

New algorithms for solving unconstrained optimization problems based on the generalized Newton method involving simple quadrature rules

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Abstract. Solving system of nonlinear equations is one of the most important problems in numerical analysis. Optimization problems can often be transformed into the equation $F(x) = 0$ with a nonsmooth function F , e.g. nonlinear complementarity problem or variational inequality problem. We consider some modifications of a generalized Newton method using some subdifferential (first of all B-differential) and based on some rules of quadrature. We use these algorithms for solving unconstrained optimization problems, in which the objective function has not differentiable gradient. Such problems can appear in optimization as subproblems. The proposed methods are locally and at least superlinearly convergent under mild conditions imposed on the gradient of the objective function. Finally, we present results of numerical tests.

Keywords: unconstrained optimization problems, generalized Newton method, B-differential, quadrature rules, superlinear convergence.

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1. Introduction

We consider nonlinear unconstrained programming problem

$$\min f(x), x \in D \subset R^n \tag{1}$$

where $f : D \subset R^n \rightarrow R$ (D is an open convex set) is assumed to be only LC^1 but not C^2 . The LC^1 property means that the objective function f is continuously differentiable and its gradient ∇f is only locally Lipschitzian (in older papers LC^1 functions were also called $C^{1,1}$ functions). If f is LC^1 , then (1) is called an unconstrained LC^1 optimization problem.

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The second-order differentiability is the property, which may not hold for some problems. In effect, proposed methods could be apply more often than only for solving equations which come from the reformulation of nonlinear complementarity problems or variational inequalities. The augmented Lagrangian of a twice smooth nonlinear programming problem is a LC^1 function ([17]). Such functions and problems were discussed in [15]. Because really in many problems functions don't possess a sufficient degree of smoothness, algorithms for solving nondifferentiable unconstrained problems can be important tools to solve them. The efficient Newton-like methods for solving some optimization problems with nonsmooth gradient were introduced for LC^1 optimization problem e.g. in [16, 6]. In turn, an interesting construction of the unconstrained optimization problem with the objective function, which may not be twice differentiable, with usage of penalty functions or Lagrange multiplier functions was presented in [4, 5].

As is well-known, finding the solution of problem (1) is equivalent to solving of nonsmooth equation $F(x) = 0$, where function F is a gradient of f ($F = \nabla f$). The generalized Jacobian-based Newton method is one of the standard methods for solving nonsmooth equations. Methods of this class were introduced e.g. in [17, 14, 19, 7] and have superlinear convergence. The basic form of the method is defined by

$$x^{(k+1)} = x^{(k)} - (V^{(k)})^{-1} F(x^{(k)}), \quad k = 0, 1, \dots \quad (2)$$

where $V^{(k)}$ is taken from some subdifferential of F at $x^{(k)}$. This subdifferential may be the Clarke generalized Jacobian (Qi and Sun [17]), the B-differential (Qi [14]), the b-differential (Sun and Han [19]) and the *-differential (Gao [7]). Naturally, the increment $x^{(k+1)} - x^{(k)}$ can be obtained as the solution of a linear system with matrix $V^{(k)}$ by any iterative or direct method.

Some new variants of classic Newton's method for solving smooth equations, based on various quadrature rules, were proposed in [2, 3]. It was proved, that these methods have local and quadratic convergence for a continuously differentiable function F . Some algorithms were extended in [20] to the nonsmooth case.

The paper is organized as follows. In Section 2, we recall fundamental results for the generalized Jacobian, various subdifferentials and semismoothness. Some new versions of the generalized Newton method for solving unconstrained LC^1 optimization problem and the convergence analysis are studied in Section 3. In Section 4, we give some numerical examples.

2. Preliminaries

Let $F : R^n \rightarrow R^n$ be a locally Lipschitz function and $f_i : R^n \rightarrow R$ be the i -th component of F for $i = 1, \dots, n$. According to Rademacher's theorem, the local Lipschitz continuity of F implies that F is differentiable almost everywhere. Let D_F denotes the set of points at which F is differentiable and $JF(x)$ - the usual Jacobian matrix of partial derivatives of F at x .

Then the set

$$\partial_B F(x) = \left\{ \lim_{x_i \rightarrow x} JF(x_i), x_i \in D_F \right\}, \tag{3}$$

is called the *B-differential* (the Bouligand subdifferential) of F at x . If all elements of $\partial_B F(x)$ are nonsingular, then F is called *BD-regular* at x^* . The *generalized Jacobian* of F at x in the sense of Clarke [1] is the convex hull of the B-differential i.e.

$$\partial F(x) = \text{conv} \partial_B F(x), \tag{4}$$

In turn, the following set

$$\partial_b F(x) = \partial_B f_1(x) \times \dots \times \partial_B f_n(x) \tag{5}$$

is called the *b-differential* of F at x ([19]). And the **-differential* $\partial_* F(x)$ introduced in [7] is a non-empty bounded set for each x such that

$$\partial_* F(x) \subset \partial f_1(x) \times \dots \times \partial f_n(x), \tag{6}$$

where $\partial f_i(x)$ is the Clarke generalized gradient of f_i at x .

It is well-known that if $n = 1$, then $\partial F(x)$ reduces to the Clarke generalized gradient of F at x and $\partial_b F(x) = \partial_B F(x)$. Moreover, $\partial F(x)$, $\partial_B F(x)$ and $\partial_b F(x)$ are **-differentials* for a locally Lipschitz function [7].

The notion of semismoothness was originally introduced for functionals by Mifflin [9]. The following definition is taken from [17]. A function F is *semismooth* at a point x if F is locally Lipschitzian at x and

$$\lim_{V \in \partial F(x+th'), h' \rightarrow h, t \downarrow 0} Vh' \tag{7}$$

exists for any $h \in R^n$.

Semismoothness implies some important properties for the convergence analysis of methods in nonsmooth optimization.

Lemma 2.1 (Lemma 2.2, [17]). *Suppose that $F'(x; h)$ exists for any h at x . Then:*

- (i) $F'(x; \cdot)$ is Lipschitzian;
- (ii) for any h , there exists a $V \in \partial F(x)$ such that

$$F'(x; h) = Vh. \tag{8}$$

Proposition 2.2 (Theorem 2.3, [17]). *The following statements are equivalent:*

- (i) F is semismooth at x ;
- (ii) for $V \in \partial F(x + h)$, $h \rightarrow 0$,

$$Vh - F'(x; h) = o(\|h\|); \tag{9}$$

(iii)

$$\lim_{h \rightarrow 0} \frac{F'(x + h; h) - F'(x; h)}{\|h\|} = 0. \tag{10}$$

Remark 2.3. *In the original version of the statement (iii) in the above proposition there is the assumption $x + h \in D_F$. Without loss of generality, this assumption may be removed, because the proof is analogous. Moreover, it follows from (10) that if F has a strong Fréchet derivative at x , then F is semismooth at x .*

If for any $V \in \partial F(x + h)$, as $h \rightarrow 0$,

$$Vh - F'(x, h) = O\left(\|h\|^{1+p}\right), \quad (11)$$

where $0 < p \leq 1$, then we say that F is p -order semismooth at x . Clearly, p -order semismoothness implies semismoothness.

Qi and Sun [17] remarked that if F is semismooth at x , then for any $h \rightarrow 0$,

$$F(x + h) - F(x) - F'(x; h) = o(\|h\|), \quad (12)$$

and if F is p -order semismooth at x , then for any $h \rightarrow 0$,

$$F(x + h) - F(x) - F'(x; h) = O\left(\|h\|^{1+p}\right). \quad (13)$$

If $p = 1$ then the function F is called *strongly semismooth* ([11]).

Lemma 2.4 (Lemma 2.6, [14]). *If F is BD-regular at x , then there are a neighborhood N of x and a constant $C > 0$ such that for any $y \in N$ and $V \in \partial_B F(y)$, V is nonsingular and*

$$\|V^{-1}\| \leq C. \quad (14)$$

If F is also semismooth at $y \in N$, then, for any $h \in \mathbb{R}^n$,

$$\|h\| \leq C \|F'(y; h)\|. \quad (15)$$

Instead of semismoothness we can use the following more general assumption on the function F :

Assumption A. *Assume that function F is Lipschitz continuous. We say that F satisfies A at x if for any $y \in \mathbb{R}^n$ and any $V_y \in \partial_B F(y)$, the following equality holds:*

$$F(y) - F(x) = V_y(y - x) + o(\|y - x\|). \quad (16)$$

Moreover, we say that F satisfies A at x with degree p if F is Lipschitz continuous and the following equality holds:

$$F(y) - F(x) = V_y(y - x) + O\left(\|y - x\|^{1+p}\right). \quad (17)$$

Remark 2.5. *It is easy to check that if F is BD-regular at x and satisfies assumption A at x , then there exist a neighborhood N of x and a constant $C > 0$ such that for any $y \in N$ and $V \in \partial_B F(y)$,*

$$\|y - x\| \leq C \|V_y(y - x)\|. \quad (18)$$

There are at least three classes of functions that satisfied Assumption A [13]. Beside semismoothness, the second-order C-differentiability (see [15]) and H-differentiability

(see [8]) are properties that imply A. Moreover, it is easy to prove that the p -order semismoothness implies A with degree p .

Notation: Throughout the whole paper $S(x, r)$ denotes an open ball in R^n with center x and radius r .

3. Quadrature-based generalized Newton methods

In this section we consider some versions of the generalized Newton method, which were constructed using some rules deriving from quadratures for numerical integration. Using methods from [20] based on ideas from [2], we apply analogous methods for solving unconstrained optimization problems. We prove a local convergence theorem for one of the methods using iteration matrices taken from the B-differential of F .

Let $x^{(0)} \in R^n$ be some approximation to solution of (1). To obtain $x^{(k+1)}$ from k th approximation $x^{(k)}$ by means of the trapezoidal generalized Newton method we use the following formula

$$x^{(k+1)} = x^{(k)} - 2[V_x^{(k)} + V_z^{(k)}]^{-1}F(x^{(k)}), \quad k = 0, 1, \dots \quad (19)$$

where $V_x^{(k)}$ and $V_z^{(k)}$ are taken from some subdifferentials of F at $x^{(k)}$ and $z^{(k)}$, respectively, and $z^{(k)} = x^{(k)} - (V_x^{(k)})^{-1}F(x^{(k)})$. Using the midpoint rule, the midpoint generalized Newton method is obtained as

$$x^{(k+1)} = x^{(k)} - (V_{xz}^{(k)})^{-1}F(x^{(k)}), \quad k = 0, 1, \dots \quad (20)$$

where $V_{xz}^{(k)}$ is an element of some subdifferential of F at $\frac{1}{2}(x^{(k)} + z^{(k)})$ and $z^{(k)} = x^{(k)} - (V_x^{(k)})^{-1}F(x^{(k)})$, as previously. Note that both formulas (19) and (20) use arithmetic means: of $V_x^{(k)}$ and $V_z^{(k)}$ in (19) and of $x^{(k)}$ and $z^{(k)}$ in (20).

Gao suggested in [7] that different $*$ -differentials $\partial_*F(x)$ generate different superlinearly convergent Newton methods based on the iteration (2). In this way we can obtain other methods from (19) and (20).

To prove convergence results for method (20) with the B-differential, we need some helpful lemma.

Lemma 3.1. *Let F be BD-regular at x^* . Then the function*

$$G(x) = x - (\bar{V}_x)^{-1}F(x), \quad (21)$$

where $\bar{V}_x \in \partial_B F(x - \frac{1}{2}(V_x)^{-1}F(x))$ and $V_x \in \partial_B F(x)$, is well-defined in a neighborhood of x^* .

Proof. Since F is BD-regular at x^* , then based on Lemma 2.4 there exist a constant $\beta > 0$ and a neighborhood N of x^* such that V_x is nonsingular and $\|V_x^{-1}\| \leq \beta$ for any $x \in N$ and $V_x \in \partial_B F(x)$.

Let ε be such that $0 < \varepsilon < 1/2\beta$. First, we claim that there is $V_{x^*} \in \partial_B F(x^*)$ such that

$$\|V_x - V_{x^*}\| < \varepsilon \quad (22)$$

for any $x \in S(x^*, \delta)$ and $V_x \in \partial_B F(x)$.

If the above inequality is not true, then there is a sequence $\{y^{(k)} : y^{(k)} \in D_F\}$ convergent to x^* such that

$$\|JF(y^{(k)}) - V_{x^*}\| \geq \varepsilon \quad \text{for all } V_{x^*} \in \partial_B F(x^*). \quad (23)$$

By passing to a subsequence, we may assume that $\{JF(y^{(k)})\}$ converges to $V_{x^*} \in \partial_B F(x^*)$, which contradicts the above inequality.

Now, we consider $z = x - \frac{1}{2}(V_x)^{-1}F(x)$, where $V_x \in \partial_B F(x)$. By the local convergence of the generalized Newton method (see [14]), it can be guaranteed that $z \in S(x^*, \delta)$ and (22) holds. So, using the Banach perturbation lemma (see [10]), we obtain that \bar{V}_x is nonsingular and

$$\|(\bar{V}_x)^{-1}\| = \|(V_z)^{-1}\| = \|[V_{x^*} + (V_z - V_{x^*})]^{-1}\| \quad (24)$$

$$\leq \frac{\|(V_{x^*})^{-1}\|}{1 - \|(V_{x^*})^{-1}\|\|V_z - V_{x^*}\|} \leq \frac{\beta}{1 - \beta\varepsilon} < 2\beta. \quad (25)$$

for $x \in S(x^*, \delta)$.

So, the function $G(x)$ is well-defined in $S(x^*, \delta)$. □

Theorem 3.2. *Suppose that F satisfies assumption A at x^* , F is BD-regular at x^* and $\|V_{x^*}\| \leq \gamma$ for all $V_{x^*} \in \partial_B F(x^*)$. Then there exists a neighborhood of x^* such that for any starting point $x^{(0)}$ belonging to this neighborhood, the sequence $\{x^{(k)}\}$ generated by the method (20) with the B-differential converges superlinearly to x^* . Moreover, if $F(x^{(k)}) \neq 0$ for all k , then the norm of F decreases superlinearly in a neighborhood of x^* , i.e.*

$$\lim_{k \rightarrow \infty} \frac{\|F(x^{(k+1)})\|}{\|F(x^{(k)})\|} = 0. \quad (26)$$

If F satisfies assumption A with degree 1 at x^ , then the convergence is quadratic.*

Proof. By Lemmas 2.4 and 3.1, the iterative schema (20) is well-defined in a neighborhood of x^* for the first step $k = 0$. Further, if we consider $z = x - \frac{1}{2}(V_x)^{-1}F(x)$, where $V_x \in \partial_B F(x)$, then it can be guaranteed that $z \in S(x^*, \delta)$ (like in Lemma 3.1) and

$$\begin{aligned} \|x^{(k+1)} - x^*\| &= \|x^{(k)} - (V_{x_z^{(k)}})^{-1}F(x^{(k)}) - x^*\| \\ &= \|(V_{x_z^{(k)}})^{-1}\| \|F(x^{(k)}) - F(x^*) - V_{x_z^{(k)}}(x^{(k)} - x^*)\| = o(\|x^{(k)} - x^*\|). \end{aligned} \quad (27)$$

The last equality is due to Lemma 2.4 and Assumption A. This shows that the sequence $\{x^{(k)}\}$ is superlinearly convergent to x^* .

Now, we prove (26). By Lemma 2.4, there are a scalar C and $\delta_1 > 0$ such that if $x \in S(x^*, \delta_1)$ and $V \in \partial_B F(x)$ then V is nonsingular and (14) holds. By Assumption A, for any $\alpha \in (0, 1)$, there is a $\delta_2 \in (0, \delta_1)$ such that if $x \in S(x^*, \delta_2)$,

$$\|F(x) - V(x - x^*)\| \leq \alpha \|x - x^*\|. \quad (28)$$

By (27) there is a $\delta \in (0, \delta_2)$ such that if $x^{(k)} \in S(x^*, \delta)$, then

$$\|x^{(k+1)} - x^*\| \leq \alpha \|x^{(k)} - x^*\|. \quad (29)$$

Since $\{x^{(k)}\}$ converges to x^* , there is an integer k_δ such that $\|x^{(k)} - x^*\| \leq \delta$ for all $k \geq k_\delta$. By (29), $\|x^{(k+1)} - x^*\| \leq \delta \leq \delta_2$. Furthermore, (22) implies $\|V_{xz}^{(k+1)}\| \leq \varepsilon + \|V_{x^*}\| \leq \varepsilon + \gamma$. By (28) and (29) we have

$$\begin{aligned} \|F(x^{(k+1)})\| &\leq \|V_{xz}^{(k+1)}(x^{(k+1)} - x^*)\| + \alpha \|x^{(k+1)} - x^*\| \\ &\leq (\varepsilon + \gamma + \alpha) \|x^{(k+1)} - x^*\| \leq \alpha(\varepsilon + \gamma + \alpha) \|x^{(k)} - x^*\|. \end{aligned} \quad (30)$$

By (20), (29) and (14) we obtain

$$\begin{aligned} \|x^{(k)} - x^*\| &\leq \|x^{(k+1)} - x^{(k)}\| + \|x^{(k+1)} - x^*\| \\ &\leq \|(V_{xz}^{(k)})^{-1}F(x^{(k)})\| + \alpha \|x^{(k)} - x^*\| \\ &\leq C \|F(x^{(k)})\| + \alpha \|x^{(k)} - x^*\|. \end{aligned}$$

So,

$$\|x^{(k)} - x^*\| \leq \frac{C}{1 - \alpha} \|F(x^{(k)})\|. \quad (31)$$

By (30) and (31),

$$\begin{aligned} \|F(x^{(k+1)})\| &\leq \alpha(\varepsilon + \gamma + \alpha) \|x^{(k)} - x^*\| \\ &\leq \frac{C\alpha(\varepsilon + \gamma + \alpha)}{1 - \alpha} \|F(x^{(k)})\|. \end{aligned}$$

Since $F(x^{(k)}) \neq 0$ for all k and α may be arbitrarily small as k tends to infinity, we have (26).

If the function F satisfies A with degree 1, then we have

$$F(x) - F(x^*) - V(x - x^*) = O(\|x - x^*\|^2). \quad (32)$$

Hence the sequence $\{x^{(k)}\}$ defined by (20) with the B-differential is quadratically convergent to x^* . \square

Remark 3.3. *The convergence of the other variants of the generalized Newton method may be proved in a similar way.*

4. Numerical tests and conclusions

The method proposed here can be applied to solve the following constrained optimization problem

$$\begin{cases} \min_{x \in R^n} h(x) \\ g_i(x) \leq 0, i = 1, \dots, m, \end{cases} \quad (33)$$

where h and g_i are twice differentiable. Similar as in [5], we can construct an unconstrained optimization problem (1) with use the Di Pillo-Grippe type Lagrange multiplier function $f : R^{n+m} \rightarrow R$ in the form

$$f(x, \mu, C) = h(x) + \sum_{i=1}^m \frac{(\max\{0, \mu_i + Cg_i(x)\})^2 - \mu_i^2}{2C} + C\|P(x)[\nabla h(x) + \sum_{i=1}^m \mu_i \nabla g_i(x)]\|^2, \quad (34)$$

where $\mu = (\mu_1, \dots, \mu_m)$ are Lagrange multipliers, $P(x)$ is a $m \times n$ matrix and $C > 0$ is a constant. If h and g_i are twice continuously differentiable, f may not be twice differentiable at (x, μ, C) with $\mu_i + Cg_i(x) = 0$, but it has LC^1 gradient and satisfies Assumption A at such points.

We use a constant matrix P as $P(x)$ and large enough parameter C to ensure the equivalence problems (33) and (34), see [12].

To illustrate a performance of the considered methods (19) and (20), we present numerical results of computational tests. Calculations were performed in Dev-C++ in double-precision arithmetic. We declare a failure of the algorithm when the stopping criterion $\|x^{(k+1)} - x^{(k)}\|_2 \leq 10^{-10}$ or $\|F(x^{(k)})\|_2 \leq 10^{-12}$ is not reached after 1000 iterations ($\|\cdot\|_2$ denotes the Euclidean norm). Tables summarize the results in terms of the number of iterations N for miscellaneous starting points $x^{(0)}$. A symbol “ \times ” denotes that the test failed.

We consider problems (33) with the following functions (examples were taken from [18]):

Example 1.

$$\begin{cases} f(x) = (x_1 - 2)^2 + (x_2 - 1)^2 \\ g_1(x) = x_1^2 - x_2 \\ g_2(x) = x_2^2 - x_1 \end{cases}$$

Example 2.

$$\begin{cases} f(x) = -\frac{1}{27\sqrt{3}}(9 - (x_1 - 3)^2)x_2^3 \\ g_1(x) = -(\frac{1}{\sqrt{3}}x_1 - x_2) \\ g_2(x) = -(x_1 + \sqrt{3}x_2) \\ g_3(x) = -(6 - x_1 - \sqrt{3}x_2) \end{cases}$$

Table 1
Numerical results for Problem 1

initial data			Method		
$x^{(0)}$	μ	C	midpoint	trapezoid	classic
(0.5, 0.5)	1	10	6	9	13
(0.5, 0.5)	2	10	7	10	15
(1, 1)	1	10	8	11	17
(1, 1)	2	10	11	14	21
(1, 1)	1	20	12	18	23
(5, 5)	2	10	×	16	×
(5, 5)	2	20	11	15	22
(5, 5)	2	50	10	17	21
(10, 10)	2	20	14	19	×
(-10, -10)	1	20	×	28	×

Table 2
Numerical results for Problem 2

initial data			Method		
$x^{(0)}$	μ	C	midpoint	trapezoid	classic
(2, 0.5)	(1, 1, 1)	10	7	11	15
(2, 0.5)	(2, 2, 2)	10	8	10	15
(4, 1)	(1, 1, 1)	10	8	11	15
(4, 1)	(2, 2, 2)	10	7	11	×
(4, 2)	(2, 2, 2)	20	×	12	17
(4, 2)	(3, 3, 3)	20	8	13	×
(6, 1.5)	(2, 2, 2)	20	6	9	13
(6, 1.5)	(3, 3, 3)	20	×	14	×

We presented some new versions of the generalized Newton algorithms for solving unconstrained LC^1 optimization problems. First, we proved that the sequence generated by the midpoint variant of the method with the B-differential is locally and superlinearly convergent to the solution of problem (1) under mild assumptions. Some stronger condition imposed on the equation guarantees that the method has quadratic convergence.

The performance of the methods is evaluated first of all in the terms of the number of iterations required. The important conclusion is that the generalized Newton methods based on quadrature rules allow us to find the solutions of nonsmooth equations usually more efficiently than the classic version. Really, the computational cost of one step of the quadrature-based method is double that for one step of the classic method, because two matrices are required. Comparing the trapezoidal variant with the midpoint one, the convergence may be, roughly speaking, quite weak (see Table 2). This is not surprising if we recall that we use the arithmetic mean of $V_x^{(k)}$ and $V_z^{(k)}$ in the trapezoidal version and the arithmetic mean of $x^{(k)}$ and $z^{(k)}$ in the midpoint

one. So, the efficiency of the generalized Newton method depends on the successive iteration points rather than on matrices taken from the subdifferential.

Moreover, behavior of the values of functions F at successive iteration points indicates that $\|F(x^{(k+1)})\| / \|F(x^{(k)})\|$ converges to 0 as $k \rightarrow \infty$, which was proved in Theorem 5. However, not all of the problems considered above were solved with a satisfactory convergence.

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