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

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

(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

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

(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

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

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

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

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

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

$$\det(\nabla^2 f(x^*)) = 0, \text{ and } \|\nabla f(x)\| \geq c \|x - x^*\|^2, \ c > 0, \ x \in D,$$  \hspace{1cm} (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

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

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

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

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

$$B_k = (B^i_k, B^2_k, \ldots, B^n_k), B^i_k \in R^{n \times n}, B^i_k = (B^i_k)^T, \ i = 1, 2, \ldots, n$$  \hspace{1cm} (11)

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

$$B'_{k+1} = B'_k - \frac{B'_k s_k y^i_k B'_k}{s_k^T B'_k s_k} + \frac{y^i_k (y^i_k)^T}{(y^i_k)^T s_k}, \ i = 1, 2, \ldots, n.$$  \hspace{1cm} (12)
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Note that the operators \( B_{k+1} \) satisfy the equation
\[
B_{k+1}s_k = \nabla^2 f(x_{k+1}) - \nabla^2 f(x_k), \ k = 0,1,2,\cdots \tag{13}
\]
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
\[
\frac{\partial^3 f(x)}{\partial x_i \partial x_j \partial x_l} = \frac{\partial^3 f(x)}{\partial x_i \partial x_j \partial x_l} = \cdots = \frac{\partial^3 f(x)}{\partial x_i \partial x_j \partial x_l}, \ i,j,l = 1,2,\cdots, n . \tag{14}
\]
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
\[
B_{k+1} = B_k + E , \tag{15}
\]
then
\[
E s_k = \nabla^2 f(x_{k+1}) - \nabla^2 f(x_k) - B_k s_k = Y . \tag{16}
\]
In that case we have to solve the problem
\[
\min \|E\|^2, \ |E|^2 = \sum_{i=1}^{n} \sum_{j=1}^{n} \sum_{k=1}^{n} E_{ijk}^2 \tag{17}
\]
under constraints
\[
E s = Y, \ s \in R^n, \ Y \in R^{n \times n}, \ Y = Y^T \tag{18}
\]
and
\[
E_{ijk} = E_{ikj} = E_{jik} = E_{jki} = E_{kij} = E_{kji}, \ i,j,k = 1,2,\cdots, n . \tag{19}
\]

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
\[
L(E, \Lambda) = \frac{1}{2} \|E\|^2 + \sum_{i=1}^{n} \sum_{j=1}^{n} \sum_{k=1}^{n} \Lambda_{ij} (\sum_{k=1}^{n} E_{ijk} s_k - Y_{ij}) . \tag{20}
\]
From this we have

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

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

\[
E_{pq} = -\frac{1}{3} (\Lambda_{pq} s_r + \Lambda_{pr} s_q + \Lambda_{rq} s_p) \quad 1 \leq p \leq q \leq r \leq n. \tag{22}
\]

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

\[
\sum_{i=1}^{n} (\Lambda_{qi} s_i + \Lambda_{ji} s_j + \Lambda_{ji} s_i) s_i = -3Y_i \quad 1 \leq i \leq j \leq n \tag{23}
\]

or is in the matrix form

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

Therefore

\[
s^T \Lambda s = -\frac{1}{\|s\|^2} s^T Y s, \quad u = \Lambda s = \frac{1}{2\|s\|^2} (-3Ys + s^T Y s) \tag{25}
\]

Finally

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

To calculate the new threefold symmetric update \( B_{k+1} = B_k + E \) we use the formulæ (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 \( B_0 = (B_1^0, B_2^0, \cdots, B_n^0) \) - 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 formulæ 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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\begin{equation}
H_k = \frac{1}{t} \int_0^t \nabla^3 f(x_k + t(x_{k+1} - x_k)) dt,
\end{equation}

\begin{equation}
L_k = \{ X \in \mathbb{R}^{n \times n \times n} : Xs_k = \nabla^2 f(x_{k+1}) - \nabla^2 f(x_k) \},
\end{equation}

\begin{equation}
Q = \{ X \in \mathbb{R}^{n \times n \times n} : X \text{ is threefold symmetric operator} \}.
\end{equation}

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

\begin{equation}
H_k s_k = \nabla^2 f(x_{k+1}) - \nabla^2 f(x_k),
\end{equation}

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

\begin{equation}
\| B_{k+1} - H_k \|^2 + \| B_k - B_{k+1} \|^2 = \| B_k - H_k \|^2 \quad k = 0, 1, 2, \ldots
\end{equation}

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

\begin{equation}
\sum_{k=0}^{\infty} \| B_{k+1} - B_k \|^2 < \infty.
\end{equation}

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

References


