Superquadraticly convergent methods for minimization functions

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Abstract

In the paper locally superquadraticly 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

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

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

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

Let \( B_k \) be a matrix, \( B_k \in \mathbb{R}^{n \times n} \), \( B_k = (B_k^i) \), \( i = 1,2,\ldots, n \). The sequence \( \{x_k\} \) is 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
\[
B_{k+1} = B_k - \frac{B_k s_k s_k^T B_k}{s_k^T B_k s_k} + \frac{y_k y_k^T}{y_k^T s_k}, \quad y_k = \nabla f(x_{k+1}) - \nabla f(x_k).
\]

The DFP formula, for nonsingular problems, guarantees local superlinear convergence of the method
\[
x_{k+1} = x_k + s_k, \quad B_k s_k = -\nabla f(x_k), \quad k = 0,1,2,\ldots
\]

We may use the DFP formula to approximate the operator \( \nabla^2 f(x_k) \). Namely, let
\[
B_k = (B_k^i), \quad B_k^i \in \mathbb{R}^{n \times n}, \quad B_k^i = (B_k^i)^T, \quad i = 1,2,\ldots, n
\]

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
\[
B_{k+1}^i = B_k^i - \frac{B_k^i s_k s_k^T B_k^i}{s_k^T B_k^i s_k} + \frac{y_k^i (y_k^i)^T}{y_k^i s_k}, \quad i = 1,2,\ldots, n.
\]
Note that the operators $B_{k+1}$ satisfy the equation

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

(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

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

(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

$$\min \|E\|^2, \ \|E\|^2 = \sum_{i=1}^{n} \sum_{j=1}^{n} \sum_{k=1}^{n} E_{ijk}^2$$

(17)

under constraints

$$Es = Y, \ s \in R^n, \ Y \in R^{n \times n}, \ Y = Y^T$$

(18)

and

$$E_{ijk} = E_{skj} = E_{jisk} = E_{ksij} = E_{jski}, \ i,j,k = 1,2,\cdots,n.$$  

(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
\[
\frac{\partial L(E, \Lambda)}{\partial E_{pqr}} = E_{pqr} + \Lambda_{pq} s_r = 0 .
\] (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
\[
E_{pqr} = -\frac{1}{3}(\Lambda_{pq} s_r + \Lambda_{pr} s_q + \Lambda_{qp} s_p) \quad \text{for} \quad 1 \leq p \leq q \leq r \leq n .
\] (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
\[
\Lambda s^T s + \Lambda s^T s = -3Y .
\] (24)

Therefore
\[
s^T \Lambda s = -\frac{1}{2} \frac{s^T Ys}{\|s\|^2} + \frac{1}{2} \frac{s^T Ys}{\|s\|^2} (\Lambda s^T s + \Lambda s^T s) .
\] (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 \(x_0 \in \mathbb{R}^n\) 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
Superquadratically convergent methods for minimization functions

\[ H_k = \frac{1}{0} \nabla^3 f(x_k + t(x_{k+1} - x_k))dt \tag{27} \]

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

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

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

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

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

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

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

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

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

References