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A NOTE ON THE USAGE OF NONDIFFERENTIABLE EXACT PENALTIES IN SOME SPECIAL OPTIMIZATION PROBLEMS

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The usage of exact nondifferentable penalties for the numerical solution of optimization problems with a special constraint structure is recommended. Vectors from generalized gradients of appropriate objectives are computed so that effective nondifferentiable minimization methods can be applied.

1. INTRODUCTION

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Based on the connection of an exact penalization technique with nondifferentiable optimization (NDO) methods we propose a numerical approach for the treatment of special inequality constraints involving min-terms.

In the next section we study constraints of the form

(1.1)
$$\psi(x, y) = f_2(x, y) - \min_{s \in \Omega} f_2(x, s) \le 0,$$

where $f_2[\mathbb{R}^n \times \mathbb{R}^m \to \mathbb{R}]$ is continuously differentiable with respect to x, convex continuous with respect to y and $\nabla_x f_2$ is continuous on $\mathbb{R}^n \times \mathbb{R}^m$. $\Omega \subset \mathbb{R}^m$ is assumed to be nonempty, convex and compact. Such constraints arise if we solve optimization problems of the form

(1.2)
$$f_1(x, y) \to \inf$$
 subj. to

(1.3)
$$y \in \underset{s \in \Omega}{\operatorname{argmin}} f_2(x, s)$$

and replace relation (1.3) by the optimality condition

(1.4)
$$\psi(x, y) \leq 0, \quad y \in \Omega$$

Problems (1.2)-(1.3) are termed Stackelberg problems and occur frequently in economic modelling or optimum design problems, cf. [2], [6].

Section 3 is devoted to constraints of the form

(1.5)
$$\beta(x) = \min_{i=1,...,m} \{q^i(x)\} \le 0$$

(1.6)
$$\tilde{\beta}(x) = \min Q(x, s) \leq 0,$$

where functions $q^{i}[\mathbb{R}^{n} \to \mathbb{R}]$, i = 1, 2, ..., m, are continuously differentiable on \mathbb{R}^{n} , function $Q[\mathbb{R}^{n} \times \mathbb{R}^{m} \to \mathbb{R}]$ is continuously differentiable on $\mathbb{R}^{n} \times \mathbb{R}^{m}$ and convex with respect to s and $\varkappa \subset \mathbb{R}^{m}$ is nonempty, convex and compact. Constraints of the type (1.5) arise mostly due to a combinatorial structure in the problem in question. Semi-infinite constraint (1.6) may appear in some CAD problems or special control problems.

For the understanding of the paper a certain basic knowledge of nonsmooth analysis is required. We refer the reader to Chapter 2 of [1]. The following notation is employed:

 $\partial f(x)$ is the generalized gradient of a function f at x, $\partial_x f(x, y)$ is the partial generalized gradient with respect to x, for an $\alpha \in \mathbb{R}$ (α)⁺ = max {0, α }, \mathbb{R}^n_+ is the nonnegative orthant of \mathbb{R}^n , x^j is the *j*th coordinate of a vector $x \in \mathbb{R}^n$ and E is the unit matrix.

2. STACKELBERG PROBLEMS

We will assume that in problem (1.2)-(1.3) the function $f_1[\mathbb{R}^n \times \mathbb{R}^m \to \mathbb{R}]$ is regular (in the sense of Clarke), locally Lipschitz on $\mathbb{R}^n \times \mathbb{R}^m$ and

(2.1)
$$\Omega = \{ y \in \mathbb{R}^m \mid \Phi^i(y) \le 0, \ i = 1, 2, ..., k \}$$

where the functions $\Phi^{i}[\mathbb{R}^{m} \to \mathbb{R}]$ are convex continuous. Under the assumptions being imposed (cf. [1]) ψ is locally Lipschitz. The inner optimization problem $\min_{s\in\Omega} f_{2}(x, s)$ possesses a solution so that constraints (1.4) are consistent. Hence, the existence of a solution (\hat{x}, \hat{y}) of problem (1.2) - (1.3) may be guaranteed by some coercivity assumption on f_{1} with respect to x or by adding an additional constraint

$$(2.2) x \in \omega \subset \mathbb{R}^n,$$

where ω is nonempty and compact. Throughout this section it is assumed that a solution (\hat{x}, \hat{y}) exists.

Let us assume that the rewritten problem

(2.3)
$$f_1(x, y) \to \inf$$
$$\text{subj. to}$$
$$\psi(x, y) \leq 0, \quad y \in \Omega$$

is calm at its solution (\hat{x}, \hat{y}) with respect to vertical perturbations of the constraint $\psi(x, y) \leq 0$. Then it has been proved in [1] that there exists a positive scalar r_0

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or

such that for $r \ge r_0$ the function

(2.4)
$$\Theta = f_1 + r(\psi)^{-1}$$

attains its minimum over $\mathbb{R}^n \times \Omega$ at (\hat{x}, \hat{y}) . Hence, we may solve instead of (1.2)–(1.3) the augmented problem

(2.5)
$$\Theta(x, y) \to \mathrm{mf}$$

 $y \in \Omega$

with a suitably chosen penalty parameter r > 0. Θ is nondifferentiable so that for its numerical solution an NDO method is needed. Then, under the appropriate calmness assumption with respect to vertical perturbations of constraints $\Phi^i(x) \leq 0$, i = 1, 2, ..., k, we may handle also the constraint $y \in \Omega$ by the same technique, arriving thus at the unconstrained minimization problem

(2.6)
$$\widetilde{\Theta}(x, y) = f_1(x, y) + r(\psi(x, y))^+ + \sum_{i=1}^{n} r_i(\Phi^i(y))^+ \to \inf_{i=1}^{n} f_i(y)$$
$$(x, y) \in \mathbb{R}^n \times \mathbb{R}^m,$$

where r_i , i = 1, 2, ..., k, are positive penalty parameters. The objective $\tilde{\Theta}$ is locally Lipschitz and directionally derivable; hence the chance for a successful implementation of an NDO routine is satisfactory. However, if we want to use a bundle or subgradient algorithm, we must be able to compute at any pair (x, y) one arbitrary vector from $\partial \tilde{\Theta}(x, y)$.

Proposition 2.1. Θ is regular on $\mathbb{R}^n \times \mathbb{R}^m$ and one has

(2.7)
$$\begin{bmatrix} \xi \\ \eta \end{bmatrix} + r \begin{bmatrix} \nabla_x f_2(x, y) & -\nabla_x f_2(x, z) \\ \mu \end{bmatrix} \in \partial \Theta(x, y)$$

provided $(\xi, \eta) \in \partial f_1(x, y)$, $z \in \arg \min_{s \in \Omega} f_2(x, s)$, $\mu \in \partial_y f_2(x, y)$ and $\psi(x, y) \ge 0$. If $\psi(x, y) \le 0$, then

$$\begin{bmatrix} \xi \\ \eta \end{bmatrix} \in \partial \Theta(x, y)$$

 $g \circ \psi$ is regular and

Proof. $\Theta = f_1 + rg \circ \psi$, where $g = (\cdot)^+$. f_1 is regular by assumption and $\psi(x, y) = f_2(x, y) + \sup_{s\in\Omega} (-f_2(x, s))$ so that it is also regular due to the assumptions being imposed, cf. Th. 2.8.2 of [1]. For any $\alpha \in \mathbb{R}$ $\partial g(\alpha) \subset \mathbb{R}_+$ which implies that

$$\gamma \begin{bmatrix} \lambda \\ \gamma \end{bmatrix} \in \partial(g \circ \psi)(x, y),$$

whenever $\gamma \in \partial g(\psi(x, y))$ and $(\lambda, \gamma) \in \partial \psi(x, y)$ because of Chain Rule I of Clarke. λ may be computed according to Cor. 2 of the above mentioned Th. 2.8.2, meanwhile the computation of v and γ is trivial. The assertion has been proved.

The same argumentation implies also the regularity of penalty terms $(\Phi^i(y))^+$, i = 1, 2, ..., k, and the validity of relations

(2.9) $\vartheta_i \in \partial((\Phi^i(y))^+),$

where

$$\begin{split} \vartheta_i &\in \; \partial \Phi^i(y) \quad \text{if} \quad \Phi^i(y) > 0 \\ \vartheta_i &= 0 \qquad \text{if} \quad \Phi^i(y) \leq 0 \;, \quad i = 1, 2, \dots, k \end{split}$$

All terms of $\tilde{\Theta}$ are regular functions and hence the desired gradient information for a bundle or subgradient algorithm can be obtained by summing up a vector from $\partial \Theta$ computed according to Proposition 2.1 with a vector

$$\begin{bmatrix} 0\\ \sum_{i=1}^{k} r_i \vartheta_i \end{bmatrix}$$

 ϑ_i being given by (2.9). Of course, the solution z of the inner optimization problem must be sufficiently precise, otherwise the NDO algorithm could fail.

This approach was used to solve the three following simple test examples. In all of them $x \in \mathbb{R}$, $y \in \mathbb{R}^2$, $f_1 = \frac{1}{2}[(y^1 - 3)^2 + (y^2 - 4)^2]$, $\Omega = \{(y^1, y^2) \in \mathbb{R}^2_+ | -0.333y^1 + y^2 \leq 2, y^1 - 0.333y^2 \leq 2\}$ and

$$f_2 = \frac{1}{2} \langle y, H(x) y \rangle - \langle b(x), y \rangle, b(x) = \begin{bmatrix} 1 + 1 \cdot 333x \\ x \end{bmatrix},$$

where the $[2 \times 2]$ matrix H(x) varies.

Example 1.

$$H(x) = E \; .$$
 Starting point: $x = y^1 = y^2 = 0 \; .$ Solution: $x = 2 \cdot 07$, $y^1 = 3$, $y^2 = 3$, $f_1 = 0 \cdot 5 \; .$

Example 2.

 $H(x) = \begin{bmatrix} 1 + x & 0 \\ 0 & 0 \end{bmatrix}$ Starting point: x = 5, $y^1 = y^2 = 0$. Solution: x = 0, $y^1 = 3$, $y^2 = 3$, $f_1 = 0.5$.

Example 3.

$$H(x) = \begin{bmatrix} 1 + x & 0 \\ 0 & 1 + 0.1x \end{bmatrix}$$

Starting point: $x = y^1 = y^2 = 0$.
Solution: $x = 3.456$, $y^1 = 1.707$, $y^2 = 2.569$, $f_1 = 1.859$

All examples have been solved by means of the code M1FC1 written by Cl. Lemaréchal according to the bundle method [4]. The inner quadratic programming problems have been solved by the SOL/QPSOL code of Gill and al.

3. COMBINATORIAL INEQUALITY CONSTRAINTS

Let us investigate the optimization problem

(3.1)
$$f_0(x) \to \inf$$

subj. to $\beta(x) \le 0$, $x \in \Omega$,

where $f_0[\mathbb{R}^n \to \mathbb{R}]$ is continuously differentiable on \mathbb{R}^n , β is given by (1.5) and $\Omega \subset \mathbb{R}^n$ is nonempty, convex and compact. As function q^i , i = 1, 2, ..., m, are continuously differentiable, β is locally Lipschitz and hence problem (3.1) possesses a solution \hat{x} whenever

$$\{x \in \Omega \mid \beta(x) \le 0\} \neq \emptyset.$$

We will assume that relation (3.2) holds and problem (3.1) is calm at \hat{x} with respect to vertical perturbations of the constraint $\beta(x) \leq 0$. Then, as in Section 2, we may conclude that \hat{x} provides a minimum of the function

$$(3.3) \qquad \qquad \Xi = f_0 + r(\beta)^+$$

over Ω , whenever the penalty parameter r > 0 is sufficiently large. The calmness property can be ensured e.g. by using the generalized Mangasarian-Fromowitz constraint qualification, cf. [1]. The augmented objective Ξ is clearly locally Lipschitz and semismooth (cf. [5]) so that a bundle or subgradient algorithm may be applied to the problem $\Xi(x) \rightarrow \inf$

$$x \in \Omega$$
,

provided the constraint $x \in \Omega$ can be handled directly within the used minimization routine. The vectors from $\partial \Xi(x)$ may be computed according to the following assertion.

Proposition 3.1. Let $x \in \mathbb{R}^n$, $\beta(x) > 0$ and $i \in I(x) = \{i \in \{1, 2, ..., m\} \mid q^i(x) = \beta(x)\}$. Then (3.5) $\nabla f_0(x) + r \nabla q^i(x) \in \partial \Xi(x)$. If $\beta(x) \leq 0$, then (3.6) $\nabla f_0(x) \in \partial \Xi(x)$.

Proof. $\Xi = f_0 + rg \circ \beta$, where $g = (\cdot)^+$. If $\beta(x) > 0$, then due to Chain Rule I of Clarke

$$\partial(g \circ \beta)(x) = \partial\beta(x) = -\partial(\max_{i=1,\dots,m} \{-q'(x)\}).$$

Hence, by Prop. 2.3.12 of $\begin{bmatrix} 1 \end{bmatrix}$ for $i \in I(x)$

$$\nabla q^i(x) \in \partial(g \circ \beta)(x)$$

so that relation (3.5) holds. If $\beta(x) \leq 0$, then x is a global minimizer of $g \circ \beta$ which implies relation (3.6).

Differently from function $(\psi)^+$ discussed in the previous section, function $(\beta)^+$ is nonregular (in the sense of Clarke). This is the reason why we require f_0 to be continuously differentiable; otherwise relations (3.5), (3.6) do not hold.

The structure of Ω is also important. If Ω consists merely of lower and upper bounds on single coordinates of x, e.g. the effective code M2FC1 of Cl. Lemaréchal written according to the bundle method [4] may be applied with the necessary gradient information being computed according to Proposition 3.1.

If, however, Ω is given by (2.1) and we use (under the appropriate calmness assumption) the same penalization technique to the constraints $\Phi^{i}(x) \leq 0$, i = 1, 2, ..., k, we may have difficulties with the computation of a vector from $\partial \vec{\Xi}$, where

(3.7)
$$\widetilde{\Xi} = \Xi + \sum_{i=1}^{k} r_i (\Phi^i)^+ ,$$

 r_i , i = 1, 2, ..., k, being some suitably chosen positive penalty parameters. $\tilde{\Xi}$ is locally Lipschitz and semismooth, but we do not know any computationally acceptable way of evaluating a vector $\xi \in \partial \tilde{\Xi}(x)$ provided

$$\beta(x) > 0 \, ,$$

cardinality of I(x) is greater than 1, and

$$\exists i \in \{1, 2, ..., k\}$$
 such that $\Phi^{i}(x) = 0$.

In all other situations one has

$$\xi = \xi_1 + \sum_{i=1}^k r_i \vartheta_i \in \partial \widetilde{\Xi}(x) ,$$

where $\xi_1 \in \partial \Xi(x)$ is computed according to (3.5), (3.6) and vectors ϑ_i , i = 1, 2, ..., k, are computed according to (2.9).

This obstacle will certainly not cause any difficulties in a majority of problems. If, however, some line-search difficulties occur, it might be due to a bad gradient information and we have then either to augment the constraints $\Phi^i(x) \leq 0$ by some smooth penalty or apply some algorithm of Kiwiel [3], capable of treating general inequality constraints within the nonsmooth minimization method.

If the constraint $\beta(x) \leq 0$ is replaced in (3.1) by the semi-infinite constraint $\tilde{\beta}(x) \leq 0$ with $\tilde{\beta}$ given by (1.6), then all the above considerations remain true, only Proposition 3.1 must be replaced by the following statement:

Proposition 3.2. Let $x \in \mathbb{R}^n$, $\tilde{\beta}(x) > 0$ and $R(x) = \{y \in \varkappa \mid Q(x, y) = \tilde{\beta}(x)\}$. Then, on denoting

(3.8) $\Lambda = f_0 + r(\tilde{\beta})^+, \quad r > 0,$

(3.9)
$$\nabla f_0(x) + r \nabla_x Q(x, z) \in \partial A(x)$$

provided $z \in R(x)$. If $\tilde{\beta}(x) \leq 0$, then

$$(3.10) \qquad \nabla f_0(x) \in \partial A(x)$$

The proof can be performed along the same lines as the proof of Prop. 3.1, but instead of Prop. 2.3.12 we have now to exploit Th. 2.8.2 of [1]. \Box

We conclude this section by an illustrative optimal control example. Let us consider the problem

$$F(x_m) + \sum_{i=0}^{m-1} \varphi_i(x_i, u_i) \to \inf$$

(3.11) subj. to $x_{i+1} = f_i(x_i, u_i), \quad i = 0, 1, ..., m-1, \quad x_0 = a, \quad u_i \in \omega \subset \mathbb{R}^k,$

$$\max_{i=1,\dots,m} x_i^1 \ge L$$

where $x = (x_1, x_2, ..., x_m) \in \mathbb{R}^{n \times m}$ is the trajectory, $u = (u_0, u_1, ..., u_{m-1}) \in \mathbb{R}^{k \times m}$ is the control, ω is the set of admissible controls, $a \in \mathbb{R}^n$ is a given initial state and the functions $F[\mathbb{R}^n \to \mathbb{R}]$, $\varphi_i[\mathbb{R}^n \times \mathbb{R}^k \to \mathbb{R}]$, $f_i[\mathbb{R}^n \times \mathbb{R}^k \to \mathbb{R}^n]$, i = 0, 1, ..., m - 1, are supposed to be continuously differentiable. The inequality (3.12) expresses the requirement that the first coordinate x_i^1 must be at some *i* greater or equal to the given scalar *L*.

Remark. If x is a discretized trajectory of a rocket, we may require that a certain prescribed altitude must be achieved. If x^1 represents the temperature measured at a given point of a heated object, condition (3.12) means that during the heating a certain prescribed temperature must be reached.

If we denote by S_i the operator which assigns to each control $u \in \mathbb{R}^{k \times m}$ the state $x_{i+1} \in \mathbb{R}^n$, corresponding to u with respect to the system equation, the problem (3.11)-(3.12) may be written in the form

$$J(u) = F \circ S_{m-1}(u) + \varphi_0(a, u_0) + \sum_{i=1}^{n} \varphi_i(S_{i-1}(u), (u_i)) \to \inf$$
(3.13) subj. to $u_i \in \omega, \quad i = 0, 1, ..., m - 1$

$$\min_{\substack{i=1,...,m}} \{L - (S_{i-1}(u))^1\} \leq 0.$$

Problem (3.13) is exactly of the type (3.1). Proposition 3.1, the assumptions of which are here clearly satisfied, implies the following assertion:

Proposition 3.3. Let u be an admissible control, x be the corresponding trajectory and $I(u) = \{i \in \{1, 2, ..., m\} \mid x_i^1 = \max_{\substack{j=1,...,m}} x_j^1\}.$

Assume that

$$\Xi(u) = J(u) + r (\min_{i=1,...,m} \{L - x_{i}^{1}\})^{+}$$

is the augmented objective with a suitably chosen penalty parameter r > 0. Finally, let $(p_1, p_2, ..., p_m) \in \mathbb{R}^{n \times m}$ be the solution of the adjoint equation

$$(3.14) \quad p_i = \left[\nabla_{x_i} f_i(x_i, u_i)\right]^{\mathrm{T}} p_{i+1} - \nabla_{x_i} \varphi_i(x_i, u_i), \quad i = 1, 2, ..., m-1,$$

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with the terminal condition

$$p_m = -\nabla F(x_m)$$

Then $(v_0, v_1, \ldots, v_{m-1}) \in \partial \Xi(u)$ if

(3.15) $v_i = \nabla_{u_i} \varphi_i(x_i, u_i) - [\nabla_{u_i} f_i(x_i, u_i)]^T p_{i+1}, \quad i = 0, 1, ..., m-1$ and there exists a $j \in \{1, 2, ..., m\}$ such that $x_j^1 \ge L$. If $x_i^1 < L$ for all i = 1, 2, ..., m, then formula (3.15) remains true provided we replace the adjoint equation (3.14) at some $i \in I(u)$ by the equation

$$p_i = \left[\nabla_{x_i} f_i(x_i, u_i)\right]^{\mathrm{T}} p_{i+1} - \nabla_{x_i} \varphi_i(x_i, u_i) + \xi,$$

 $\boldsymbol{\xi} = (r, 0, 0, \dots, 0)^{\mathrm{T}} \in \mathbb{R}^{n}.$

In the proof we just need to combine Proposition 3.1 with the standard way of constructing the adjoint equations. Thus, combinatorial optimal control problems of the type (3.11)-(3.12) can easily be solved by the proposed approach provided the appropriate calmness assumption holds.

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