Superquadraticly convergent methods for minimization functions

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Abstract
In the paper locally superquadratically convergent methods for minimization functions are considered. Threetfold 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

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

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

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

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

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

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

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

(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.

\section{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

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

(10)

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

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

(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

\[
B_{k+1}^i = B_k^i - \frac{B_k^i s_k s_k^T B_k^i}{s_k^T B_k^i s_k} + \frac{y_k^i (y_k^i)^T}{(y_k^i)^T s_k}, \quad i = 1, 2, \cdots, n.
\]

(12)
Note that the operators $B_{k+1}$ satisfy the equation

$$B_{k+1} = \nabla^2 f(x_{k+1}) - \nabla^2 f(x_k), \quad k = 0, 1, 2, \ldots$$  \hspace{1cm} (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

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

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

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

then

$$E s_k = \nabla^2 f(x_{k+1}) - \nabla^2 f(x_k) - B_k s_k = Y. \hspace{1cm} (16)$$

In that case we have to solve the problem

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

under constraints

$$E s = Y, \quad s \in R^n, \quad E \in R^{n \times n}, \quad Y = Y^T \hspace{1cm} (18)$$

and

$$E_{ijk} = E_{skj} = E_{jik} = E_{ksj} = E_{kj} = E_{ki}, \quad i, j, k = 1, 2, \ldots, n. \hspace{1cm} (19)$$

**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

$$L(E, \Lambda) = \frac{1}{2} \|E\|^2 + \sum_{i=1}^{n} \sum_{j=1}^{n} \Lambda_{ij} (\sum_{k=1}^{n} E_{ijk} s_k - Y_{ij}) \hspace{1cm} (20)$$
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
\[
\sum_{i=1}^{n} (\Lambda_{ij}s_i + \Lambda_{ji}s_j + \Lambda_{ji}s_j)s_i = -3Y_{ij} \quad 1 \leq i \leq j \leq n
\] (23)
or is in the matrix form
\[
\Lambda \|s\|^2 + \Lambda ss^T + ss^T \Lambda = -3Y.
\] (24)

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

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

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

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

The set \( Q \) is linear subspace in \( R^{n \times n} \) 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