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

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

If the matrix $\nabla^2 f(x^*)$ is nonsingular then Newton method is locally quadraticly convergent to x^*, i.e. there exist $c > 0$ and $\varepsilon > 0$ such that, if $\|x^* - x_0\| < \varepsilon$, then

$$\|x_{k+1} - x^*\| \le c \|x_k - x^*\|^2. \tag{2}$$

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

$$x_{k+1} = x_k + t_k s_k,\ t_k \in R,\ k = 0,1,2,\cdots \tag{3}$$

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

$$x_{k+1} = x_k + s_k,\ k = 0,1,2,\cdots \tag{4}$$

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where s_k is the solution of the system of quadratic equations

$$\nabla f(x_k) + \nabla^2 f(x_k)s_k + \frac{1}{2}(\nabla^3 f(x_k)s_k, s_k) = 0\,. \tag{5}$$

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 superquadraticly convergent to x^*, i.e.

$$\lim_{k\to\infty} \frac{\left\| x_{k+1} - x^* \right\|}{\left\| x_k - x^* \right\|^2} = 0\,. \tag{6}$$

Let $B_k = (B_k^1, B_k^2, \cdots, B_k^n)$, $B_k^i \in R^{n\ x\ n}$, $B_k^i = (B_k^i)^T$, $i = 1,2,\cdots,n$. 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 $\min_{x\in D} f\left(x\right)$ is regularly singular at x^*, i.e.

$$\det(\nabla^2 f(x^*)) = 0, \ \text{ and } \ \left\|\nabla f(x)\right\| \geq c\left\|x - x^*\right\|^2,\ c > 0,\ x \in D\,, \tag{8}$$

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

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

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

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

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

$$B_k = (B_k^1, B_k^2, \cdots, B_k^n),\ B_k^i \in R^{n\ x\ n},\ B_k^i = (B_k^i)^T,\ i = 1,2,\cdots,n \tag{11}$$

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

$$B_{k+1}^i = B_k^i - \frac{B_k^i s_k s_k^T B_k^i}{s_k^T B_k^i s_k} + \frac{y_k^i (y_k^i)^T}{(y_k^i)^T s_k},\ i = 1,2,\cdots,n\,. \tag{12}$$

Note that the operators B_{k+1} satisfy the equation

$$B_{k+1}s_k = \nabla^2 f(x_{k+1}) - \nabla^2 f(x_k),\ k = 0,1,2,\cdots \tag{13}$$

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

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

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

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

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

$$Es = Y,\ s \in R^n,\ Y \in R^{n\ x\ n},\ Y = Y^T \tag{18}$$

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 $\Lambda \in R^{n\ x\ n}$. In our case the lagrangian has the form

$$L(E,\Lambda) = \frac{1}{2}\|E\|^2 + \sum_{i=1}^{n}\sum_{j=1}^{n}\Lambda_{ij}\left(\sum_{k=1}^{n} E_{ijk}s_k - Y_{ij}\right). \tag{20}$$

From this we have

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

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

$$E_{pqr} = -\frac{1}{3}(\Lambda_{pq} s_r + \Lambda_{pr} s_q + \Lambda_{qr} s_p) \quad \text{for} \quad 1 \le p \le q \le r \le n \,. \tag{22}$$

Now, the equation $Es = Y$ has the form

$$\sum_{l=1}^{n} (\Lambda_{ij} s_l + \Lambda_{il} s_j + \Lambda_{jl} s_i) s_l = -3Y_{ij} \quad 1 \le i \le j \le n \tag{23}$$

or is in the matrix form

$$\Lambda \|s\|^2 + \Lambda s s^T + s s^T \Lambda = -3Y \,. \tag{24}$$

Therefore

$$s^T \Lambda s = -\frac{1}{\|s\|^2} s^T Y s, \; u = \Lambda s = \frac{1}{2\|s\|^2}(-3Ys + \frac{s^T Y s}{\|s\|^2} s) \,. \tag{25}$$

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 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 $B_0 = (B_0^1, B_0^2, \cdots, B_0^n)$ - 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

$$H_k = \int_0^1 \nabla^3 f(x_k + t(x_{k+1} - x_k))dt\,, \tag{27}$$

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

$$Q = \{X \in R^{n\,x\,n\,x\,n} : X \text{ is threefold symmetric operator}\}. \tag{29}$$

The set Q is linear subspace in $R^{n\,x\,n\,x\,n}$ 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

$$\|B_{k+1} - H_k\|^2 + \|B_k - B_{k+1}\|^2 = \|B_k - H_k\|^2 \quad k = 0,1,2,\cdots \tag{31}$$

The inequality $\|B_{k+1} - H_k\| \le \|B_k - H_k\|$ 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].

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