde{\alpha}^0, \epsilon, q_1) \mapsto (\tilde{x}, \tilde{\mu}, \tilde{\alpha}^0, \tilde{\alpha}^{max})$

Data. $\gamma > 0, \theta \in (0, 1)$.

Step 1. (Computation of search directions)
Choose a set of directions $D = \{p^1, \dots, p^r\}$ satisfying Assumption 3.

Step 2. (Minimization on the cone $\{D\}$)

Step 2.1. (Initialization)
Set $i = 1, y^i = x, \tilde{\alpha}^i = \tilde{\alpha}^0$.

Step 2.2. (Computation of the initial stepsize)
Compute the maximum steplength $\tilde{\alpha}^i$ such that $A(y^i + \tilde{\alpha}^i p^i) \leq b$ and set $\hat{\alpha}^i = \min\{\tilde{\alpha}^i, \tilde{\alpha}^i\}$.

Step 2.3. (Test on the search direction)
If $(\hat{\alpha}^i > 0$ and $Z(y^i + \hat{\alpha}^i p^i; \mu, \epsilon) < Z(y^i; \mu, \epsilon) - \gamma(\hat{\alpha}^i)^2$ and $y^i + \hat{\alpha}^i p^i \in \mathcal{S}_\alpha$), then
compute $\alpha^i = \text{expansion step}(\tilde{\alpha}^i, \hat{\alpha}^i, y^i, p^i)$
and set $\tilde{\alpha}^{i+1} = \alpha^i$;
otherwise set $\alpha^i = 0$ and $\tilde{\alpha}^{i+1} = \theta \tilde{\alpha}^i$.

Step 2.4. (New point)
Set $y^{i+1} = y^i + \alpha^i p^i$.

Step 2.5. (Test on the minimization on the cone $\{D\}$)
If $i = r$, go to Step 3;
otherwise set $i = i + 1$ and go to Step 2.2.

Step 3. (Iterate outputs)
Set $\tilde{x} = y^{i+1}$.
Set $\tilde{\alpha}^0 = \tilde{\alpha}^{i+1}$ and $\tilde{\alpha}^{max} = \max_{i=1, \dots, r+1} \{\tilde{\alpha}^i\}$; choose $\tilde{\mu} = \min\{\mu, (\tilde{\alpha}^{max})^{q_1}\}$.
return $(\tilde{x}, \tilde{\mu}, \tilde{\alpha}^0, \tilde{\alpha}^{max})$.

Therefore the expansion step in Step 2.3 is defined as follows:

Expansion step $(\tilde{\alpha}^i, \hat{\alpha}^i, y^i, p^i) \mapsto \alpha$

Data. $\gamma > 0, \delta \in (0, 1)$.

Step 1. Set $\alpha = \hat{\alpha}^i$.

Step 2. Let $\tilde{\alpha} = \min\{\tilde{\alpha}^i, (\alpha/\delta)\}$.

Step 3. If $y^i + \tilde{\alpha} p^i \notin \mathcal{S}_\alpha$ or $\alpha = \tilde{\alpha}^i$ or

$$Z(y^i + \tilde{\alpha} p^i; \mu, \epsilon) \geq Z(y^i; \mu, \epsilon) - \gamma(\tilde{\alpha})^2$$

return α .

Step 4. Set $\alpha = \tilde{\alpha}$ and go to Step 2.

We note that the iteration map \mathcal{M} takes, as input arguments, current values for the iterate x , the smoothing parameter μ , the initial step size $\tilde{\alpha}^0$, the penalty parameter ϵ , and exponent q_1 and returns, as output arguments, the newly computed

iterate \tilde{x} , smoothing parameter $\tilde{\mu}$, initial stepsize for subsequent calls $\tilde{\alpha}^0$, and maximum stepsize $\tilde{\alpha}^{max}$. For a thorough description of the iteration map \mathcal{M} we refer the interested reader to [21].

On the basis of the iteration map \mathcal{M} so far described, we can define our derivative-free method for the solution of problem (1).

Algorithm. DeFCon

Data. $\tilde{x} \in \mathcal{S}_\alpha$, $\tilde{\alpha}_0^0 > 0$, $\epsilon_0 > 0$, $\mu_{max} > 0$, $\gamma > 0$, $\delta \in (0, 1)$, $\theta \in (0, 1)$, $0 < q_1 < q_2 < 1$, and $\tau \in (0, 1)$.

Step 0. Set $\mu_0 = \mu_{max}$, $x_0 = \tilde{x}$, $j = 0$, and $\epsilon = \epsilon_j$.

Step 1. Set $k = 0$.

Step 2. (Main iteration)

Compute $\mathcal{M}(x_k, \mu_k, \tilde{\alpha}_k^0, \epsilon, q_1) \mapsto (x_{k+1}, \mu_{k+1}, \tilde{\alpha}_{k+1}^0, \tilde{\alpha}_{k+1}^{max})$.

Set $k = k + 1$.

Step 3. (Penalty parameter testing)

If $\frac{(\tilde{\alpha}_k^{max})^{q_2}}{\mu_k} < \min\{\epsilon, \max\{0, g_1(x_k), \dots, g_m(x_k)\}\}$, then set $\epsilon = \frac{(\tilde{\alpha}_k^{max})^{q_2}}{\tau \mu_k}$.

If $Z(\tilde{x}; \mu_k, \epsilon) \leq Z(x_k; \mu_k, \epsilon)$, then set $x_0 = \tilde{x}$ else $x_0 = x_k$.

Set $\epsilon_{j+1} = \epsilon$, $j = j + 1$, $\mu_0 = \mu_k$ and go to Step 1.

Else go to Step 2.

As mentioned earlier in this section, the crucial aspect of Algorithm DeFCon resides in Step 3, that is, in the penalty parameter testing and updating formula.

We remark that the requirement that $0 < q_1 < q_2 < 1$ is essential to prove convergence. In particular, $q_1 \in (0, 1)$ is required to prove convergence of the method proposed in [21]; $q_2 \in (0, 1)$ is needed to prove that the penalty parameter is updated only a finite number of times. Finally, $q_1 < q_2$ is essential to prove that a feasible point is obtained in the limit by Algorithm DeFCon.

The quantity $(\tilde{\alpha}_k^{max})^{q_2}$ can be viewed as a stationarity measure of the current iterate with respect to the smoothing function (see [16]). Then, on the basis of the analysis carried out in [16], we can say that $(\tilde{\alpha}_k^{max})^{q_2} / \mu_k$ roughly measures the stationarity of the current iterate with respect to problem (4). Thus, the rationale behind the penalty parameter updating is to decrease ϵ whenever an improvement of the quality of the solution of problem (4) does not correspond to a reduction of the infeasibility of the current iterate with respect to problem (1). Note, in particular, that if x_k is feasible with respect to the nonlinear inequality constraints, then the penalty parameter is left unchanged.

The following proposition is an important result in that it guarantees that the penalty parameter ϵ is reduced finitely many times.

PROPOSITION 10. *Let $J = \{0, 1, \dots\}$ be the index set generated by Algorithm DeFCon at Step 3. Then, J is finite.*

Proof. Suppose that, each time that the penalty parameter satisfies the condition tested at Step 3 and before incrementing the counter j , the following quantities are stored: $\sigma_j^{max} = \tilde{\alpha}_k^{max}$, $\tilde{\sigma}_j^i = \tilde{\alpha}_j^i$, $\sigma_j^i = \alpha_j^i$ for all $i = 1, \dots, r_{k-1} + 1$, $w_j^i = y_{k-1}^i$ and $d_j^i = p_{k-1}^i$ for all $i = 1, \dots, r_{k-1}$, and $t_j = r_{k-1}$, $z_j = x_k$, $\rho_j = \mu_k$. For the sake of completeness, we set $\rho_{-1} = \mu_{max}$.

Reasoning by contradiction, we suppose that J is infinite. By the test of Step 3 of Algorithm DeFCon we have that

$$\frac{(\sigma_j^{max})^{q_2}}{\rho_j} \leq \epsilon_j;$$

hence

$$\epsilon_{j+1} = \tau \frac{(\sigma_j^{max})^{q_2}}{\rho_j} \leq \tau \epsilon_j$$

so that we get

$$(36) \quad \lim_{j \rightarrow \infty} \epsilon_j = 0.$$

Let $\{z_j\}$ be the sequence produced by Algorithm DeFCon. Then, by Assumption 1, an accumulation point $\bar{z} \in \bar{\mathcal{S}}_\alpha$ exists. Let us relabel $\{z_j\}$ the subsequence which converges to \bar{z} . Suppose, furthermore, that $\bar{z} \in \partial\mathcal{D}_\alpha$. By the instructions at Step 3 of Algorithm DeFCon, iteration map \mathcal{M} , and by point (i) of Proposition 6, we get that

$$(37) \quad Z(z_j; \epsilon_j) \leq Z(z_j; \rho_j, \epsilon_j) \leq Z(x_0^{(j)}; \mu_0^{(j)}, \epsilon_j) \leq Z(x_0^{(j)}; \rho_{j-1}, \epsilon_j),$$

where we denote by $\{x_k^{(j)}\}$ and $\{\mu_k^{(j)}\}$ the sequences produced by Algorithm DeFCon when $\epsilon = \epsilon_j$.

Furthermore, by the second test at Step 3 of Algorithm DeFCon and by relation (12), we get

$$(38) \quad Z(x_0^{(j)}; \rho_{j-1}, \epsilon_j) \leq Z(\tilde{x}; \rho_{j-1}, \epsilon_j) \leq Z(\tilde{x}; \epsilon_j) + \rho_{j-1} \ln m.$$

Hence, by (37) and (38) and multiplying by ϵ_j , we obtain

$$(39) \quad \epsilon_j Z(z_j; \epsilon_j) \leq \epsilon_j Z(\tilde{x}; \epsilon_j) + \epsilon_j \rho_{j-1} \ln m.$$

Since, when $j \rightarrow \infty$, $z_j \rightarrow \bar{z} \in \partial\mathcal{D}_\alpha$, an index $i \in \{1, \dots, m\}$ must exist such that $g_i(z_j) \rightarrow \alpha_i$ so that $\hat{g}_i(z_j; \epsilon_j) \rightarrow +\infty$. Therefore, we get that

$$(40) \quad \lim_{j \rightarrow \infty} \epsilon_j Z(z_j; \epsilon_j) = \lim_{j \rightarrow \infty} \max\{0, \hat{g}_1(z_j; \epsilon_j), \dots, \hat{g}_m(z_j; \epsilon_j)\} = +\infty.$$

Noting that, by the expression of $\hat{g}_i(x; \epsilon)$, $\lim_{j \rightarrow \infty} \hat{g}_i(\tilde{x}; \epsilon_j) = g_i(\tilde{x})$, $i = 1, \dots, m$, we can write that

$$(41) \quad \lim_{j \rightarrow \infty} \epsilon_j Z(\tilde{x}; \epsilon_j) + \epsilon_j \rho_{j-1} \ln m = \max\{0, g_1(\tilde{x}), \dots, g_m(\tilde{x})\} < +\infty.$$

Thus, (39), (40), and (41) prove that \bar{z} cannot be on $\partial\mathcal{D}_\alpha$; therefore $\bar{z} \in \mathcal{S}_\alpha$.

Now, the test and the instructions at Step 3 of Algorithm DeFCon yield that for every index j ,

$$(42) \quad \frac{(\sigma_j^{max})^{q_2}}{\rho_j} < \min \left\{ \epsilon, \max\{0, g_1(z_j), \dots, g_m(z_j)\} \right\} \leq \epsilon = \epsilon_j,$$

which, recalling that the sequence $\{\rho_j\}$ is bounded above, implies that $\lim_{j \rightarrow \infty} (\sigma_j^{max})^{q_2} = 0$; hence

$$(43) \quad \lim_{j \rightarrow \infty} \sigma_j^{max} = 0.$$

Now we show that $\lim_{j \rightarrow \infty} w_j^i = \bar{z}$ for all $i = 1, \dots, t_j$. To this aim, recalling the definition of σ_j^{max} and the instructions at Step 2.3 of iteration map \mathcal{M} , we can write

$$\|w_j^i - z_j\| \leq t_j \sigma_j^{max} \quad \forall i \in \{1, \dots, t_j\},$$

which, by (43) and by the boundedness of t_j , by Assumption 3, yield

$$(44) \quad \lim_{j \rightarrow \infty} \|w_j^i - z_j\| = 0 \quad \forall i \in \{1, \dots, t_j\}.$$

Hence, by the fact that $z_j \rightarrow \bar{z}$, we obtain that

$$(45) \quad w_j^i \rightarrow \bar{z} \quad \forall i = 1, \dots, t_j.$$

By (45), (43), and the fact that $\bar{z} \in \mathcal{S}_\alpha$, we have that, for sufficiently large values of j , $w_j^i + \tilde{\sigma}_j^i d_j^i \in \mathcal{S}_\alpha$ and $w_j^i + \sigma_j^i d_j^i \in \mathcal{S}_\alpha$. We recall that point (ii) of Proposition 6 in [21] holds. Therefore, by the instructions of Step 3 and (44), we obtain that, for sufficiently large values of j , either

$$w_j^i + \frac{\sigma_j^i}{\delta} d_j^i \in \mathcal{S}_\alpha \text{ and } Z\left(w_j^i + \frac{\sigma_j^i}{\delta} d_j^i; \rho_j, \epsilon_j\right) \geq Z(w_j^i; \rho_j, \epsilon_j) - \gamma \left(\frac{\sigma_j^i}{\delta}\right)^2$$

or

$$w_j^i + \tilde{\sigma}_j^i d_j^i \in \mathcal{S}_\alpha \text{ and } Z(w_j^i + \tilde{\sigma}_j^i d_j^i; \rho_j, \epsilon_j) \geq Z(w_j^i; \rho_j, \epsilon_j) - \gamma (\tilde{\sigma}_j^i)^2$$

are satisfied. Now, setting $\xi_j^i = \frac{\sigma_j^i}{\delta}$ in the first case and $\xi_j^i = \tilde{\sigma}_j^i$ in the second one, we have, for sufficiently large values of j ,

$$(46) \quad w_j^i + \xi_j^i d_j^i \in \mathcal{S}_\alpha \text{ and } Z(w_j^i + \xi_j^i d_j^i; \rho_j, \epsilon_j) \geq Z(w_j^i; \rho_j, \epsilon_j) - \gamma (\xi_j^i)^2.$$

From the updating formula for y^i in Step 2.4 of iteration map \mathcal{M} , we note that

$$(47) \quad \|w_j^i - z_j\| \leq \sum_{l=1}^{i-1} \sigma_j^l \leq \delta \sum_{l=1}^{i-1} \xi_j^l \leq \delta t_j \max_{l=1, \dots, t_j} \{\xi_j^l\},$$

from which we get that

$$(48) \quad \max_{i=1, \dots, t_j} \{\xi_j^i, \|z_j - w_j^i\|\} \leq \max\{1, \delta t_j\} \max_{i=1, \dots, t_j} \{\xi_j^i\} \leq t_j \max_{i=1, \dots, t_j} \{\tilde{\sigma}_j^i, \sigma_j^i\}.$$

From (42), we have that, for every index j ,

$$\max_{i=1, \dots, t_j} \{(\tilde{\sigma}_j^i)^{q_2}, (\sigma_j^i)^{q_2}\} = (\sigma_j^{max})^{q_2} < \rho_j \epsilon_j,$$

which implies that

$$(49) \quad (\epsilon_j \rho_j)^{1/q_2} > \sigma_j^{max},$$

so that, by (48) and (49), we obtain $\max_{i=1, \dots, t_j} \{\xi_j^i, \|z_j - w_j^i\|\} < t_j (\epsilon_j \rho_j)^{1/q_2}$, from which, recalling that $0 < q_2 < 1$, we get

$$(50) \quad \lim_{j \rightarrow \infty} \frac{\max_{i=1, \dots, t_j} \{\xi_j^i, \|z_j - w_j^i\|\}}{\epsilon_j \rho_j} = 0.$$

By considering (36), (46), and (50), we have that the hypotheses of point (ii) of Proposition 9 are satisfied so that a $\bar{j} \geq 0$ exists such that, for all $j \geq \bar{j}$, z_j is feasible for problem (1).

On the other hand, by the instruction of Step 3 of Algorithm DeFCon, we have that, for every index j ,

$$\frac{(\sigma_j^{max})^{q_2}}{\rho_j} < \max\{0, g_1(z_j), \dots, g_m(z_j)\},$$

which means that $z_j \in \mathcal{S}_\alpha$ and $g(z_j) \not\leq 0$, for every index j . The latter contradicts what has just been proved, namely, that z_j is feasible for problem (1) for j sufficiently large, thus completing the proof. \square

The previous proposition guarantees that, after finitely many times, the test at Step 3 of Algorithm DeFCon is never satisfied so that the penalty parameter ϵ stays fixed at its last value, say $\epsilon_{\bar{j}}$, and $\{\epsilon_j\}$, $\{z_j\}$, $\{\rho_j\}$ are all finite sequences. Therefore, from now on, we shall assume that $\epsilon = \epsilon_{\bar{j}}$.

The following proposition describes some properties concerning the sequences of points and of objective function values generated by Algorithm DeFCon and the sampling technique adopted.

PROPOSITION 11 (see [21]). *Let $\{x_k\}$, $\{\mu_k\}$ be the sequences generated by Algorithm DeFCon when $\epsilon = \epsilon_{\bar{j}}$. Then*

- (a) $\{x_k\}$ is well defined;
- (b) the sequence $\{x_k\}$ is bounded;
- (c) the following limits hold:

$$(51) \quad \lim_{k \rightarrow \infty} \max_{i=1, \dots, r_k} \{\alpha_k^i\} = 0,$$

$$(52) \quad \lim_{k \rightarrow \infty} \max_{i=1, \dots, r_k} \{\tilde{\alpha}_k^i\} = 0,$$

$$(53) \quad \lim_{k \rightarrow \infty} \max_{i=1, \dots, r_k} \|x_k - y_k^i\| = 0.$$

As shown in [21], by carrying out the convergence analysis, a significant role is played by the index set K defined as follows:

$$(54) \quad K = \{k : \mu_{k+1} < \mu_k\}.$$

Indeed, the following proposition shows that every accumulation point of the sequence $\{x_k\}_K$ is a KKT point for problem (1).

PROPOSITION 12. *Let $\{x_k\}$ be the sequence generated by Algorithm DeFCon when $\epsilon = \epsilon_{\bar{j}}$. Then the sequence $\{x_k\}$ is bounded and every accumulation point \bar{x} of $\{x_k\}_K$, where K is defined by (54), is a KKT point for problem (1).*

Proof. First of all we prove that \bar{x} is feasible for problem (1). Since ϵ is no longer updated, from the instruction of Step 3 of Algorithm DeFCon we know that, for every index $k \in K$,

$$0 \leq \min\{\epsilon_{\bar{j}}, \max\{0, g_1(x_{k+1}), \dots, g_m(x_{k+1})\}\} \leq \frac{(\tilde{\alpha}_{k+1}^{max})^{q_2}}{\mu_{k+1}},$$

and, by the instruction at Step 3 of iteration \mathcal{M} ,

$$\frac{(\tilde{\alpha}_{k+1}^{max})^{q_2}}{\mu_{k+1}} = (\tilde{\alpha}_{k+1}^{max})^{q_2 - q_1},$$

which, taking the limit for $k \rightarrow \infty, k \in K$, recalling the results of Proposition 11, and the fact that $q_1 < q_2$, implies that

$$(55) \quad \lim_{k \rightarrow \infty, k \in K} \max\{0, g_1(x_{k+1}), \dots, g_m(x_{k+1})\} = 0.$$

Now let \bar{x} be an accumulation point of sequence $\{x_{k+1}\}_K$; that is, an infinite index set $\hat{K} \subseteq K$ exists such that

$$\lim_{k \rightarrow \infty, k \in \hat{K}} x_{k+1} = \bar{x}.$$

On account of relation (55), we have that

$$\lim_{k \rightarrow \infty, k \in \hat{K}} \max\{0, g_1(x_{k+1}), \dots, g_m(x_{k+1})\} = 0,$$

which means that \bar{x} is such that $\bar{x} \in \mathcal{F}$.

By employing (53) of Proposition 11 and the definition of iteration \mathcal{M} , we have that

$$\lim_{k \rightarrow \infty} \|x_k - x_{k+1}\| = 0.$$

Hence, we know that

$$\lim_{k \rightarrow \infty, k \in \hat{K}} x_k = \lim_{k \rightarrow \infty, k \in \hat{K}} x_{k+1},$$

so that $\lim_{k \rightarrow \infty, k \in \hat{K}} x_k = \bar{x} \in \mathcal{F}$.

Finally, we show that \bar{x} is a KKT point for problem (1). By the instructions of iteration map \mathcal{M} , every point $x_k \in \mathcal{S}_\alpha$: whose closure is compact by Assumption 1. Hence, the sequence $\{x_k\}$ is bounded and therefore it admits limit points.

Now let \bar{x} be any accumulation point of the subsequence $\{x_k\}_K$, where K is defined by (54). By the first part of the proof, we know that $\bar{x} \in \mathcal{F}$. Furthermore, by Corollary 1 of [21], we have that \bar{x} is a stationary point of the exact penalty function $Z(x; \epsilon)$, so that, by Proposition 3, \bar{x} is a KKT point for problem (1). \square

5. Case study: Constrained parameter estimation for glucose kinetics model. The aim of this paper is mainly theoretical. Thus, the development of an efficient code based on the proposed algorithm and the analysis of its numerical performance are beyond the scope of the present paper. We refer to [12] for a numerical experimentation on standard test problems. In [12] an asynchronous parallel generating set search approach has been used to minimize many different penalty functions. The influence of the penalty function has been analyzed from a computational point of view. In particular, Griffin and Kolda employ as penalty functions the nondifferentiable ℓ_1, ℓ_2 , and ℓ_∞ plus their smoothed versions s_1, s_2 , and s_∞ . All of these penalization techniques are compared against the standard ℓ_2^2 differentiable penalty function. An extensive numerical experimentation is carried out on a large set of test problems from the CUTER collection [11]. The conclusion of [12] is that the use of a smooth approximation s_∞ of an ℓ_∞ exact penalty function leads to a derivative-free algorithm which shows a good compromise between quality of the final point and number of function evaluations required to get convergence.

Encouraged by these results we wanted to understand if the proposed derivative-free algorithm was able to efficiently solve a real world application. To this aim, we

used a rough MATLAB implementation of Algorithm DeFCon to solve a problem connected with the study of an insulin-glucose model of the human body. To solve the problem we also used the constrained nonlinear minimization MATLAB routine `fmincon` and the freely available derivative-free MATLAB package NOMADm [2]. The latter is a recent implementation of a class of mesh-adaptive direct search (MADS) algorithms for solving nonlinear and mixed variable optimization problems with general nonlinear constraints. In particular, the employment of `fmincon` is useful to understand to what extent the unavailability of the derivatives can be overcome by finite difference approximations. On the other hand, the comparison with the derivative-free package NOMADm is needed to point out that the proposed algorithm is at least as efficient as an existing derivative-free code.

The study and understanding of circulatory models of glucose kinetics are of great importance in medicine and biology. Such models study the response of body tissues to an impulsive injection of a glucose bolus of known quantity. The intravenous glucose tolerance test (IVGTT) is a simple and standardized test that allows one to measure the reaction of the organism to the mentioned impulsive perturbation of the steady state. IVGTT has a documented ability to assess the functioning of the key organs involved in glucose homeostasis. Moreover, it is a powerful tool in the study of diabetes mellitus in that it is able to provide information on beta-cell function and insulin sensitivity (both peripheral and hepatic).

The IVGTT experimental protocol used prescribes the following operations [27]:

- Collection of 3ml blood basal samples at -30 , -15 , and 0 min. to glucose injection.
- Injection of a 300mg/kg glucose bolus at 0 min. immediately after the collection of the last basal sample.
- Infusion, at 20 min. from injection, of $0.03U/kg$ insulin at a constant rate for 5 minutes.
- Collection of 3ml blood samples at 2, 3, 4, 5, 6, 8, 10, 15, 20, 25, 30, 40, 60, 80, 100, 120, 140, 160, 180, 210, and 240 min. from injection of glucose, for measurements of glucose, glucose tracer, insulin, and C-peptide concentrations.

In the circulatory model of glucose kinetics studied in [24, 26, 25], the body tissues are lumped into two blocks. The heart-lungs block represents the heart chambers and the lungs, i.e., the tissues in between the right atrium and left ventricle. The periphery block represents all the remaining tissues, nourished by the entire arterial tree originating from the left ventricle (including the heart tissues nourished by the coronaries).

The dynamics of the exogenous arterial glucose concentration during the IVGTT can be modelled by the following system of ordinary differential equations:

$$(56a) \quad \frac{dG_A(t)}{dt} = -\lambda G_A(t) + \lambda [G_1(t) + G_2(t) + J/F],$$

$$(56b) \quad \frac{dG_1(t)}{dt} = -\alpha_1 G_1(t) + \alpha_1 \vartheta [1 - E_b - \gamma Z(t)] G_A(t),$$

$$(56c) \quad \frac{dG_2(t)}{dt} = -\alpha_2 G_2(t) + \alpha_2 (1 - \vartheta) [1 - E_b - \gamma Z(t)] G_A(t),$$

$$(56d) \quad \frac{dZ(t)}{dt} = -\beta Z(t) + \beta [I(t) - I_b], \quad Z(0) = 0.$$

Here, $G_A(t)$ denotes the exogenous arterial glucose concentration, the sum between $G_1(t)$ and $G_2(t)$ denotes the mixed-venous glucose concentration, $Z(t)$ denotes the increment from the basal level of whole-body insulin fractional extraction, $I(t)$ is the insulin concentration during the exam, $J = 300 \text{ mg/kg}$ is the known intravenous glucose infusion, $F = 2688 \text{ ml} \cdot \text{min}^{-1} \cdot \text{m}^{-2}$ is the cardiac output, $\lambda = 3.84 \text{ min}^{-1}$ is the reciprocal of the mean heart-lungs transit time [17] and is patient-independent, and I_b is the basal value of insulin concentration and is patient-specific; we used $I_b = 50 \text{ pmol/l}$. The numerical solution of the system of ODE (56) requires that the insulin concentration increment $I(t) - I_b$ in (56d) is available at every time instant. For this purpose, the measured values of $I(t) - I_b$ have been smoothed and interpolated by a continuous function of time as detailed in [28]. Finally, $\alpha_1, \alpha_2, \beta, \gamma, \vartheta, E_b$ are the model parameters to be estimated in such a way that $G_A(t)$ approximates as well as possible the measurements gathered during the IVGTT. The model parameters, as suggested by biomedical engineers, can be sensibly bounded both from below and above as follows:

$$\begin{aligned} 0.5 \leq \alpha_1 \leq 5, \quad 0.01 \leq \alpha_2 \leq 0.5, \quad 0.3 \leq \vartheta \leq 0.9, \quad 0.01 \leq \beta \leq 1, \\ 0.01 \leq E_b \leq 0.1, \quad 5 \cdot 10^{-5} \leq \gamma \leq 5 \cdot 10^{-4}. \end{aligned}$$

Let us define $t = (2, 3, 4, 5, 6, 8, 10, 15, 20, 25, 30, 40, 60, 80, 100, 120, 140, 160, 180, 210, 240)^\top$, and let g_i denote the exogenous glucose concentration measured at time t_i during the IVGTT. Then

$$f(\alpha_1, \alpha_2, \beta, \gamma, \vartheta, E_b) = \sum_{i=1}^{21} (G_A(t_i) - g_i)^2$$

is the sum of squared errors between model prediction and actual measurements. Moreover, among all the possible models, we are interested in those for which the mean periphery transit time $\vartheta/\alpha_1 + (1 - \vartheta)/\alpha_2$ is greater than or equal to 2.5 minutes. This time limit is necessary to prevent models that are not representative of a human patient with medium body mass index. Thus, we end up with the following constrained problem:

$$\begin{aligned} (57) \quad & \min f(\alpha_1, \alpha_2, \beta, \gamma, \vartheta, E_b) \\ & \text{s.t. } g(\alpha_1, \alpha_2, \vartheta) = \vartheta/\alpha_1 + (1 - \vartheta)/\alpha_2 \geq 2.5, \\ & \quad 0.5 \leq \alpha_1 \leq 5, \\ & \quad 0.01 \leq \alpha_2 \leq 0.5, \\ & \quad 0.3 \leq \vartheta \leq 0.9, \\ & \quad 0.01 \leq \beta \leq 1, \\ & \quad 0.01 \leq E_b \leq 0.1, \\ & \quad 5 \cdot 10^{-5} \leq \gamma \leq 5 \cdot 10^{-4}. \end{aligned}$$

The circulatory model of glucose has been implemented in MATLAB/Simulink [29]. The solution of the system of ODE (56), which is at the basis of the model, is done numerically with a precision ξ that can be set by the user.

We started our experimentation by comparing the outcomes of Algorithm DeF-Con with that of the constrained nonlinear minimization MATLAB routine `fmincon` and of the derivative-free package NOMADm, selecting a precision level of the ODE solver $\xi = 10^{-3}$. We ran `fmincon` and NOMADm by using default values for their parameters apart from the tolerances in the stopping criterion which we set to 10^{-6} as for Algorithm DeF-Con. Moreover, both `fmincon` and NOMADm were ran by appropriately specifying the scale of the optimization variables.

Initial values for the parameters, as suggested by biomedical engineers, are

α_1	α_2	β	γ	ϑ	E_b
1.0089	0.40794	0.16481	$3.932 \cdot 10^{-4}$	0.84496	0.020991

In Figure 1 we report the actual measurements of exogenous glucose during IVGTT as crosses and plot the curve $G_A(t)$ obtained in correspondence to the initial values of the parameters as listed above.

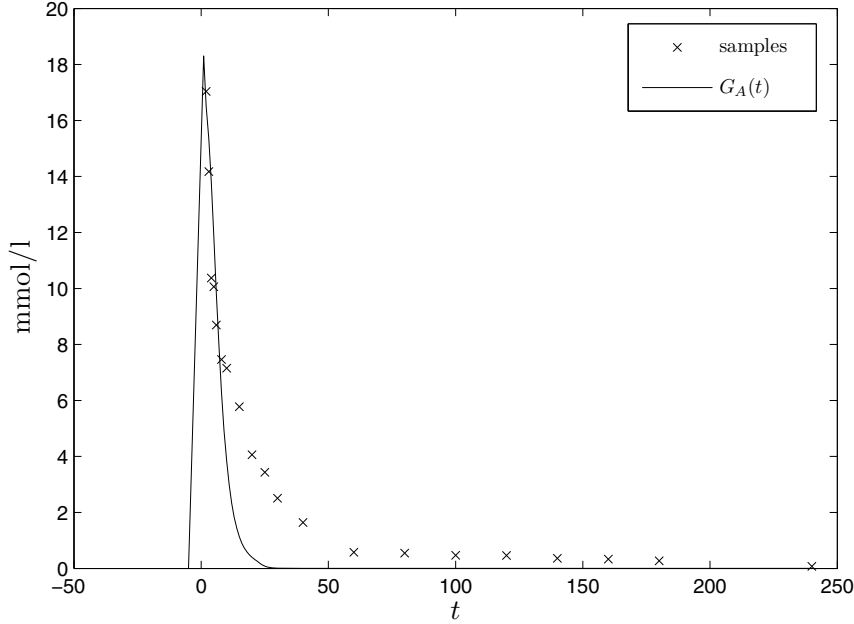


FIG. 1. *Initial configuration.*

Starting from this initial point, the proposed derivative-free algorithm (DeFCon), NOMADm, and the MATLAB routine `fmincon` yield the results reported in Table 1, where (n.it.) and (n.f.) denote, respectively, the number of iterations and number

TABLE 1
Results obtained by Algorithm *DeFCon*, *NOMADm*, and *fmincon* for $\xi = 10^{-3}$.

	DeFCon	NOMADm	fmincon
n.it.	46	144	12
n.f.	627	480	245
α_1^*	2.0228	1.3995	0.80479
α_2^*	0.11881	0.081768	0.011788
β^*	0.055959	0.010513	1.0
γ^*	$1.6529 \cdot 10^{-4}$	$1.4906 \cdot 10^{-4}$	$5.0 \cdot 10^{-5}$
ϑ^*	0.7409	0.84496	0.9
E_b^*	0.01	0.052241	0.01
f^*	2.0959	5.4409	27.6094
g^*	2.547	2.5	9.6017

of functions evaluations. $\alpha_1^*, \alpha_2^*, \beta^*, \gamma^*, \vartheta^*$, and E_b^* represent the final values of the model parameters to be estimated. Finally, f^* and g^* represent, respectively, the final values of the objective function and of the nonlinear constraint (which should be greater than or equal to 2.5). Looking at the results it can be noted that, even though all the methods manage to achieve feasibility of the final point, Algorithm DeFCon and NOMADm are able to produce a point whose objective function value is much better than that produced by fmincon. Algorithm DeFCon and NOMADm produce almost the same points. Indeed, the parameter values obtained by Algorithm DeFCon and NOMADm yield almost the same curves $G_A(t)$ even though Algorithm DeFCon reaches a better objective function value than that achieved by NOMADm, which converges in fewer function evaluations. As concerns the result computed by fmincon, it yields a curve $G_A(t)$ which is substantially different in terms of approximation of the glucose measurements (see Figure 2) from that yielded by Algorithm DeFCon and NOMADm. Comprehensibly, this better behavior of Algorithm DeFCon and NOMADm over fmincon is achieved at the expense of a higher computational burden and points out the noisy nature of the approximation problem which is at the basis of the inefficiency of fmincon.

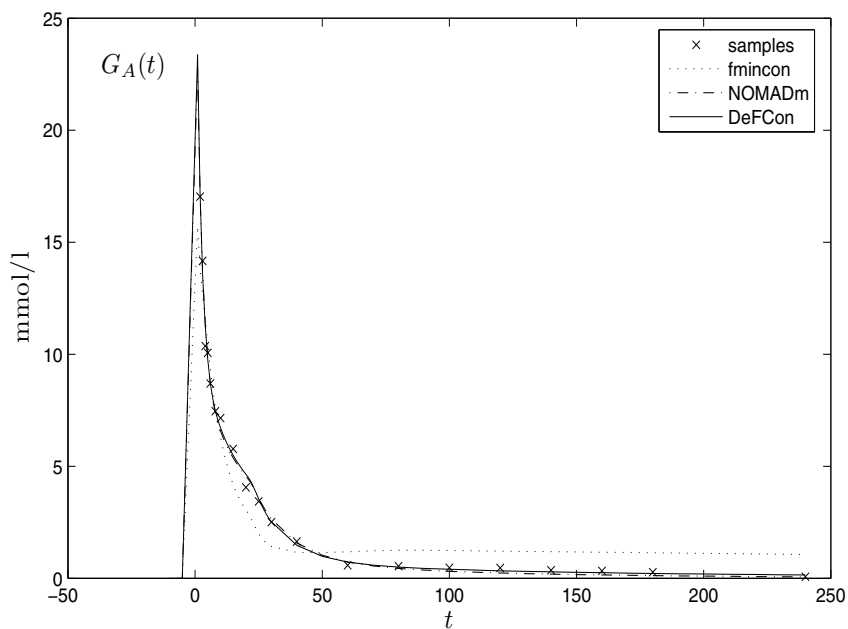


FIG. 2. *Optimal curves.*

The inefficiency of the MATLAB solver fmincon along with the modest number of iterations and function evaluations to get convergence might indicate that the ODE solver tolerance is too high for estimation of first order derivatives by finite differences to be reliable. Hence, we tried to solve the problem with increasing precision levels for the ODE solver; namely we set the precision $\xi = 10^{-4}, 10^{-5}, 10^{-6}$ and compared the results in Table 2.

As concerns the above comparison, we first note that there is only a slight change

TABLE 2
Comparison between Algorithm DeFCon, NOMADm, and fmincon.

ξ	10^{-6}			10^{-5}		
	DeFCon	NOMADm	fmincon	DeFCon	NOMADm	fmincon
n.it.	97	1211	21	68	1253	9
n.f.	1410	3408	316	994	3542	157
α_1^*	2.1468	1.9386	2.2779	2.1659	1.9386	0.58594
α_2^*	0.12418	0.11473	0.049484	0.12401	0.11473	0.012527
β^*	0.067333	0.046646	0.95153	0.067373	0.046646	1.0
γ^*	$1.5 \cdot 10^{-4}$	$1.5 \cdot 10^{-4}$	$5.0 \cdot 10^{-5}$	$1.5 \cdot 10^{-4}$	$1.5 \cdot 10^{-4}$	$5.0 \cdot 10^{-5}$
θ^*	0.73186	0.75805	0.86005	0.73182	0.75805	0.9
E_p^*	0.01	0.020991	0.033761	0.01	0.020991	0.01
f^*	2.0061	2.3219	63.7352	2.0075	2.3217	69.183
g^*	2.5002	2.5000	3.2058	2.5005	2.5000	9.5193

ξ	10^{-4}		
	DeFCon	NOMADm	fmincon
n.it.	57	187	9
n.f.	827	562	146
α_1^*	2.1261	1.5948	0.5
α_2^*	0.12318	0.091778	0.036089
β^*	0.06504	0.015396	0.01
γ^*	$1.5 \cdot 10^{-4}$	$1.5 \cdot 10^{-4}$	$5.0 \cdot 10^{-4}$
θ^*	0.73407	0.81762	0.89948
E_p^*	0.01	0.046137	0.01
f^*	2.0146	4.1823	103.9875
g^*	2.504	2.5001	4.5842

in the points produced by Algorithm DeFCon and NOMADm. Namely, as the ODE solver precision ξ increases, Algorithm DeFCon and NOMADm, though requiring more iterations and function evaluations to converge, produce points which are very close to each other. This is confirmed by the objective and constraint function values which gain more and more accuracy as the precision ξ becomes finer. However, Algorithm DeFCon seems to be more efficient than NOMADm when the precision ξ is less than or equal to 10^{-5} . Slightly better results both for Algorithm DeFCon and NOMADm can be obtained by performing a tuning of their parameters.

On the contrary, fmincon exhibits a more unpredictable behavior converging to points that are largely different from each other in terms of parameter, objective, and constraint function values. The outcomes of fmincon seem to be unrelated to the precision level of the ODE solver apart for the fact that the computational burden increases as ξ gets finer. This inefficiency of fmincon is most probably due to the lack of derivative knowledge on the problem which fmincon tries to overcome by computing gradients by finite difference approximation. This, in turn, makes fmincon more subject to the numerical noise introduced by the ODE solver thus explaining the apparent instability of the code.

6. Conclusions. In this paper we presented a derivative-free algorithm for the solution of inequality constrained nonlinear programming problems. The method is based on the derivative-free minimization of a smooth approximation of a new (nondifferentiable) ℓ_∞ exact penalty function. We proved that the method is globally convergent towards a KKT point of the constrained problem. In order to stress the ability of our method to tackle real world problems, we reported the results obtained on a constrained problem concerning the parameter estimation of an insulin-glucose model of the human body. A comparison with another derivative-free optimization routine shows the effectiveness of the proposed method.

The convergence properties and the theoretical analysis of the proposed method has been carried out in the case where only inequality constraints are present. The method can be adapted to handle both equality and inequality constraints, preserving

its convergence properties but at the expense of some nontrivial technicalities which considerably complicate the analysis. Furthermore, we remark that the realization of an efficient code was not the main aim of this paper. For this reason a fine tuning of the parameters and an efficient computation of the search directions have not been done but are the subject of continuing work.

Appendix.

Proof of Proposition 3. Since $\bar{x} \in \mathcal{F}$, then $B(\bar{x}; \epsilon) = I_0(\bar{x})$. Therefore, by Proposition 2, we have

$$\left(\nabla f(\bar{x}) + \sum_{i \in I_0(\bar{x})} \frac{\lambda_i((\alpha_i - g_i(\bar{x}))^2 + \epsilon \alpha_i)}{\epsilon(\alpha_i - g_i(\bar{x}))^2} \nabla g_i(\bar{x}) \right)^\top d \geq 0 \quad \forall d \in T(\bar{x}).$$

Then, by setting $\bar{\lambda}_i = \frac{\lambda_i((\alpha_i - g_i(\bar{x}))^2 + \epsilon \alpha_i)}{\epsilon(\alpha_i - g_i(\bar{x}))^2}$, $i \in I_0(\bar{x})$, and $\bar{\lambda}_i = 0$, $i \in \{1, \dots, m\} \setminus I_0(\bar{x})$, we have that there does not exist any direction $d \in R^n$ such that

$$\left(\nabla f(\bar{x}) + \sum_{i \in I_0(\bar{x})} \bar{\lambda}_i \nabla g_i(\bar{x}) \right)^\top d < 0, \\ a_j^\top d \leq 0 \quad \forall j \in J(\bar{x}).$$

Hence, by using the Motzkin theorem [23], we have that $y_0 > 0$ and $\mu_j \geq 0$, $j \in J(\bar{x})$, exist such that

$$y_0 \left(\nabla f(\bar{x}) + \sum_{i \in I_0(\bar{x})} \bar{\lambda}_i \nabla g_i(\bar{x}) \right) + \sum_{j \in J(\bar{x})} a_j \mu_j = 0.$$

The result follows by taking $\bar{\mu}_j = \mu_j / y_0$ for $j \in J(\bar{x})$, and $\bar{\mu}_j = 0$ for $j \notin J(\bar{x})$. \square

In order to complete the proof of the exactness results of the penalty function $Z(x; \epsilon)$, we need some technical results which are reported in the following propositions.

PROPOSITION 13. *Let $\hat{x} \in \mathcal{S}_\alpha$; then there exist numbers $\epsilon(\hat{x}) > 0$ and $\sigma(\hat{x}) > 0$ such that, for all $\epsilon \in (0, \epsilon(\hat{x})]$ and for all $x \in \mathcal{B}(\hat{x}, \sigma(\hat{x})) \cap \mathcal{S}_\alpha$ and $g(x) \not\leq 0$, there exists a direction $d \in T(\hat{x})$ satisfying $DZ(x, d; \epsilon) < 0$.*

Proof. By Assumption 2, we have that the hypotheses of Lemma 1 are satisfied at \hat{x} for $I = I_\pi(\hat{x})$. Let $\mathcal{B}(\hat{x}, \rho)$ and $d \in T(\hat{x})$ be the neighborhood and the direction considered in Lemma 1. We have that $d \in T(\hat{x})$ is such that

$$(58) \quad \nabla \hat{g}_i(x; \epsilon)^\top d \leq -1$$

for all $i \in I_\pi(\hat{x})$. By continuity, we can find a neighborhood $\mathcal{B}(\hat{x}, \sigma(\hat{x})) \subseteq \mathcal{B}(\hat{x}, \rho)$ such that, for $i \notin I_\pi(\hat{x})$ and $x \in \mathcal{B}(\hat{x}, \sigma(\hat{x})) \cap \mathcal{S}_\alpha$, we have $g_i(x) < 0$; it follows that $I_\pi(x) \subseteq I_\pi(\hat{x})$ for $x \in \mathcal{B}(\hat{x}, \sigma(\hat{x})) \cap \mathcal{S}_\alpha$.

Now let $x \in \mathcal{B}(\hat{x}, \sigma(\hat{x})) \cap \mathcal{S}_\alpha$ be an infeasible point, that is, $g(x) \not\leq 0$. Then, there must exist at least an index $i \in I_\pi(\hat{x})$ such that $g_i(x) > 0$ and $\hat{g}_i(x; \epsilon) > 0$, so that it results in $B(x; \epsilon) \subseteq I_\pi(x)$.

Therefore, recalling the expression of the directional derivative of $Z(x; \epsilon)$ and (58), we get

$$DZ(x, d; \epsilon) = \nabla f(x)^\top d + \frac{1}{\epsilon} \max_{i \in B(x; \epsilon)} \{ \nabla \hat{g}_i(x; \epsilon)^\top d \} \leq \nabla f(x)^\top d - \frac{1}{\epsilon},$$

from which it follows that a value $\epsilon(\hat{x}) > 0$ exists such that, for all $\epsilon \in (0, \epsilon(\hat{x})]$ and $x \in \mathcal{B}(\hat{x}, \sigma(\hat{x})) \cap \mathcal{S}_\alpha$ with $x \notin \mathcal{F}$, it must hold that

$$DZ(x, d; \epsilon) < 0,$$

which concludes the proof. \square

PROPOSITION 14. Let $\bar{\lambda} \in R^m$ and $\bar{\mu} \in R^p$ be multipliers such that $(\bar{x}, \bar{\lambda}, \bar{\mu})$ is a KKT triple for problem (1). Then the following bound holds:

$$\|\bar{\lambda}\|_q \leq \nabla f(\bar{x})^\top z,$$

where $z \in T(\bar{x})$ is a vector such that

$$(59) \quad \nabla g_i(\bar{x})^\top z \leq -1, \quad i \in I_0(\bar{x}).$$

Proof. From the fact that $(\bar{x}, \bar{\lambda}, \bar{\mu})$ is a KKT triple, it follows that, for any $z \in T(\bar{x})$ satisfying (59), we have

$$\nabla f(\bar{x})^\top z = - \sum_{i \in I_0(\bar{x})} \bar{\lambda}_i \nabla g_i(\bar{x})^\top z - \sum_{j \in J(\bar{x})} \bar{\mu}_j a_j^\top z \geq 0.$$

Therefore, the following linear program and its dual are both feasible and bounded:

$$(60) \quad \begin{aligned} \min_z \quad & \nabla f(\bar{x})^\top z \\ & \nabla g_i(\bar{x})^\top z \leq -1, \quad i \in I_0(\bar{x}), \\ & a_j^\top z \leq 0, \quad j \in J(\bar{x}), \end{aligned}$$

$$(61) \quad \begin{aligned} \max_{u,v} \quad & \sum_{i \in I_0(\bar{x})} u_i \\ & \sum_{i \in I_0(\bar{x})} \nabla g_i(\bar{x}) u_i + \sum_{j \in J(\bar{x})} a_j v_j = -\nabla f(\bar{x}), \\ & u, v \geq 0. \end{aligned}$$

Let z^* and (u^*, v^*) be optimal solutions of (60) and (61), respectively. Recalling that every KKT multipliers (λ, μ) of problem (1) satisfy the constraints of problem (61), we then have

$$\|\bar{\lambda}\|_q \leq \|\bar{\lambda}\|_1 \leq \sum_{i \in I_0(\bar{x})} u_i^* = \nabla f(\bar{x})^\top z^* \leq \nabla f(\bar{x})^\top z$$

for any $z \in T(\bar{x})$ satisfying (59). \square

PROPOSITION 15 (see [7, Proposition 8]). A number Λ exists such that $\|\bar{\lambda}\|_\infty \leq \Lambda$ for all KKT triples $(\bar{x}, \bar{\lambda}, \bar{\mu})$ of problem (1).

Proof. The proof follows using Proposition 14 and the same reasoning of Proposition 8 in [7]. \square

Now, we can finally prove Propositions 4 and 5.

Proof of Proposition 4.

“If”-part: it follows from Proposition 10 in [9].

“Only if”-part: as $(\bar{x}, \bar{\lambda}, \bar{\mu})$ is a KKT triple for problem (1) we can write

$$(62) \quad \nabla f(\bar{x}) = - \left(\sum_{i \in I_0(\bar{x})} \bar{\lambda}_i \nabla g_i(\bar{x}) + \sum_{j \in J(\bar{x})} \bar{\mu}_j a_j \right).$$

Recalling that $\bar{x} \in \mathcal{F}$ and that, by definition, $\hat{g}_0(x; \epsilon) = 0$, so that $B(\bar{x}; \epsilon) = I_0(\bar{x}) \cup \{0\}$, the directional derivative of $Z(x; \epsilon)$ along direction d can be written as follows:

$$\begin{aligned} DZ(x, d; \epsilon) &= \nabla f(x)^\top d + \frac{1}{\epsilon} \max_{i \in B(x; \epsilon)} \{\nabla \hat{g}_i(x; \epsilon)^\top d\} \\ &= \nabla f(\bar{x})^\top d + \frac{1}{\epsilon} \max_{i \in I_0(\bar{x})} \{\max\{\nabla \hat{g}_i(\bar{x}; \epsilon)^\top d, 0\}\}. \end{aligned}$$

By using (62) in the above expression we get

$$\begin{aligned} DZ(\bar{x}, d; \epsilon) &= \frac{1}{\epsilon} \max_{i \in I_0(\bar{x})} \{\max\{\nabla \hat{g}_i(\bar{x}; \epsilon)^\top d, 0\}\} - \left(\sum_{i \in I_0(\bar{x})} \bar{\lambda}_i \nabla g_i(\bar{x})^\top d + \sum_{j \in J(\bar{x})} \bar{\mu}_j a_j^\top d \right) \\ &\geq \frac{1}{\epsilon} \max_{i \in I_0(\bar{x})} \{\max\{\nabla \hat{g}_i(\bar{x}; \epsilon)^\top d, 0\}\} - \left(\sum_{i \in I_0(\bar{x})} \bar{\lambda}_i \max\{\nabla g_i(\bar{x})^\top d, 0\} + \sum_{j \in J(\bar{x})} \bar{\mu}_j a_j^\top d \right). \end{aligned}$$

Whenever $d \in T(\bar{x})$, by definition of $T(\bar{x})$, we get

$$DZ(\bar{x}, d; \epsilon) \geq \frac{1}{\epsilon} \max_{i \in I_0(\bar{x})} \{\max\{\nabla \hat{g}_i(\bar{x}; \epsilon)^\top d, 0\}\} - \sum_{i \in I_0(\bar{x})} \bar{\lambda}_i \max\{\nabla g_i(\bar{x})^\top d, 0\}.$$

By considering the expression of $\nabla \hat{g}_i(x; \epsilon)$, it results, for $i \in I_0(\bar{x})$,

$$\nabla \hat{g}_i(\bar{x}; \epsilon) = \left(1 + \frac{\epsilon}{\alpha_i}\right) \nabla g_i(\bar{x}),$$

so that we obtain

$$DZ(\bar{x}, d; \epsilon) \geq \frac{1}{\epsilon} \max_{i \in I_0(\bar{x})} \{\max\{\nabla \hat{g}_i(\bar{x}; \epsilon)^\top d, 0\}\} - \sum_{i \in I_0(\bar{x})} \bar{\lambda}_i \frac{\alpha_i}{\alpha_i + \epsilon} \max\{\nabla \hat{g}_i(\bar{x}; \epsilon)^\top d, 0\}.$$

Now, recalling Proposition 15, we have that

$$\begin{aligned} \sum_{i \in I_0(\bar{x})} \bar{\lambda}_i \frac{\alpha_i}{\alpha_i + \epsilon} \max\{\nabla \hat{g}_i(\bar{x}; \epsilon)^\top d, 0\} &\leq \max_{i \in I_0(\bar{x})} \{\max\{\nabla \hat{g}_i(\bar{x}; \epsilon)^\top d, 0\}\} \sum_{i \in I_0(\bar{x})} \bar{\lambda}_i \\ &\leq \max_{i \in I_0(\bar{x})} \{\max\{\nabla \hat{g}_i(\bar{x}; \epsilon)^\top d, 0\}\} m\Lambda, \end{aligned}$$

so that we can say that \bar{x} is a critical point of problem (4) for all $\epsilon \in (0, \epsilon^*]$, where $\epsilon^* = 1/m\Lambda$.

Proof of Proposition 5. The proof follows by considering Propositions 3 and 13 and [8, 9]. \square

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