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

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

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

$$\|x_{k+1} - x^*\| \leq c \|x_k - x^*\|^2. \quad (2)$$

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

$$x_{k+1} = x_k + t_k s_k, \ t_k \in \mathbb{R}, \ k = 0,1,2, \ldots \quad (3)$$

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

$$x_{k+1} = x_k + s_k, \ k = 0,1,2, \ldots \quad (4)$$

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where $s_k$ is the solution of the system of quadratic equations
\[ \nabla f(x_k) + \nabla^2 f(x_k) s_k + \frac{1}{2}(\nabla^3 f(x_k) s_k, s_k) = 0. \] (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 $B_k = (B^1_k, B^2_k, \cdots, B^n_k)$, $B_k \in \mathbb{R}^{n \times n}$, $B^i_k = (B^i_k)^T$, $i = 1, 2, \cdots, n$. 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.
\[ \det(\nabla^2 f(x^*)) = 0, \quad \|\nabla f(x)\| \geq c\|x - x^*\|^2, \quad c > 0, \quad x \in D, \] (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.

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
\[ B_{k+1} = B_k - \frac{B_k s_k s_k^T y_k y_k^T}{s_k^T B_k s_k} + \frac{y_k y_k^T}{y_k^T s_k}, \quad y_k = \nabla f(x_{k+1}) - \nabla f(x_k). \] (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
\[ B^i_k = (B^1_k, B^2_k, \cdots, B^n_k), \quad B^i_k \in \mathbb{R}^{n \times n}, \quad B^i_k = (B^i_k)^T, \quad i = 1, 2, \cdots, n \] (11)
and let $\nabla^2_i f(x_k)$ denote i-th column of the matrix $\nabla^2 f(x_k)$, $y^i_k = \nabla^2 f(x_{k+1}) - \nabla^2_i f(x_k)$. Then
\[ B^i_{k+1} = B^i_k - \frac{B^i_k s_k s_k^T B^i_k}{s_k^T B^i_k s_k} + \frac{y^i_k (y^i_k)^T}{(y^i_k)^T s_k}, \quad i = 1, 2, \cdots, n. \] (12)
Note that the operators $B_{k+1}$ satisfy the equation

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

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

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

and

$$E_{g_{ik}} = E_{g_{kj}} = E_{jik} = E_{jki} = E_{s_{ij}} = E_{s_{ji}} \quad i, j, k = 1, 2, \ldots, n.$$ \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

$$L(E, \Lambda) = \frac{1}{2} \|E\|^2 + \sum_{i=1}^{n} \sum_{f=1}^{n} \Lambda_{ij} (\sum_{k=1}^{n} E_{g_{ik}} s_{k} - Y_{ij}).$$ \hspace{1cm} (20)
From this we have
\[ \frac{\partial L(E, \Lambda)}{\partial E_{pq}} = E_{pq} \Lambda + \Lambda_{pq} s_r = 0. \] (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
\[ E_{pq} = -\frac{1}{3} (\Lambda_{pq} s_r + \Lambda_{pr} s_q + \Lambda_{qr} s_p) \text{ for } 1 \leq p \leq q \leq r \leq n. \] (22)

Now, the equation \( E s = Y \) has the form
\[ \sum_{i=1}^{n} (\Lambda_{ij} s_i + \Lambda_{ji} s_j + \Lambda_{ij} s_i) s_i = -3Y_{ij} \quad 1 \leq i \leq j \leq n \] (23)

or is in the matrix form
\[ \Lambda \|s\|^2 + \Lambda s s^T + s s^T \Lambda = -3Y. \] (24)

Therefore
\[ s^T \Lambda s = -\frac{1}{\|s\|^2} s^T Y s, \quad u = \Lambda s = \frac{1}{2\|s\|^2} (-3Y s + s^T Y s). \] (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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\[ H_k = \frac{1}{t} \int_0^t \nabla^3 f(x_k + t(x_{k+1} - x_k)) dt, \quad (27) \]
\[ L_k = \{ X \in R^{n \times n \times n} : Xs_k = \nabla^2 f(x_{k+1}) - \nabla^2 f(x_k) \}, \quad (28) \]
\[ Q = \{ X \in R^{n \times n \times n} : X \text{ is threefold symmetric operator} \}. \quad (29) \]

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