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Superquadraticly convergent methods for minimization functions

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Abstract

In the paper locally superquadraticly convergent methods for minimization functions are considered. Threefold symmetric approximations to partial derivatives of the third order are constructed.

1. Introduction

Let $f: D \subset \mathbb{R}^n \to \mathbb{R}$, $f \in \mathbb{C}^3(D)$, D - open set. We want to find $x^* \in D$ such that $\nabla f(x^*) = 0$. For a given $x_0 \in D$ the Newton method defines the sequence $\{x_k\}$ in the following way

$$\nabla^2 f(x_k) s_k = -\nabla f(x_k), \ x_{k+1} = x_k + s_k, \ k = 0, 1, 2, \cdots.$$
 (1)

If the matrix $\nabla^2 f(x^*)$ is nonsingular then Newton method is locally quadraticly convergent to x^* , i.e. there exist c>0 and $\varepsilon>0$ such that, if $\|x^*-x_0\|<\varepsilon$, then

$$||x_{k+1} - x^*|| \le c ||x_k - x^*||^2$$
. (2)

To assure global convergence of the method one should consider a sequence

$$x_{k+1} = x_k + t_k s_k, \ t_k \in \mathbb{R}, \ k = 0, 1, 2, \cdots$$
 (3)

and the parameter t_k should satisfy the global convergence conditions. If the matrix $\nabla^2 f(x^*)$ is singular, then the Newton method is divergent or at most linearly convergent to x^* . To assure a great speed of convergence for singular problems one applies the method of the third rate of convergence: for a given $x_0 \in D$ the sequence $\{x_k\}$ is defined as

$$x_{k+1} = x_k + s_k, \ k = 0, 1, 2, \cdots$$
 (4)

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where s_k is the solution of the system of quadratic equations

$$\nabla f(x_k) + \nabla^2 f(x_k) s_k + \frac{1}{2} (\nabla^3 f(x_k) s_k, s_k) = 0.$$
 (5)

When the calculation of the operator $\nabla^3 f(x_k)$ is too expensive or is not attainable for computation then we propose a new class of the methods which are locally superquadraticly convergent to x^* , i.e.

$$\lim_{k \to \infty} \frac{\left\| x_{k+1} - x^* \right\|}{\left\| x_k - x^* \right\|^2} = 0.$$
 (6)

Let $B_k = (B_k^1, B_k^2, \dots, B_k^n)$, $B_k^i \in R^{n \times n}$, $B_k^i = (B_k^i)^T$, $i = 1, 2, \dots, n$. The sequence $\{x_k\}$ is defined by (1.4) and

$$\nabla f(x_k) + \nabla^2 f(x_k) s_k + \frac{1}{2} (B_k s_k, s_k) = 0.$$
 (7)

If the problem $\min_{x \in D} f(x)$ is regularly singular at x^* , i.e.

$$\det(\nabla^2 f(x^*)) = 0, \text{ and } \|\nabla f(x)\| \ge c \|x - x^*\|^2, \ c > 0, \ x \in D,$$
 (8)

then the sequence $\{x_k\}$ defined by (1.4) and (1.7) is locally superlinearly convergent to x^* , if the operators B_k are constructed in an adequate way. In this paper such algorithms are given.

2. The BFGS method

The DFP (Davidon [1], Fletcher and Powell [2]) method is very well known as the method of approximation to the Hessian $\nabla^2 f(x_k)$. This formula has the form

$$B_{k+1} = B_k - \frac{B_k s_k s_k^T B_k}{s_k^T B_k s_k} + \frac{y_k y_k^T}{y_k^T s_k}, \ y_k = \nabla f(x_{k+1}) - \nabla f(x_k).$$
 (9)

The DFP formula, for nonsingular problems, guarantees local superlinear convergence of the method

$$x_{k+1} = x_k + s_k, \ B_k s_k = -\nabla f(x_k), \ k = 0, 1, 2, \cdots$$
 (10)

We may use the DFP formula to approximate the operator $\nabla^3 f(x_k)$. Namely, let

$$B_k = (B_k^1, B_k^2, \dots, B_k^n), \ B_k^i \in \mathbb{R}^{n \times n}, \ B_k^i = (B_k^i)^T, \ i = 1, 2, \dots, n$$
 (11)

and let $\nabla_i^2 f(x_k)$ denote i-th column of the matrix $\nabla^2 f(x_k)$, $y_k^i = \nabla_i^2 f(x_{k+1}) - \nabla_i^2 f(x_k)$. Then

$$B_{k+1}^{i} = B_{k}^{i} - \frac{B_{k}^{i} s_{k} s_{k}^{T} B_{k}^{i}}{s_{k}^{T} B_{k}^{i} s_{k}} + \frac{y_{k}^{i} (y_{k}^{i})^{T}}{(y_{k}^{i})^{T} s_{k}}, \quad i = 1, 2, \dots, n.$$

$$(12)$$

Note that the operators B_{k+1} satisfy the equation

$$B_{k+1}S_k = \nabla^2 f(x_{k+1}) - \nabla^2 f(x_k), \ k = 0, 1, 2, \cdots$$
 (13)

Now, from the general theory for the systems of nonlinear equations [3], [4] local superquadratic convergence of the method results (4), (7) with the update (12). On the other hand, the DFP updates do not satisfy the following properties of the partial derivatives

$$\frac{\partial^3 f(x)}{\partial x_i \partial x_j \partial x_l} = \frac{\partial^3 f(x)}{\partial x_i \partial x_l \partial x_j} = \dots = \frac{\partial^3 f(x)}{\partial x_l \partial x_j \partial x_l}, i, j, l = 1, 2, \dots, n.$$
(14)

In this case, we say the operator $\nabla^3 f(x)$ is threefold symmetric (T-symmetric).

It is worth remarking that the operator $\nabla^3 f(x)$ has only $P(n) = \frac{1}{6}n(n+1)(n+2)$

different elements and the DFP approximations have $Q(n) = \frac{1}{2}n^2(n+1)$ different elements, which means that the BFGS formula is not adequate for approximation to $\nabla^3 f(x)$. In the next Section we give a new formula for the update of B_k and B_k will be T-symmetric.

3. New approximation to $\nabla^3 f(x)$

The approximation B_k to $\nabla^3 f(x)$ satisfies secant equation (13) and operators B_k should be threefold symmetric. If we take

$$B_{k+1} = B_k + E , (15)$$

then

$$Es_{k} = \nabla^{2} f(x_{k+1}) - \nabla^{2} f(x_{k}) - B_{k} s_{k} = Y.$$
 (16)

In that case we have to solve the problem

$$\min \|E\|^2, \ \|E\|^2 = \sum_{i=1}^n \sum_{k=1}^n \sum_{k=1}^n E_{ijk}^2$$
 (17)

under constraints

$$Es = Y, \ s \in \mathbb{R}^n, \ Y \in \mathbb{R}^{n \times n}, \ Y = Y^T$$
 (18)

and

$$E_{ijk} = E_{ikj} = E_{jik} = E_{jki} = E_{kij} = E_{kij}, i, j, k = 1, 2, \dots, n.$$
 (19)

Remark. If we take another norm of the operator E, then we get another formula for the update B_k .

Let $\Lambda \in \mathbb{R}^{n \times n}$. In our case the lagrangian has the form

$$L(E,\Lambda) = \frac{1}{2} ||E||^2 + \sum_{i=1}^n \sum_{j=1}^n \Lambda_{ij} \left(\sum_{k=1}^n E_{ijk} s_k - Y_{ij} \right).$$
 (20)

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From this we have

$$\frac{\partial L(E,\Lambda)}{\partial E_{pqr}} = E_{pqr} + \Lambda_{pq} s_r = 0.$$
 (21)

The fact $E_{pqr} = E_{qpr}$ implies $\Lambda = \Lambda^T$. Since the operator E is threefold symmetric then equation (21) may be written as

$$E_{pqr} = -\frac{1}{3} \left(\Lambda_{pq} s_r + \Lambda_{pr} s_q + \Lambda_{qr} s_p \right) \quad \text{for } 1 \le p \le q \le r \le n.$$
 (22)

Now, the equation Es = Y has the form

$$\sum_{l=1}^{n} (\Lambda_{ij} s_l + \Lambda_{il} s_j + \Lambda_{jl} s_i) s_l = -3Y_{ij} \quad 1 \le i \le j \le n$$
 (23)

or is in the matrix form

$$\Lambda \|s\|^2 + \Lambda s s^T + s s^T \Lambda = -3Y. \tag{24}$$

Therefore

$$s^{T} \Lambda s = -\frac{1}{\|s\|^{2}} s^{T} Y s, \ u = \Lambda s = \frac{1}{2\|s\|^{2}} (-3Y s + \frac{s^{T} Y s}{\|s\|^{2}} s) \ . \tag{25}$$

Finally

$$\Lambda = -\frac{1}{\|s\|^2} (3Y + us^T + su^T).$$
 (26)

To calculate the new threefold symmetric update $B_{k+1} = B_k + E$ we use the formulae (22), (25) and (26).

4. Remarks on the local superquadratic convergence of the method

At first we describe the proposed algorithm:

- a) Let $x_0 \in \mathbb{R}^n$ and $B_0 = (B_0^1, B_0^2, \dots, B_0^n)$ threefold operator be given. Let k = 0.
- b) Solve, using for example the Newton method, the system of quadratic equations

$$\nabla f(x_k) + \nabla^2 f(x_k) s_k + \frac{1}{2} (B_k s_k, s_k) = 0$$
,

- c) Calculate $x_{k+1} = x_k + s_k$, $\nabla f(x_{k+1})$, $\nabla^2 f(x_{k+1})$,
- d) Update the operator B_k using the formulae from Section 3,
- e) If a stop criterion is not satisfied, then k := k+1 and return to point b. To explain a character of convergence of the method we introduce some notations. Let

$$H_k = \int_0^1 \nabla^3 f(x_k + t(x_{k+1} - x_k)) dt, \qquad (27)$$

$$L_{k} = \{ X \in \mathbb{R}^{n \times n \times n} : X s_{k} = \nabla^{2} f(x_{k+1}) - \nabla^{2} f(x_{k}) \},$$
 (28)

$$Q = \{X \in \mathbb{R}^{n \times n \times n} : X \text{ is threefold symmetric operator}\}.$$
 (29)

The set Q is linear subspace in $R^{n \times n \times n}$ and $H_k \in Q$. Applying Theorem 3.2.7 [5] we have

$$H_{\nu}s_{\nu} = \nabla^{2} f(x_{\nu+1}) - \nabla^{2} f(x_{\nu}),$$
 (30)

which means that $Q \cap L_k$ is a nonempty linear set. The proposed norm is generated by inner product, so the operator B_{k+1} is defined as the orthogonal projection of the operator B_k onto the set $Q \cap L_k$, and from Pitagoras Theorem (see [3]) we get

$$\|B_{k+1} - H_k\|^2 + \|B_k - B_{k+1}\|^2 = \|B_k - H_k\|^2 \quad k = 0, 1, 2, \cdots$$
 (31)

The inequality $||B_{k+1} - H_k|| \le ||B_k - H_k||$ implies local linear convergence of the sequence $\{x_k\}$. From equations (31) it results additionally

$$\sum_{k=0}^{\infty} \|B_{k+1} - B_k\|^2 < \infty. \tag{32}$$

The last inequality and the secant equation (13) assure local superquadratic convergence of the proposed algorithm [4].

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