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

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

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

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

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

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

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

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

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where $s_k$ is the solution of the system of quadratic equations

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

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.

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

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

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

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

$$\det(\nabla^2 f(x^*)) = 0, \quad \|\nabla f(x)\| \geq c \|x - x^*\|^2, \quad c > 0, \quad x \in D, \tag{8}$$

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

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

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

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

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

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

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

$$B_{k+1}^i = B_k^i - \frac{B_k^i s_k s_k^T B_k^i}{s_k^T B_k^i s_k} + \frac{y_k^i (y_k^i)^T}{(y_k^i)^T s_k}, \quad i = 1, 2, \cdots, n. \tag{12}$$
Note that the operators $B_{k+1}$ satisfy the equation
\[ B_{k+1} s_k = \nabla^2 f(x_{k+1}) - \nabla^2 f(x_k), \quad k = 0, 1, 2, \ldots \] \hfill (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
\[ \frac{\partial^3 f(x)}{\partial x_i \partial x_j \partial x_l} = \frac{\partial^3 f(x)}{\partial x_l \partial x_j \partial x_i} = \cdots = \frac{\partial^3 f(x)}{\partial x_i \partial x_j \partial x_l}, \quad i, j, l = 1, 2, \ldots, n. \] \hfill (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
\[ B_{k+1} = B_k + E, \] \hfill (15)
then
\[ E s_k = \nabla^2 f(x_{k+1}) - \nabla^2 f(x_k) - B_k s_k = Y. \] \hfill (16)

In that case we have to solve the problem
\[ \min \|E\|^2, \quad \|E\|^2 = \sum_{i=1}^{n} \sum_{j=1}^{n} \sum_{k=1}^{n} E_{ijk}^2 \] \hfill (17)
under constraints
\[ E s = Y, \quad s \in R^n, \quad Y \in R^{n \times n}, \quad Y = Y^T \] \hfill (18)
and
\[ E_{ijk} = E_{jki} = E_{jik} = E_{kji} = E_{lijk} = E_{kjl}, \quad i, j, k = 1, 2, \ldots, n. \] \hfill (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
\[ L(E, \Lambda) = \frac{1}{2} \|E\|^2 + \sum_{i=1}^{n} \sum_{j=1}^{n} \Lambda_{ij} \left( \sum_{k=1}^{n} E_{ijk} s_k - Y_{ij} \right). \] \hfill (20)
From this we have
\[ \frac{\partial L(E, \Lambda)}{\partial E_{pq}} = E_{pqr} + \Lambda_{pq} s_r = 0. \]  
(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
\[ E_{pqr} = -\frac{1}{3}(\Lambda_{pq} s_r + \Lambda_{pr} s_q + \Lambda_{qr} s_p) \text{ for } 1 \leq p \leq q \leq r \leq n. \]  
(22)

Now, the equation \( Es = Y \) has the form
\[ \sum_{i=1}^{n} (\Lambda_{ij} s_i + \Lambda_{ji} s_j + \Lambda_{ji} s_j) s_i = -3Y_{ij} \text{ for } 1 \leq i \leq j \leq n \]  
(23)
or is in the matrix form
\[ \Lambda \|s\|^2 + \Lambda s s^T + s s^T \Lambda = -3Y. \]  
(24)

Therefore
\[ s^T \Lambda s = -\frac{1}{\|s\|^2} s^T Ys, \quad u = \Lambda s = \frac{1}{2\|s\|^2} (-3Ys + s^T Ys) / \|s\|^2 \]  
(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 \( B_0 = (B_0^1, B_0^2, \ldots, B_0^n) \) - 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
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\[ H_k = \int_0^1 \nabla^3 f(x_k + t(x_{k+1} - x_k)) dt, \quad (27) \]

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

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

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

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

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