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2001

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Technical report No. 844

September 2001

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Abstract

In this paper we propose an algorithm for solving nonlinear nonconvex programming problems which is based on the nonsmooth equation approach. This Algorithm was implemented in the interactive system for universal functional optimization UFO. Results of numerical experiments are reported.

Keywords

Nonlinear programming, nonsmooth analysis, semismooth equations, KKT systems, algorithms

[1] Work supported by grant GA ČR 201/00/0080.

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NONSMOOTH EQUATION METHOD FOR NONLINEAR NONCONVEX OPTIMIZATION [3]

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1 Introduction

In this contribution, we are concerned with a general nonlinear programming problem:

(NP): Find the minimum of function $f(x)$ on the set given by constraints $c_I(x) \leq 0$ and $c_E(x) = 0$, where $f : R^n \to R$, $c_I : R^n \to R^{m_I}$ and $c_E : R^n \to R^{m_E}$ are twice continuously differentiable mappings ($c_I \leq 0$ is considered by elements) and $I = \{1, \ldots, m_I\}$, $E = \{m_I + 1, \ldots, m_I + m_E\}$.

Necessary conditions (the KKT - conditions) for the solution of problem (NP) (if gradients of active constraints are linearly independent) have the following form

$$\begin{aligned} g(x,u) &= 0, \\ c_I(x) &\leq 0, \quad u_I \geq 0, \quad U_I C_I(x) e = 0, \\ c_E(x) &= 0, \end{aligned} \tag{1.1}$$

where

$$g(x,u) = \nabla f(x) + \sum_{i \in I} u_i \nabla c_i(x) + \sum_{i \in E} u_i \nabla c_i(x) = \nabla f(x) + A_I(x) u_I + A_E(x) u_E$$

and $A_I(x) = [\nabla c_i(x) : i \in I]$, $A_E(x) = [\nabla c_i(x) : i \in E]$. Here $u_I \in R^{m_I}$, $u_E \in R^{m_E}$ are vectors of Lagrange multipliers, $U_I = \mathrm{diag}(u_i : i \in I)$, $C_I(x) = \mathrm{diag}(c_i(x) : i \in I)$ and e is the vector with unit elements.

The second set of conditions in (1.1), so called complementarity conditions, can be transformed to equations using the Fischer-Burmeister function $\psi(a,b) = \sqrt{a^2 + b^2} - (a+b)$, which is zero if and only if $a \geq 0$, $b \geq 0$ and $ab = 0$. Therefore, complementarity conditions are satisfied if and only if $\psi(u_i, -c_i(x)) = 0$, $i \in I$ and (1.1) can be replaced by the nonlinear system

$$\begin{aligned} g(x,u) &= 0, \\ \psi_I(u_I, -c_I(x)) &= 0, \\ c_E(x) &= 0, \end{aligned} \tag{1.2}$$

where $\psi_I(u_I, -c_I(x)) = [\psi(u_i, -c_i(x)) : i \in I]^T$.

The Fischer-Burmeister function $\psi(a,b)$ is continuously differentiable at a point where $|a| + |b| \neq 0$ and is semismooth if $|a| + |b| = 0$. Moreover, function $\psi^2(a,b)$ is

[3] This work was supported by grant GAČR No. 201/00/0080

continuously differentiable everywhere [2]. Therefore, (1.2) is a system of semismooth equations, which can be solved by the Newton method [10], [2], [8]. The gradient and the Clarke subdifferential of the Fischer-Burmeister function are given by formulas

$$\nabla\psi(a,b) = \begin{bmatrix} \frac{a}{\sqrt{a^2+b^2}} - 1 \\ \frac{b}{\sqrt{a^2+b^2}} - 1 \end{bmatrix}, \quad |a| + |b| \neq 0, \tag{1.3}$$

$$\partial\psi(0,0) = \operatorname{conv} \bigcup_{\phi\in[0,2\pi]} \begin{bmatrix} \cos\phi - 1 \\ \sin\phi - 1 \end{bmatrix}. \tag{1.4}$$

Formula (1.4) implies that $[-1,-1]^T \in \partial\psi(0,0)$. Therefore, setting $r(a,b) = \sqrt{a^2+b^2}$ for $|a| + |b| \neq 0$ and $r(a,b) = 1$ for $|a| + |b| = 0$ we obtain

$$\begin{bmatrix} \frac{a}{r(a,b)} - 1 \\ \frac{b}{r(a,b)} - 1 \end{bmatrix} \in \partial\psi(a,b). \tag{1.5}$$

Linearizing system (1.2) by using (1.5), we obtain a step of the Newton method

$$\begin{bmatrix} G & A_I & A_E \\ (R_I + C_I)R_I^{-1}A_I^T & -(R_I - U_I)R_I^{-1} & 0 \\ A_E^T & 0 & 0 \end{bmatrix} \begin{bmatrix} \Delta x \\ \Delta u_I \\ \Delta u_E \end{bmatrix} = - \begin{bmatrix} g \\ \psi_I \\ c_E \end{bmatrix}, \tag{1.6}$$

where

$$G = G(x,u) = \nabla^2 f(x) + \sum_{i\in I} u_i \nabla^2 c_i(x) + \sum_{i\in E} u_i \nabla^2 c_i(x),$$

$A_I = A_I(x)$, $A_E = A_E(x)$, $C_I = C_I(x)$, $U_I = U_I(x)$, $R_I = \operatorname{diag}(r(u_i, -c_i(x)) : i \in I)$, $g = g(x,u)$, $\psi_I = \psi_I(u_I, -c_I(x))$ and $c_E = c_E(x)$. Note that linear system (1.6) is not suitable for iterative solvers in general since it is nonsymmetric and can have unsuitable diagonal elements. Therefore, an equivalent system is constructed and solved as is shown in Section 2.

The algorithm of a nonsmooth equation method can be roughly described in the following form. For given vectors $x \in R^n$, $u_I \in R^{m_I}$, $u_E \in R^{m_E}$ we determine direction vectors Δx, Δu_I, Δu_E by solving linear system equivalent to (1.6). Furthermore, we choose step-length $\alpha > 0$ and set $x := x + \alpha\Delta x$, $u_I := u_I + \alpha\Delta u_I$, $u_E := u_E + \alpha\Delta u_E$. Individual parts of the algorithm require more detailed explanation.

The use of the Fisher-Burmeister function for solving dense medium-size nonlinear programming problems is studied theoretically in [3] and [4]. Unfortunately, no computational experiments are presented. The aim of this paper is an application of the nonsmooth equation approach to the solution of large sparse problems and, especially, the use of the indefinitely preconditioned conjugate gradient method in this case.

2 Direction determination

System (1.6) is nonsymmetric with the dimension $n + m_I + m_E$. This system can be symmetrized by the multiplication of a diagonal matrix and reduced by the elimination of inactive constraints. In the subsequent text, we use the simplified notation $c_i = c_i(x)$, $r_i = r(u_i, -c_i(x))$, $\psi_i = \psi(u_i, -c_i(x)) = r_i - (u_i - c_i)$ so $\partial\psi_i/\partial u_i = (u_i - r_i)/r_i$, $\partial\psi_i/\partial c_i = (c_i + r_i)/r_i$.

Definition 1. *Let $0 < \varepsilon_0 < 1/2$. We say that the constraint with index $i \in I$ is active, if*

$$-\partial\psi_i/\partial u_i \le \varepsilon_0 \partial\psi_i/\partial c_i, \tag{2.1}$$

which can be written in the form

$$r_i - u_i \le \varepsilon_0 (r_i + c_i). \tag{2.2}$$

Lemma 1. *Let the constraint with index $i \in I$ be active. Then $u_i > 0$ and $(4/5)\varepsilon_0 < (r_i + c_i)/r_i \le 2$. Furthermore, there are numbers ε_1 and ε_2 such that the constraint with index $i \in I$ is active if $u_i > 0$ and $|c_i| \le \varepsilon_1 u_i$ and inactive if $u_i \le 0$ or $|c_i| > \varepsilon_2 u_i$.*

Proof. (a) Obviously, $0 \le (r_i - u_i)/r_i \le 2$ and $0 \le (r_i + c_i)/r_i \le 2$. Assume that $u_i \le 0$. Then $(r_i - u_i)/r_i \ge 1$ which together with the previous inequalities implies $(r_i - u_i)/(r_i + c_i) = ((r_i - u_i)/r_i)(r_i/(r_i + c_i)) \ge 1/2$, which is in contradiction with (2.2), since $\varepsilon_0 < 1/2$. Using (1.5), we obtain

$$(1 - \partial\psi_i/\partial c_i)^2 + (1 + \partial\psi_i/\partial u_i)^2 = \frac{c_i^2 + u_i^2}{r_i^2} = 1 \tag{2.3}$$

so $\partial\psi_i/\partial c_i$ and $-\partial\psi_i/\partial u_i$ lie on the unit circle centred at point $[1, 1]$. If the constraint with index $i \in I$ is active, then (2.2) implies that $-\partial\psi_i/\partial u_i$ lies under the line defined by (2.1) (with equality), see Fig. 1.

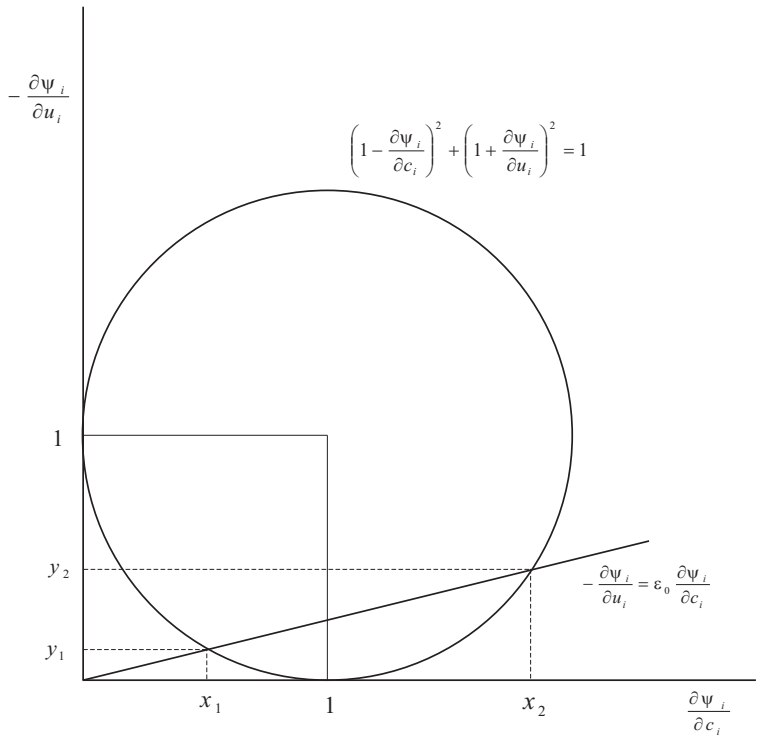

Fig. 1

Denote by (x_1, y_1) and (x_2, y_2) intersections of the circle (2.3) and the line defined by (2.1) (with $x_1 \le x_2$). Then $y = \varepsilon_0 x$ and

$$(1+\varepsilon_0^2)x^2 - 2(1+\varepsilon_0)x + 1 = 0.$$

If the constraint with index $i \in I$ is active, then

$$\frac{\partial \psi_i}{\partial c_i} \ge x_1 = \frac{1+\varepsilon_0 - \sqrt{2\varepsilon_0}}{1+\varepsilon_0^2} > \frac{4}{5}\varepsilon_0$$

(we used the inequality $\varepsilon_0 < 1/2$).
(b) Obviously, $y_1 = \varepsilon_0 x_1 > 0$. Furthermore, (2.3) implies $x_2 \le 2$, which gives $y_2 = \varepsilon_0 x_2 < 1$. If $-\partial\psi_i/\partial u_i \le y_1$, then (2.1) holds and the constraint with index $i \in I$ is active and if $-\partial\psi_i/\partial u_i > y_2$, then (2.1) cannot hold and the constraint with index $i \in I$ is inactive. We have proved above that the constraint with index $i \in I$ is inactive when $u_i \le 0$. Assuming $u_i > 0$, we can write

$$-\frac{\partial \psi_i}{\partial u_i} = 1 - \frac{u_i}{\sqrt{u_i^2 + c_i^2}} = 1 - \frac{1}{\sqrt{1+\lambda_i^2}}, \tag{2.4}$$

where $\lambda_i = |c_i|/u_i$, $i \in I$. Since the function on the right hand side of (2.4) is increasing (with the value 0 for $\lambda_i = 0$ and the limit 1 for $\lambda_i \to \infty$), there are numbers ε_1 and ε_2 such that $-\partial\psi_i/\partial u_i \le y_1$ if $|c_i|/u_i \le \varepsilon_1$ and $-\partial\psi_i/\partial u_i > y_2$ if $|c_i|/u_i > \varepsilon_2$. □

Theorem 1. *Let the pair $x^* \in R^n$ and $u_I^* \in R^{m_I}$ solve (1.1) and the strict complementarity conditions $u_i^* + |c_i(x^*)| > 0$ $\forall i \in I$ hold. Then there exist neighborhoods $\mathcal{N} \subset R^n$ and $\mathcal{M}_I \subset R^{m_I}$ of x^* and u_I^* such that the constraint with index $i \in I$ is active when $c_i(x^*) = 0$ and inactive when $u_i^* = 0$ whenever $x \in \mathcal{N}$ and $u_I \in \mathcal{M}_I$. Moreover, if $x \to x^*$ and $u_I \to u_I^*$, then $(r_i - u_i)/(r_i + c_i) \to 0$ for all active constraints and $(r_i - u_i)/(r_i + c_i) \to \infty$ for all inactive constraints.*

Proof. Let $u_i^* > 0$. Since $c_i(x^*) = 0$ and function $c_i(x)$ is continuous, there exist neighbourhoods $\mathcal{N}_i \subset R^n$ of x^* and $\mathcal{M}_i \subset R$ of u_i^* such that $u_i > u_i^*/2$ if $u_i \in \mathcal{M}_i$ and $|c_i(x)| < \varepsilon_1 u_i^*/2$ if $x \in \mathcal{N}_i$ so the constraint with index $i \in I$ is active by Lemma 1. Let $u_i^* = 0$. Since $c_i(x^*) < 0$ and function $c_i(x)$ is continuous, there exist neighbourhoods $\mathcal{N}_i \subset R^n$ of x^* and $\mathcal{M}_i \subset R$ of u_i^* such that $|c_i(x)| > |c_i(x^*)|/2$ if $x \in \mathcal{N}_i$ and $u_i < |c_i(x^*)|/(2\varepsilon_2)$ if $u_i \in \mathcal{M}_i$ so the constraint with index $i \in I$ is inactive by Lemma 1. If we set $\mathcal{N} = \cap_{i\in I}\mathcal{N}_i$ and put $\mathcal{M}_I$ equal to the Cartesian product of $\mathcal{M}_i$, $i \in I$, then the constraint with index $i \in I$ is active if $c_i(x^*) = 0$ and inactive if $u_i^* = 0$ whenever $x \in \mathcal{N}$ and $u_I \in \mathcal{M}_I$. Moreover, if $x \to x^*$ and $u_I \to u_I^*$, then $u_i \to u_i^* > 0$ and $c_i \to 0$ for all active constraints, implying $r_i \to u_i^*$ and $(r_i - u_i)/(r_i + c_i) \to 0$. Similarly, $u_i \to 0$ and $c_i \to c_i(x^*) < 0$ for all inactive constraints, implying $r_i \to |c_i(x^*)|$ and $(r_i - u_i)/(r_i + c_i) \to \infty$. □

Let us denote active quantities by $\hat{u}_i$, $\hat{c}_i$, $\hat{r}_i$, $\hat{\psi}_i$ and inactive quantities by $\check{u}_i$, $\check{c}_i$, $\check{r}_i$, $\check{\psi}_i$. Eliminating equations corresponding to inactive quantities from (1.6), we obtain

$$\Delta\check{u}_I = \check{M}_I^{-1}\left[(\check{R}_I + \check{C}_I)^{-1}\check{R}_I\check{\psi}_I + \check{A}_I^T\Delta x\right], \tag{2.5}$$

where $\check{M}_I = (\check{R}_I + \check{C}_I)^{-1}(\check{R}_I - \check{U}_I)$ and

$$\begin{bmatrix} \hat{G} & \hat{A}_I & A_E \\ \hat{A}_I^T & -\hat{M}_I & 0 \\ A_E^T & 0 & 0 \end{bmatrix} \begin{bmatrix} \Delta x \\ \Delta \hat{u}_I \\ \Delta u_E \end{bmatrix} = - \begin{bmatrix} \hat{g} \\ (\hat{R}_I + \hat{C}_I)^{-1}\hat{R}_I\hat{\psi}_I \\ c_E \end{bmatrix}, \tag{2.6}$$

where $\hat{M}_I = (\hat{R}_I + \hat{C}_I)^{-1}(\hat{R}_I - \hat{U}_I)$ and

$$\begin{aligned} \hat{G} &= G + \check{A}_I\check{M}_I^{-1}\check{A}_I^T, \\ \hat{g} &= g + \check{A}_I\check{M}_I^{-1}(\check{R}_I + \check{C}_I)^{-1}\check{R}_I\check{\psi}_I. \end{aligned}$$

Condition (2.2) guarantees that matrices $\hat{M}_I$ and $\check{M}_I^{-1}$ are bounded. Therefore also $\hat{G}$ is bounded (if G and A are bounded). Moreover, Theorem 1 insures that $\hat{M}_I \to 0$ if $x \to x^*$, $u_I \to u_I^*$ and the strict complementarity conditions hold at the solution point. The property $\hat{M}_I \to 0$ is very useful, since system (2.6) can be efficiently preconditioned by the way described in [5] if $\hat{M}_I$ has small elements. The second set of equations of (2.6) was obtained after multiplying corresponding set of equations of (1.6) by the diagonal matrix $(\hat{R}_I + \hat{C}_I)^{-1}\hat{R}_I$ whose elements lie in the bounded interval $[1/2, 5/(4\varepsilon_0)]$ by Lemma 1. If ε_0 has a reasonable value (usually $\varepsilon_0 = 1/10$), then this scaling does not influence the final inexact solution of (2.6).

Vector $\Delta\hat{u}_I$ is determined by solving system (2.6) and vector $\Delta\check{u}_I$ is computed from (2.5). System (2.6), which is symmetric and indefinite of order $n + \hat{m}_I + m_E$, can be solved either directly by using the sparse Bunch-Parlett decomposition or iteratively by using preconditioned Krylov-subspace methods for symmetric indefinite systems. Motivated by [5] and [7], we will investigate the preconditioner

$$C = \begin{bmatrix} \hat{D} & \hat{A}_I & A_E \\ \hat{A}_I^T & -\hat{M}_I & 0 \\ A_E^T & 0 & 0 \end{bmatrix}, \tag{2.7}$$

where $\hat{D}$ is a positive definite diagonal matrix derived from a diagonal of $\hat{G}$. Let us denote the matrix of system (2.6) by K. Then the following theorems are proved in [9].

Theorem 2. *Consider preconditioner (2.7) applied to system (2.6). Then matrix KC^{-1} has at least $\hat{m}_I + 2m_E$ unit eigenvalues but, if $\hat{G} - \hat{D}$ is nonsingular (the usual case), then at most $\hat{m}_I + m_E$ linearly independent eigenvectors corresponding to these eigenvalues exist. The other eigenvalues of matrix KC^{-1} are exactly eigenvalues of matrix $Z_E^T\tilde{G}Z_E(Z_E^T\tilde{D}Z_E)^{-1}$, where $[Z_E, A_E]$ is a nonsingular square matrix, $Z_E^TA_E = 0$, $Z_E^TZ_E = I$ and where $\tilde{G} = \hat{G} + \hat{A}_I\hat{M}_I^{-1}\hat{A}_I^T$, $\tilde{D} = \hat{D} + \hat{A}_I\hat{M}_I^{-1}\hat{A}_I^T$. If $Z_E^T\tilde{G}Z_E$ is positive definite then all eigenvalues are positive.*

Theorem 3. *Consider preconditioner (2.7) applied to system (2.6) and assume that $\hat{G} - \hat{D}$ is nonsingular. Then Krylov subspace $\mathcal{K} = \mathrm{span}\{\bar{r}, KC^{-1}\bar{r}, (KC^{-1})^2\bar{r}, \ldots\}$, where $\bar{r} \in R^{n+\hat{m}_I+m_E}$, has a dimension of at most $\min(n+1, n-m_E+2)$.*

Theorem 4. *Consider conjugate gradient method with preconditioner (2.7) applied to system (2.6). Assume that initial estimation of the solution is chosen in such a way that $\hat{h}_I = 0$ and $h_e = 0$ at the start of the algorithm (h_x, $\hat{h}_I$ and h_E are parts of the residual vector). Let matrix $Z_E^T \tilde{G} Z_E$ be positive definite. Then:*

(a) Vector $\Delta^* x$ (the first part of the solution) is found after $n - m_E$ iterations at most.

(b) The algorithm cannot break down before $\Delta^* x$ is found.

(c) Error $\|\Delta x - \Delta^* x\|$ converges to zero at least R - linearly with quotient

$$\frac{\sqrt{\kappa} - 1}{\sqrt{\kappa} + 1},$$

where κ is the spectral condition number of matrix $Z_E^T \tilde{G} Z_E (Z_E^T \tilde{D} Z_E)^{-1}$.

(d) If $\Delta x = \Delta^* x$, then also $\Delta \hat{u}_I = \Delta^* \hat{u}_I$ and $\Delta^* u_E$ can be determined by the formula

$$\Delta^* u_E = \Delta u_E + (A_E^T \tilde{D}^{-1} A_E)^{-1} A_E^T \tilde{D}^{-1} h_x.$$

Theorem 2 shows that the efficiency of a Krylov-subspace method preconditioned by (2.7) does not depend strongly on the choice of active and inactive variables (matrix $\tilde{G}$ is the same for every splitting). Nevertheless, the splitting significantly influences the resulting solution since the equations corresponding to inactive variables are solved precisely and only active variables are obtained by the inexact iterative process.

Although the Fisher-Burmeister function has good theoretical properties, we finally used the modified Fisher-Burmeister function in our algorithm, since it was more efficient in computational experiments. The modified Fisher-Burmeister function $\psi^\varepsilon(a,b) = \sqrt{a^2 + b^2 + \varepsilon^2} - (a+b)$, where ε is a sufficiently small positive number, is differentiable everywhere and $r = \sqrt{a^2 + b^2 + \varepsilon^2}$ is continuous at the origin. The following theorem characterizes inaccuracy, which appears in the complementarity conditions if the modified Fisher-Burmeister function is used.

Theorem 5. *Let $\psi^\varepsilon(a,b) = \delta$ and $|a| \le |b|$. Then*

$$\begin{aligned} |a| &\le 2|\delta| + \sqrt{|\varepsilon^2 - \delta^2|/2}, \\ |a||b| &\le \frac{1}{2}(\varepsilon + 3|\delta|) \max(|\varepsilon - \delta|, |a| + |b|). \end{aligned}$$

Proof. Let $\psi^\varepsilon(a,b) = \delta$. Then

$$\sqrt{a^2 + b^2 + \varepsilon^2} - a - b = \delta$$

so

$$a^2 + b^2 + \varepsilon^2 = (a + b + \delta)^2 = a^2 + b^2 + \delta^2 + 2ab + 2(a+b)\delta$$

or

$$2|a||b| \le |\varepsilon^2 - \delta^2| + 2(|a| + |b|)|\delta|. \tag{2.8}$$

This implies

$$2|a| \leq \frac{|\varepsilon^2 - \delta^2|}{|b|} + 2(\frac{|a|}{|b|} + 1)|\delta| \leq \frac{|\varepsilon^2 - \delta^2|}{|a|} + 4|\delta|,$$

so $|a|$ lies between roots of the quadratic equation $2|a|^2 - 4|a||\delta| - |\varepsilon^2 - \delta^2| = 0$ which have opposite signs. Therefore,

$$|a| \leq |\delta| + \frac{1}{2}\sqrt{4\delta^2 + 2|\varepsilon^2 - \delta^2|} \leq |\delta| + \frac{1}{2}(2|\delta| + \sqrt{2|\varepsilon^2 - \delta^2|}) = 2|\delta| + \sqrt{|\varepsilon^2 - \delta^2|/2}.$$

Using (2.8) again, we obtain

$$2|a||b| \leq |\varepsilon - \delta|(|\varepsilon| + |\delta|) + 2(|a| + |b|)|\delta|.$$

Substituting $\max(|\varepsilon - \delta|, |a| + |b|)$ for both $|\varepsilon - \delta|$ and $|a| + |b|$ we obtain the second assertion of the theorem. □

There are two important cases. First, if $\psi^\varepsilon(a, b) = 0$, then $\delta = 0$ and, therefore, $|a| \leq \varepsilon/\sqrt{2}$, $|a||b| \leq (\varepsilon/2)\max(\varepsilon, |a| + |b|)$. On the other hand, if $|\delta| = \varepsilon$ then $|a| \leq 2\varepsilon$, $|a||b| \leq 2\varepsilon(|a| + |b|)$.

The use of the modified Fisher-Burmeister function is advantageous, since the case when $|a| + |b| = 0$ is not exceptional. Moreover, the use of the basic Fisher-Burmeister function can lead to difficulties caused by computations in the finite precision arithmetic. We have tested both these possibilities and obtained better results with the modified Fisher-Burmeister function. Note that all equations used in this section hold for the modified Fisher-Burmeister function if we set $r_i = \sqrt{c_i^2 + u_i^2 + \varepsilon^2}$.

3 Step-length selection

Step-length $\alpha > 0$ can be determined in many ways. Basic requirement for the selection of step-length is the satisfying of a suitable goal criterion. This criterion is usually a merit function which is a combination of the objective function and a measure of constraint violation. Motivated by [5] and [7], we use the following merit function

$$\begin{aligned} P(\alpha) &= f(x + \alpha\Delta x) + (u_I + \Delta u_I)^T c_I(x + \alpha\Delta x) + (u_E + \Delta u_E)^T c_E(x + \alpha\Delta x) \\ &+ \frac{\sigma}{2}\|\psi_I(u_I + \alpha\Delta u_I, -c_I(x + \alpha\Delta x))\|^2 + \frac{\sigma}{2}\|c_E(x + \alpha\Delta x)\|^2, \end{aligned} \tag{3.1}$$

where $\sigma \geq 0$, which is a generalization of the merit function introduced in [5]. The following theorem holds.

Theorem 6. *Let Δx, $\hat{\Delta} u_I$, Δu_E be obtained by an inexact solution of (2.6) such that*

$$\begin{bmatrix} \hat{G} & \hat{A}_I & A_E \\ \hat{A}_I^T & -\hat{M}_I & 0 \\ A_E^T & 0 & 0 \end{bmatrix} \begin{bmatrix} \Delta x \\ \Delta \hat{u}_I \\ \Delta u_E \end{bmatrix} + \begin{bmatrix} \hat{g} \\ (\hat{R}_I + \hat{C}_I)^{-1}\hat{R}_I\hat{\psi}_I \\ c_E \end{bmatrix} = \begin{bmatrix} h_x \\ \hat{h}_I \\ h_E \end{bmatrix},$$

where h_x, $\hat{h}_I$, h_E are parts of the residual vector and let $\check{\Delta} u_I$ is given by (2.5). Then

$$\begin{aligned} P'(0) &= -(\Delta x)^T G \Delta x - \sigma\left(\|\psi_I\|^2 + \|c_E\|^2\right) \\ &+ (\Delta x)^T h_x + \sigma\left(\hat{\psi}_I^T(\hat{R}_I + \hat{C}_I)\hat{R}_I^{-1}\hat{h}_I + c_E^T h_E\right). \end{aligned} \tag{3.2}$$

If

$$\sigma > -\frac{(\Delta x)^T G \Delta x}{\|\psi_I\|^2 + \|c_E\|^2}, \tag{3.3}$$

and if (2.6) is solved with a sufficient precision, namely if

$$(\Delta x)^T h_x + \sigma \left(\hat{\psi}_I^T (\hat{R}_I + \hat{C}_I) \hat{R}_I^{-1} \hat{h}_I + c_E^T h_E \right) < (\Delta x)^T G \Delta x + \sigma \left(\|\psi_I\|^2 + \|c_E\|^2 \right), \tag{3.4}$$

then $P'(0) < 0$.

Proof. Differentiating (3.1) by α, we obtain

$$\begin{aligned} P'(0) &= (\Delta x)^T \left(\nabla f + A_I(u_I + \Delta u_I) + A_E(u_E + \Delta u_E) \right) \\ &+ \sigma \psi_I^T \left((R_I + C_I) R_I^{-1} A_I^T \Delta x - (R_I - U_I) R_I^{-1} \Delta u_I \right) + \sigma c_E^T A_E^T \Delta x. \end{aligned} \tag{3.5}$$

Using (2.5) and (2.6), we obtain equalities

$$(\Delta x)^T \left(\nabla f + A_I(u_I + \Delta u_I) + A_E(u_E + \Delta u_E) \right) = -(\Delta x)^T G \Delta x + (\Delta x)^T h_x,$$

$$\psi_I^T \left((R_I + C_I) R_I^{-1} A_I^T \Delta x - (R_I - U_I) R_I^{-1} \Delta u_I \right) = -\|\psi_I\|^2 + \hat{\psi}_I^T (\hat{R}_I + \hat{C}_I) \hat{R}_I^{-1} \hat{h}_I,$$

$$c_E^T A_E^T \Delta x = -\|c_E\|^2 + c_E^T h_E,$$

which after substituting into (3.5) give (3.2). If (3.3) holds, then the right-hand side of (3.4) is positive so if (2.6) is solved with a sufficient precision, then (3.4) holds and $P'(0) < 0$ by (3.2). □

Condition (3.3) restricts the choice of parameter σ weakly. If matrix G is positive semidefinite, any value $\sigma \geq 0$ satisfies this condition. Inequality (3.4) gives one possibility for the computation of parameter σ, which implies the inequality $P'(0) < 0$. But it is usually more efficient for practical computation to choose parameter σ as a constant and replace matrix G by some positive definite diagonal matrix if condition $P'(0) < 0$ does not hold.

To improve local convergence properties of the method, we can use another merit function

$$\begin{aligned} Q(\alpha) &= \frac{1}{2} \|g(x + \alpha \Delta x, u_I + \alpha \Delta u_I, u_E + \alpha \Delta u_E)\|^2 \\ &+ \frac{1}{2} \|\psi_I(u_I + \alpha \Delta u_I, -c_I(x + \alpha \Delta x))\|^2 + \frac{1}{2} \|c_E(x + \alpha \Delta x)\|^2. \end{aligned} \tag{3.6}$$

This function is a natural criterion for nonlinear equation solvers. Since the square of the Fisher-Burmeister function is continuously differentiable, the same property has the function $Q(\alpha)$. The following theorem characterizes properties of this function.

Theorem 7. *Let the assumptions of Theorem 6 be satisfied. Then*

$$\begin{aligned} Q'(0) &= -\|g\|^2 - \|\psi_I\|^2 - \|c_E\|^2 \\ &+ g^T h_x + \hat{\psi}_I^T (\hat{R}_I + \hat{C}_I) \hat{R}_I^{-1} \hat{h}_I + c_E^T h_E. \end{aligned} \tag{3.7}$$

If (2.6) is solved with a sufficient precision, namely if

$$g^T h_x + \hat{\psi}_I^T (\hat{R}_I + \hat{C}_I) \hat{R}_I^{-1} \hat{h}_I + c_E^T h_E < \|g\|^2 + \|\psi_I\|^2 + \|c_E\|^2, \tag{3.8}$$

then $Q'(0) < 0$.

Proof. Differentiating (3.6) by α, we obtain

$$\begin{aligned} Q'(0) &= g^T(G\Delta x + A_I\Delta u_I + A_E\Delta u_E) \\ &+ \psi_I^T\left((R_I + C_I)R_I^{-1}A_I^T\Delta x - (R_I - U_I)R_I^{-1}\Delta u_I\right) + c_E^T A_E^T\Delta x. \end{aligned} \tag{3.9}$$

Using (2.5) and (2.6), we obtain equalities

$$g^T\left(G\Delta x + A_I\Delta u_I + A_E\Delta u_E\right) = -g^T g + g^T h_x,$$

$$\psi_I^T\left((R_I + C_I)R_I^{-1}A_I^T\Delta x - (R_I - U_I)R_I^{-1}\Delta u_I\right) = -\|\psi_I\|^2 + \hat{\psi}_I^T(\hat{R}_I + \hat{C}_I)\hat{R}_I^{-1}\hat{h}_I,$$

$$c_E^T A_E^T\Delta x = -\|c_E\|^2 + c_E^T h_E,$$

which after substituting into (3.9) give (3.7). The right hand side of (3.8) is always positive so if (2.6) is solved with a sufficient precision, then (3.8) holds and $Q'(0) < 0$ by (3.7). □

Both functions $P(\alpha)$ and $Q(\alpha)$ have some advantages and disadvantages. Function $P(\alpha)$ is more closely related to the optimization problem. Using restarts, this function decreases the probability to find the saddle point of the objective function on the feasible set. Unfortunately, function $P(\alpha)$ is not sufficient to prove the global convergence. On the other hand, function $Q(\alpha)$ can be used in the globally and superlinearly convergent Newton method [2], [8]. Unfortunately, this method converges to a KKT point satisfying (1.1), which may not be the required minimum if the second order sufficient conditions do not hold. We have implemented and tested four different strategies for step-length selection. All of these strategies use function $P'(0)$ for restarts. Using a sufficiently small value of σ, we compute $P'(0)$ and if $P'(0) \geq 0$, then we replace matrix G by some positive definite diagonal matrix and repeat the direction determination. In the first strategy, using the Armijo procedure with initial estimate $\alpha = \min(1, \overline{\Delta}/\|\Delta x\|)$, we accept the first value for which $P(\alpha) < P(0)$ (since function $Q(\alpha)$ is not used, the first derivatives need not be computed during the step-length selection). In the second strategy, the value α is accepted if at least one of conditions $P(\alpha) < P(0)$ and $Q(\alpha) < Q(0)$ is satisfied. In the third strategy, condition $P(\alpha) < P(0)$ is used after restart and condition $Q(\alpha) < Q(0)$ is used otherwise. In the fourth strategy no condition for step-length selection is used, i.e., the initial estimate $\alpha = \min(1, \overline{\Delta}/\|\Delta x\|)$ is always accepted.

4 Description of the algorithm

The above considerations can be summarized in the algorithmic form.

Algorithm 1.

Data: Parameter for the active constraint definition ε_0. Minimum precision for the direction determination $0 < \varpi < 1$. Line-search parameter $0 < \beta < 1$. Step bound $\overline{\Delta} > 0$.

Input: Sparsity pattern of matrices $\nabla^2 F$ and A. Initial choice of vector x.

Step 1: *Initiation.* Choose the value $\sigma > 0$ (e.g. $\sigma = 1$). For $i \in I \cup E$ set $u_i := 0$. Compute value $f(x)$ and vectors $c_I(x)$, $c_E(x)$. Set $k := 0$.

Step 2: *Termination.* Compute matrix $A := A(x)$ and vector $g := g(x, u)$. If conditions (1.1) are satisfied with a sufficient precision, then terminate the computation. Otherwise set $k := k + 1$.

Step 3: *Approximation of the Hessian matrix.* Compute approximation G of the Hessian matrix $G(x, u)$ by using the differences of gradient $g(x, u)$ as in [1].

Step 4: *Direction determination.* Split constraints into active and inactive and build linear system (2.6). Determine positive definite diagonal matrix $\hat{D}$ as an approximation of the diagonal of $\hat{G}$ and determine a representation of the preconditioner (2.7) (Bunch-Parlett decomposition or Schur complement based representation, see [7]). Writing system (2.6) in the form $Kd = b$, set $\omega = \min(\|b\|, 1/k, \overline{\omega})$ and determine direction vectors Δx, $\Delta \hat{u}_I$ and Δu_E as an inexact solution of (2.6) (with the precision $\|Kd - b\| \leq \omega \|b\|$) by the preconditioned Krylov-subspace method. Compute vector $\Delta \check{u}_I$ by (2.5). Compute directional derivative $P'(0)$ of the merit function $P(\alpha)$ by (3.5).

Step 5: *Restart.* If $P'(0) \geq 0$, determine positive definite diagonal matrix D by the procedure given in [7], set $G = D$ and go to Step 4.

Step 6: *Step-length selection.* Find the minimum integer $l \geq 0$ using one of the following strategies. Strategy 1: $P(\beta^l) < P(0)$. Strategy 2: $P(\beta^l) < P(0)$ or $Q(\beta^l) < Q(0)$. Strategy 3: $P(\beta^l) < P(0)$ after restart and $Q(\beta^l) < Q(0)$ otherwise. Strategy 4: $l = 0$, (i.e. $\alpha = 1$). Finally, set $\alpha = \beta^l$, $x := x + \alpha \Delta x$, $u_I := u_I + \alpha \Delta u_I$, $u_E := u_E + \alpha \Delta u_E$, compute value $f(x)$ and vectors $c_I(x)$ and $c_E(x)$ and go to Step 2.

5 Numerical experiments

Algorithm 1 was tested by using five sets each containing 18 test problems. These sets were obtained as a modification of test problems for equality constrained minimization given in [6], which can be downloaded (together with report [6]) from the page `http://www.cs.cas.cz/~luksan/test.html`. In the first set, equalities $c(x) = 0$ are replaced by inequalities $c(x) \geq 0$. In the second set, equalities $c(x) = 0$ are replaced by inequalities $c(x) \leq 0$. The third set was generated from the first set by adding box constraints $x \geq 0$. The fourth set was generated from the second set by adding box constraints $x \leq 0$. The fifth set contains inequalities $-1 \leq x \leq 1$ and $-1 \leq c(x) \leq 1$. All problems used contain 1000 variables (vector x has the dimension 1000). The results of the tests are listed in Table 1 - Table 4, where NIT is the total number of iterations, NFV is the total number of function evaluations, NFG is the total number of gradient evaluations (NFG is much greater than NIT, since second order derivatives are computed by using gradient differences), NCG is the total number of CG iterations,

NRS is the total number of restarts and NFAIL gives the number of failures for a given set (the number of problems which has not been solved).

Set	NIT	NFV	NFG	NCG	NRS	TIME	NFAIL
1	1091	1444	10176	23958	89	21.78	-
2	723	1657	5142	17790	188	20.91	1
3	691	1216	5220	56643	91	22.12	-
4	341	931	2571	1483	72	7.99	2
5	580	897	4387	7196	137	12.59	-

Table 1 : Nonsmooth equation method - Strategy 1

Set	NIT	NFV	NFG	NCG	NRS	TIME	NFAIL
1	1323	1691	13858	29288	182	30.84	-
2	764	1595	6996	18113	196	22.19	1
3	735	1249	6660	68421	90	25.92	-
4	399	1261	4217	1938	84	10.29	2
5	500	705	4445	6149	86	10.53	-

Table 2 : Nonsmooth equation method - Strategy 2

Set	NIT	NFV	NFG	NCG	NRS	TIME	NFAIL
1	863	3843	9408	61887	78	23.78	2
2	630	2957	6822	19748	121	15.63	3
3	613	2533	6842	38612	114	20.21	1
4	480	2137	5340	5182	92	13.70	3
5	526	2163	5605	4467	82	12.42	1

Table 3 : Nonsmooth equation method - Strategy 3

Set	NIT	NFV	NFG	NCG	NRS	TIME	NFAIL
1	1111	1112	10295	38876	111	23.96	-
2	1386	1386	9794	31914	306	49.71	-
3	1621	1622	16566	31784	175	37.28	1
4	709	791	5311	35419	232	36.10	3
5	1395	1396	10170	11515	292	29.13	1

Table 4 : Nonsmooth equation method - Strategy 4

For a comparison, Table 5 and Table 6 contain results obtained by using the interior-point method described in [9].

Set	NIT	NFV	NFG	NCG	NRS	TIME	NFAIL
1	740	1059	5477	45935	98	27.24	-
2	736	1895	5321	58664	215	41.26	1
3	720	1378	5260	31350	82	28.33	-
4	378	538	2788	12666	20	19.50	3
5	570	723	4276	5876	55	14.48	-

Table 5 Interior-point method - Strategy 1

Set	NIT	NFV	NFG	NCG	NRS	TIME	NFAIL
1	786	786	5691	25602	55	15.08	-
2	717	717	5092	20289	119	24.07	-
3	907	907	6816	25639	84	22.66	-
4	458	458	3405	20793	49	22.76	3
5	609	612	4292	4183	21	12.24	1

Table 6: Interior-point method - Strategy 4

6 Conclusions

In this contribution, we describe an implementation of the nonsmooth-equation method for solving large and sparse general nonlinear programming problems. Computational experiments show that this approach is very reasonable. Nevertheless, KKT equations belong to the class of problems which are difficult for application of the Newton method (this observation is also known from the equality constrained optimization, see [5]). For this reason, the use of natural merit function $Q(\alpha)$, which has the best theoretical properties [2], is not efficient for practical computations, see Table 3. The simple merit function $P(\alpha)$, which was chosen to give negative directional derivative for a broad class of directions obtained as inexact solutions of system (2.6), has better practical properties. Unfortunately, this function does not allow us to prove the global convergence in general. Surprisingly good results were obtained without using a merit function, see Table 4. However, parameters ρ and $\overline{\Delta}$ have to be chosen more carefully in this case. Another conclusion, which follows from our computational experiments, is that the nonsmooth equation method based on the Fisher-Burmeister function (with Strategy 1) is competitive with the interior-point method described in [9], see Table 5. The main advantage of the nonsmooth equation approach is that no slack variables are used and matrix $\hat{M}_I$ is positive definite independently of the signs of Lagrange multipliers. Therefore, a special strategy for step-length selection ensuring positivity of slack variables and Lagrange multipliers need not be used. The nonsmooth equation method is relatively sensitive to the choice of parameters ρ and $\overline{\Delta}$ and the system (2.6) is frequently ill-conditioned due to the linear dependence of gradients of the active constraints (the number of active constraints can be greater than the number of variables).

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