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

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

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

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

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

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

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where \( s_k \) is the solution of the system of quadratic equations

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

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 aproximation 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}) \), \( B_{k}^{i} \in \mathbb{R}^{n \times n}, B_{k}^{i} = (B_{k}^{i})^T, i = 1,2,\cdots, n \) \tag{11}\]

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

\[
B_{k+1}^{i} = B_{k}^{i} - \frac{B_{k}^{i} s_k s_k^T B_{k}^{i}}{s_k^T B_{k}^{i} s_k} + \frac{y'_k (y'_k)^T}{(y'_k)^T s_k}, \quad i = 1,2,\cdots, n. \tag{12}\]
Note that the operators $B_{k+1}$ satisfy the equation
\[ B_{k+1} s_k = \nabla^2 f(x_{k+1}) - \nabla^2 f(x_k), \quad k = 0, 1, 2, \ldots \] (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
\[ \frac{\partial^3 f(x)}{\partial x_i \partial x_j \partial x_l} = \frac{\partial^3 f(x)}{\partial x_i \partial x_j \partial x_l} = \cdots = \frac{\partial^3 f(x)}{\partial x_i \partial x_j \partial x_l}, \quad i, j, l = 1, 2, \ldots, n . \] (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 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
\[ E s_k = \nabla^2 f(x_{k+1}) - \nabla^2 f(x_k) - B_k s_k = Y . \] (16)
In that case we have to solve the problem
\[ \min \|E\|^2 , \quad \|E\|^2 = \sum_{i=1}^{n} \sum_{j=1}^{n} \sum_{k=1}^{n} E_{ijk}^2 \] (17)
under constraints
\[ E s = Y, \quad s \in R^n, \quad Y \in R^{n \times n}, \quad Y = Y^T \] (18)
and
\[ E_{ijk} = E_{sij} = E_{sji} = E_{jsi} = E_{skj} = E_{ksj}, \quad i, j, k = 1, 2, \ldots, n . \] (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
\[ L(E, \Lambda) = \frac{1}{2} \|E\|^2 + \sum_{i=1}^{n} \sum_{j=1}^{n} \Lambda_{ij} (\sum_{k=1}^{n} E_{ijk} s_k - Y_{ij}) . \] (20)
From this we have
\[
\frac{\partial L(E, \Lambda)}{\partial E_{pq r}} = E_{pq r} + \Lambda_{pq s_r} = 0 .
\] (21)

The fact \( E_{pqr} = E_{qrp} \) implies \( \Lambda = \Lambda^T \). Since the operator \( E \) is threefold symmetric then equation (21) may be written as
\[
E_{pqr} = -\frac{1}{3}(\Lambda_{pq s_r} + \Lambda_{qr s_p} + \Lambda_{pr s_q}) \quad \text{for} \quad 1 \leq p \leq q \leq r \leq n .
\] (22)

Now, the equation \( Es = Y \) has the form
\[
\sum_{i=1}^{n}(\Lambda_{q,s_i} + \Lambda_{r,s_j} + \Lambda_{s,s_j})s_i = -3Y_y \quad 1 \leq i \leq j \leq n
\] (23)
or is in the matrix form
\[
\Lambda\|s\|^2 + \Lambda s s^T + s s^T \Lambda = -3Y .
\] (24)
Therefore
\[
s^T \Lambda s = -\frac{1}{\|s\|^2} s^T Y s, \quad u = \Lambda s = \frac{1}{2\|s\|^2}(-3Y_s + \frac{s^T Y}{\|s\|^2}s) .
\] (25)
Finally
\[
\Lambda = -\frac{1}{\|s\|^2}(3Y + us + su^T) .
\] (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 \( B_0 = (B^1_0, B^2_0, \cdots, B^n_0) \) - 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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\[ H_k = \int_0^1 \nabla^3 f(x_k + t(x_{k+1} - x_k)) dt, \]  
(27)

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

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

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

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

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

References


