Superquadraticly convergent methods for minimization functions

Stanisław M. Grzegórski[*], Edyta Łukasik

Department of Computer Science, Lublin University of Technology,
Nadbystrzycka 36b, 20-618 Lublin, Poland

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

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

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

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

---

[*] Corresponding author: *e-mail address*: s.grzegorski@pollub.pl

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

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

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

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

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

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

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

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

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

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

From this we have

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

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

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

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

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

Therefore

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

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

$$\nabla f(x_k) + \nabla^2 f(x_k)s_k + \frac{1}{2}(B_ks_k, s_k) = 0 ,$$

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

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

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

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

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

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

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].

References

[1] Davidon W.C.,*Variable metric method for minimization*, Report ANL-5990 Rev (1959), Argonne National Laboratories, Ill.

[2] Fletcher R., Powell M.J.D., *A rapidly convergent descent method for minimization*, Comput. J., 6 (1963) 163.

[3] Grzegórski S.M., *Orthogonal projections on convex sets for Newton-like methods*, SIAM J. on Numer. Anal., 22 (1985) 1208.

[4] Grzegórski S.M., Łukasik E., *Theory of convergence for 2-rank iterative methods*, prepared for publication.

[5] Ortega J.M., Rheinboldt W.C., *Iterative Solution of Nonlinear Solution in Several Variables*, Academic Press, New York, London, (1970).