Superquadratically convergent methods for minimization functions

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Abstract

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

1. Introduction

Let \( f : D \subset R^n \rightarrow R, \ f \in C^3(D) \), \( D \) - 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

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

(1)

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

\[
\|x_{k+1} - x^*\| \leq c\|x_k - x^*\|^2.
\]

(2)

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

\[
x_{k+1} = x_k + t_k s_k, \ t_k \in R, \ k = 0,1,2,\ldots
\]

(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

\[
x_{k+1} = x_k + s_k, \ k = 0,1,2,\ldots
\]

(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 superquadratically convergent to $x^*$, i.e.

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

(6)

Let $B_k = (B^1_k, B^2_k, \ldots, B^n_k)$, $B^i_k \in R^{n \times n}$, $B^i_k = (B^i_k)^T$, $i = 1,2,\ldots,n$. 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.

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

(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

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

(9)

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

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

(10)

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

$$
B_k = (B^1_k, B^2_k, \ldots, B^n_k), \quad B^i_k \in R^{n \times n}, \quad B^i_k = (B^i_k)^T, \quad i = 1,2,\ldots,n
$$

(11)

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

$$
B_{k+1}^i = B^i_k - \frac{B^i_k s_k s_k^T B^i_k}{s_k^T B^i_k s_k} + \frac{y^i_k (y^i_k)^T}{(y^i_k)^T s_k}, \quad i = 1,2,\ldots,n.
$$

(12)
Note that the operators \( B_{k+1} \) satisfy the equation
\[
B_{k+1} s_k = \nabla^2 f(x_{k+1}) - \nabla^2 f(x_k), \quad k = 0,1,2,\ldots
\]  
(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
\[
\frac{\partial^3 f(x)}{\partial x_i \partial x_j \partial x_l} = \frac{\partial^3 f(x)}{\partial x_j \partial x_i \partial x_l} = \cdots = \frac{\partial^3 f(x)}{\partial x_l \partial x_j \partial x_i}, \quad i, j, l = 1,2,\ldots, n .
\]  
(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 aproximations 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
\[
E s_k = \nabla^2 f(x_{k+1}) - \nabla^2 f(x_k) - B_k s_k = Y .
\]  
(16)

In that case we have to solve the problem
\[
\min \left\| E \right\|^2 , \quad \left\| E \right\|^2 = \sum_{i=1}^{n} \sum_{j=1}^{n} \sum_{k=1}^{n} E_{ijk}^2
\]  
(17)

under constraints
\[
E s = Y , \quad s \in R^n , \quad Y \in R^{n \times n} , \quad Y = Y^T
\]  
(18)

and
\[
E_{ijk} = E_{ikj} = E_{jik} = E_{jki} = E_{kij} , \quad i, j, k = 1,2,\ldots, n .
\]  
(19)

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

Let \( \Lambda \in R^{n \times n} \). In our case the lagrangian has the form
\[
L(E, \Lambda) = \frac{1}{2} \left\| E \right\|^2 + \sum_{i=1}^{n} \sum_{j=1}^{n} \sum_{k=1}^{n} \Lambda_{ij} \left( \sum_{k=1}^{n} E_{ijk} s_k - Y_{ij} \right) .
\]  
(20)
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

\[
E_{pqr} = -\frac{1}{3} (\Lambda_{pq} s_r + \Lambda_{pr} s_q + \Lambda_{qr} s_p) \quad \text{for} \quad 1 \leq p \leq q \leq r \leq n.
\]

(22)

Now, the equation \( Es = Y \) has the form

\[
\sum_{i=1}^{n} (\Lambda_{ji} s_i + \Lambda_{ij} s_j + \Lambda_{ji} s_i) s_i = -3Y_i \quad 1 \leq i \leq j \leq n
\]

(23)

or is in the matrix form

\[
\Lambda s^T + ss^T \Lambda = -3Y.
\]

(24)

Therefore

\[
s^T \Lambda s = \frac{1}{\|s\|^2} s^T Ys, \quad u = \Lambda s = \frac{1}{2\|s\|^2} (-3Ys + s^T Ys s). \]

(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 \( x_0 \in R^n \) and \( B_0 = (B_1^0, B_2^0, \ldots, B_n^0) \) - 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
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\[ H_k = \frac{1}{t} \int_0^t \nabla^3 f(x_k + t(x_{k+1} - x_k)) dt, \quad (27) \]

\[ L_k = \{ X \in \mathbb{R}^{n \times n} : X s_k = \nabla^2 f(x_{k+1}) - \nabla^2 f(x_k) \}, \quad (28) \]

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

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

\[ H_k s_k = \nabla^2 f(x_{k+1}) - \nabla^2 f(x_k), \quad (30) \]

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

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

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

\[ \sum_{k=0}^{\infty} \|B_{k+1} - B_k\|^2 < \infty. \quad (32) \]

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

References