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带有广义 Wolfe 线搜索的变尺度算法的收敛性

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摘 要

本文提出一类广义 Wolfe 线搜索模型, 并且把它与著名的 BFGS 方法相结合, 对于所得到的算法证明了: 对于凸函数算法具有全局收敛性和超线性收敛速度. 这推广了参考文献[1]中的结果.

Global Convergence of the Variable Metric Algorithms with a Generalized Wolfe Linesearch *

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Abstract In this paper, we present a generalized Wolfe linesearch method, and apply it to the well-known BFGS algorithm, for which we obtain the global convergence and superlinear convergence, our results are extension of those in [1].

Keywords BFGS method, generalized Wolfe linesearch, global convergence, super-linear convergence.

Classification AMS(1991) 90C30/CCL O221.2

1. Introduction

We discuss the unconstrained optimization problem:

$$\min f(z)$$

where $f : R^n \rightarrow R^1, f \in C^1$, which is solved by means of iterative methods, $x_{k+1} = x_k + \lambda_k d_k (k = 0, 1, \dots)$, in which x_0 is any given starting point, $d_0 = -H_0 g_0$, H_0 is any given $n \times n$ symmetric positive definite matrix, and $d_k = -H_k g_k$, $H_k = B_k^{-1}$ is iterated by the following BFGS formula

$$B_{k+1} = B_k - \frac{B_k S_k S_k^T B_k}{S_k^T B_k S_k} + \frac{y_k y_k^T}{S_k^T y_k}, \quad (1)$$

where $S_k = x_{k+1} - x_k$, $y_k = g(x_{k+1}) - g(x_k)$, g denotes the gradient ∇f of f . The BFGS algorithm is regarded as one of the most efficient algorithm in nonlinear optimization, and used more often, so in the following sections we shall discuss its properties.

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It is known to us that the Wolfe linesearch method is often used in both the theoretical analysis and application of algorithms. Applying Wolfe linesearch method to the BFGS algorithm, Powell ([1]) got some nice properties of BFGS algorithm. We extend Wolfe linesearch to a generalized Wolfe linesearch, which is described as **GW linesearch method**: Select the steplength λ_k satisfying

$$f(x_{k+1}) \leq f(x_k) + \varepsilon_1 \lambda_k g_k^T d_k, \quad (2)$$

$$g(x_{k+1})^T d_k \geq \max\{\varepsilon_2, 1 - (\lambda_k \|d_k\|)^p\} g_k^T d_k, \quad (3)$$

where $\varepsilon_1 \in (0, 1)$, $\varepsilon_2 \in (0, \frac{1}{2})$, $p \in (-\infty, 1)$. Using this new linesearch method, we shall extend the results of [1].

2. Some Lemmas

We give the assumption

- (H) (i) the level set $L_0 = \{x | f(x) \leq f(x_1)\}$ is bounded.
(ii) the objective function f is convex on L_0 .
(iii) $f \in C^2$, moreover, there exists a constant $M > 0$, such that

$$\|G(x)\| \leq M,$$

where $G(x) = \nabla^2 f(x)$.

Lemma 1^[2] Assume that (H) holds. Then there exists a positive number M_1 such that

$$\frac{\|y_k\|^2}{y_k^T S_k} \leq M_1, \quad k = 1, 2, \dots$$

Lemma 2 If the sequence of nonnegative numbers $m_k, k = 1, 2, \dots$ is such that

$$\prod_{j=1}^k m_j \geq c_1^k, \quad c_1 > 0, k = 1, 2, \dots$$

Then $\limsup_k m_k > 0$.

Proof We, by contradiction, assume that $\limsup_k m_k = 0$, then, for $0 < \varepsilon < c_1$, there exist $k_0 > 0$, such that $m_k < \varepsilon$, for all $k \geq k_0$. Hence, for all $k > k_0$,

$$c_1^k \leq \prod_{j=1}^{k_0-1} m_j \prod_{j=k_0}^k \varepsilon, \quad \left(\frac{c_1}{\varepsilon}\right)^k \leq \left(\prod_{j=1}^{k_0-1} m_j\right) \varepsilon^{1-k_0},$$

$$+\infty = \limsup_k \left(\frac{c_1}{\varepsilon}\right)^k \leq \left(\prod_{j=1}^{k_0-1} m_j\right) \varepsilon^{1-k_0} < +\infty,$$

which is a contradiction, thus, $\limsup_k m_k > 0$.

Lemma 3^[4] $\det(B_{k+1}) = \det(B_k) \frac{y_k^T S_k}{S_k^T B_k S_k}$, where $\det(B_k)$ denotes the determinate of B_k .

Lemma 4 Assume that (H) (i),(iii) hold. Then

$$\lim_k \|g_k\| \cos \theta_k = 0,$$

where $\cos \theta_k = \frac{-g_k^T d_k}{\|g_k\| \|d_k\|}$.

Proof From (H) (iii) it follows that

$$[g(x_k + \lambda_k d_k) - g_k]^T d_k = \lambda_k d_k^T \int_0^1 G(x_k + t\lambda_k d_k) dt \leq \lambda_k \|d_k\|^2 M.$$

On the other hand, from (3) it follows that

$$[g(x_k + \lambda_k d_k) - g_k]^T d_k \geq \max\{\varepsilon_2 - 1, -\|S_k\|^p\} g_k^T d_k = -\min\{1 - \varepsilon_2, \|S_k\|^p\} g_k^T d_k. \quad (4)$$

Thus,

$$\lambda_k \|d_k\|^2 M \geq -\min\{1 - \varepsilon_2, \|S_k\|^p\} g_k^T d_k,$$

i.e.,

$$\|S_k\| \geq \frac{1}{M} \min\{1 - \varepsilon_2, \|S_k\|\} \gamma_k, \quad (5)$$

where $\gamma_k = \frac{-g_k^T d_k}{\|d_k\|}$.

Comparing $\|S_k\|^p$ with $1 - \varepsilon_2$, we easily derive from (5) that

$$\|S_k\| \geq \min\left\{\frac{1 - \varepsilon_2}{M} \gamma_k, \left(\frac{\gamma_k}{M}\right)^{\frac{1}{1-p}}\right\}.$$

Substitute it into (2), we have

$$f(x_{k+1}) \leq f(x_k) - \varepsilon_1 \lambda_k \|d_k\| \gamma_k \leq f(x_k) - \varepsilon_2 \min\left\{\frac{1 - \varepsilon_2}{M} \gamma_k, \left(\frac{\gamma_k}{M}\right)^{\frac{1}{1-p}}\right\} \gamma_k.$$

The assumption (H) (i) implies that $\lim_k [f(x_k) - f(x_{k+1})] = 0$. Therefore,

$$\lim_{k \rightarrow \infty} \|g_k\| \cos \theta_k = \lim_{k \rightarrow \infty} \gamma_k = 0.$$

Lemma 5 Assume that (H) (i),(iii) hold. Then

$$\lim_{k \rightarrow \infty} \max\{\|S_k\|, \|S_k\|^{1-p}\} \|g_k\| \cos \theta_k = 0.$$

Proof (2) implies that

$$\begin{aligned} \varepsilon_1 \lambda_k \|d_k\| \gamma_k &\leq f(x_k) - f(x_{k+1}), \\ \|S_k\| &\leq \frac{f(x_k) - f(x_{k+1})}{\varepsilon_1 \|g_k\| \cos \theta_k}, \end{aligned}$$

hence,

$$0 \leq \max\{\|S_k\|, \|S_k\|^{1-p}\} \|g_k\| \cos \theta_k \leq \max\left\{\frac{f(x_k) - f(x_{k+1})}{\varepsilon_1}, (M_0)^{1-p} \|g_k\| \cos \theta_k\right\},$$

where M_0 is a constant satisfying $\|S_k\| \leq M_0$.

From Lemma 4 and (H) (i) it is easy to see that this lemma is true.

3. Global Convergence of BFGS Algorithm Using the GW Linesearch Method

Theorem 1 Assume that (H) holds. Suppose that x_0 is any starting point, B_0 is any symmetric positive definite matrix, and that the sequence $\{x_k\}$ is generated by the BFGS algorithm, in which the stepsize λ_k is determined by the GW linesearch method (2),(3). Then $\lim_k \inf \|g_k\| = 0$.

Proof We, by contradiction, assume that $\liminf_k \|g_k\| > 0$, i.e., there exists $c_2 > 0$ such that

$$\|g_k\| \geq c_2, \quad k = 0, 1, \dots \quad (6)$$

From (1) we have

$$\text{Tr}(B_{k+1}) = \text{Tr}(B_k) - \frac{\|B_k S_k\|^2}{S_k^T B_k S_k} + \frac{\|y_k\|^2}{y_k^T S_k}, \quad (7)$$

where $\text{Tr}(B_k)$ denotes the trace of B_k . From (6), (7) and Lemma 1 we have

$$\begin{aligned} 0 < \text{Tr}(B_{k+1}) &\leq \text{Tr}(B_k) - \frac{\|g_k\|^2}{g_k^T H_k g_k} + M_1 \\ &\leq \dots \\ &\leq \text{Tr}(B) - \sum_{j=1}^k \frac{c_2^2}{g_j^T H_j g_j} + kM_1. \end{aligned}$$

Hence

$$\begin{aligned} \text{Tr}(B_{k+1}) &\leq \text{Tr}(B_1) + kM_1. \\ \sum_{j=1}^k \frac{1}{g_j^T H_j g_j} &\leq \frac{\text{Tr}(B_1) + kM_1}{c_2^2} \end{aligned} \quad (8)$$

From the geometric-arithmetic mean value formula we have

$$\prod_{j=1}^k g_j^T H_j g_j \geq \left[\frac{kc_2^2}{\text{Tr}(B_1) + kM_1} \right]^k \quad (9)$$

(4) and Lemma 3 imply that

$$\det(B_{k+1}) = \det(B_k) \frac{[g(x_{k+1}) - g_k]^T d_k}{\lambda_k g_k^T H_k g_k}$$

$$\begin{aligned}
&\geq \det(B_k) \frac{\min\{1 - \epsilon_2, \|S_k\|^p\}}{\lambda_k} \\
&\geq \det(B_1) \prod_{j=1}^k \frac{\min\{1 - \epsilon_2, \|S_j\|^p\}}{\lambda_j}, \\
\prod_{j=1}^k \max\left\{\frac{\lambda_j}{1 - \epsilon_2}, \frac{\lambda_j}{\|S_j\|}\right\} &\geq \frac{\det(B_1)}{\det(B_{k+1})}. \tag{10}
\end{aligned}$$

Again using the geometric-arithmetic mean value formula, we have

$$\det(B_{k+1}) \leq \left[\frac{\text{Tr}(B_{k+1})}{n}\right]^n.$$

Therefore, from (8),(10), we have

$$\begin{aligned}
\prod_{j=1}^k \max\left\{\frac{\lambda_j}{1 - \epsilon_2}, \frac{\lambda_j}{\|S_j\|}\right\} &\geq \frac{\det(B_1)n^n}{[\text{Tr}(B_1) + kM_1]^n} \geq \frac{1}{k^n} \frac{\det(B_1)n^n}{[\text{Tr}(B_1) + M_1]^n} \\
&\geq \left(\frac{1}{e^n}\right)^k \min\left\{\frac{\det(B_1)n^n}{[\text{Tr}(B_1) + M_1]^n}, 1\right\} \geq c_3^k, \tag{11}
\end{aligned}$$

where $c_3 \leq \frac{1}{e^n} \min\left\{\frac{\det(B_1)n^n}{[\text{Tr}(B_1) + M_1]^n}, 1\right\}$.
(9) times (11),

$$\begin{aligned}
&\prod_{j=1}^k \max\left\{\frac{\|S_j\| \|g_j\| \cos \theta_j}{1 - \epsilon_2}, \|g_j\| \cos \theta_j \|S_j\|^{1-p}\right\} \\
&\geq c_3^k \left[\frac{kc_2^2}{\text{Tr}(B_1) + kM_1}\right]^k \geq \left[\frac{c_3c_2^2}{\text{Tr}(B_1) + M_1}\right]^k
\end{aligned}$$

Since

$$\begin{aligned}
&\prod_{j=1}^k \max\left\{\frac{\|S_j\| \|g_j\| \cos \theta_j}{1 - \epsilon_2}, \|g_j\| \cos \theta_j \|S_j\|^{1-p}\right\} \\
&\leq \left(\frac{1}{1 - \epsilon_2}\right)^k \prod_{j=1}^k \max\{\|S_j\|, \|S_j\|^{1-p}\} \|g_j\| \cos \theta_j.
\end{aligned}$$

Thus

$$\prod_{j=1}^k \max\{\|S_j\|, \|S_j\|^{1-p}\} \|g_j\| \cos \theta_j \geq \left[\frac{(1 - \epsilon_2)c_3c_2^2}{\text{Tr}(B_1) + M_1}\right]^k,$$

from Lemma 2 it immediately follows that

$$\limsup_k \max\{\|S_j\|, 1\} \|g_j\| \cos \theta_j > 0,$$

which contradicts Lemma 5. Therefore,

$$\liminf_k \|g_k\| = 0.$$

Theorem 2 Assume that all of the assumptions in Theorem 1 hold, and assume in addition that $G(x)$ is positive definite for all $x \in L_0$. Then $x_k \rightarrow x^*$, $g(x^*) = 0$.

Proof By Theorem 1, we know

$$\liminf_k \|g_k\| = 0.$$

i.e., there exists a subset K of $N = \{1, 2, \dots\}$ such that $\lim_{k \rightarrow K} \|g_k\| = 0$, since the sequence $\{x_k\}$ is bounded, without loss of generality, we assume that

$$\lim_{k \in K} x_k = x^*, \quad \|g(x^*)\| = 0.$$

We shall prove that $\lim_{k \rightarrow \infty} x_k = x^*$. We, by contradiction, assume that,

$$\lim_{k \in K_1} x_k = x^{**}, \quad x^{**} \neq x^*.$$

It is easy to see that $x^* \in L_0$, $x^{**} \in L_0$, and L_0 is a convex set. Since $\{f(x_k)\}$ is monotonically decreasing, we have

$$f(x^*) = \lim_{k \in K} f(x_k) = \lim_{k \in K_1} f(x_k) = f(x^{**}). \quad (12)$$

However, by Taylor formula and (H) we have

$$f(x^{**}) = f(x^*) + (x^{**} - x^*)^T G(\theta x^* + (1 - \theta)x^{**})(x^{**} - x^*) > f(x^*),$$

which contradicts (12). Therefore, $\lim_{k \rightarrow \infty} x_k = x^*$.

4. Superlinear convergence analysis

In this section, we shall assume that f is a uniform convex function, i.e.,

(H') there exists constants $m > 0$ and $M_2 > 0$ such that

$$M_2 y^T y \geq y^T G(x) y \geq m y^T y.$$

In order to get the superlinear convergence of algorithms, as done by most paper, we make the further assumption (\bar{H}): the Hessian matrix G is Lipschitz continuous at x^* , i.e.,

(\bar{H}) there exists a positive constant L such that

$$\|G(x) - G(x^*)\| \leq L \|x - x^*\|,$$

for all x in a neighborhood of x^*

It is easy to verify that the assumption (H') implies the positive definiteness of $G(x)$ on L_0 , and stonger than (H). Under the stonger assumption (H'), we get the following better results.

Lemma 6^[3] Under the assumption (H'), we have

$$\frac{m}{2} \|x_k - x^*\|^2 \leq f(x_k) - f(x^*) \leq \frac{1}{m} \|g_k\|^2.$$

Lemma 7 Under the assumption (H'), there must exist two constants $c_4 > 0$ and $c_5 > 0$ such that

$$\frac{\|y_k\|^2}{y_k^T S_k} \leq c_4, \quad \frac{\|S_k\|^2}{y_k^T S_k} \leq c_5.$$

Proof Noticing

$$y_k = \int_0^1 G(x_k + \xi \lambda_k d_k) d\xi S_k,$$

we can easily derive this Lemma from (H').

Lemma 8 Assume that there exist $c_4 > 0, c_5 > 0$ such that

$$\frac{\|y_k\|^2}{y_k^T S_k} \leq c_4, \quad \frac{\|S_k\|^2}{y_k^T S_k} \leq c_5.$$

Then there exists $c_6 > 0$ such that for all $k \geq 1, \prod_{j=1}^k \cos^2 \theta_j \geq c_6^k$.

Proof From (1) we deduce

$$\begin{aligned} \text{Tr}(B_{k+1}) &= \text{Tr}(B_k) - \frac{\|g_k\|^2}{g_k^T H_k g_k} + c_4 = \text{Tr}(B_k) - \frac{\|g_k\|}{\|H_k g_k\| \cos \theta_k} + c_4 \\ &\leq \dots \leq \text{Tr}(B_1) - \sum_{j=1}^k \frac{\|g_j\|}{\|H_j g_j\| \cos \theta_j} + c_4 k \\ \text{Tr}(B_{k+1}) &\leq \text{Tr}(B_1) + c_4 k, \end{aligned} \quad (13)$$

$$\sum_{j=1}^k \frac{\|g_j\|}{\|H_j g_j\| \cos \theta_j} \leq \text{Tr}(B_1) + c_4 k,$$

$$\prod_{j=1}^k \frac{\|g_k\|}{\|H_j g_j\| \cos \theta_j} \leq \left[\frac{\text{Tr}(B_1) + c_4 k}{k} \right]^k \leq [\text{Tr}(B_1) + c_4]^k. \quad (14)$$

From Lemma 3 and the assumptions in this Lemma we have

$$\det(B_{k+1}) = \det(B_k) \frac{y_k^T S_k}{S_k^T B_k S_k} \geq \det(B_k) \frac{c_5 \|S_k\|^2}{S_k^T B_k S_k}$$

$$\begin{aligned}
&\geq \cdots \geq \det(B_1)c_5^k \prod_{j=1}^k \frac{\|S_j\|^2}{S_j^T B_j S_j} \\
&= \det(B_1)c_5^k \prod_{j=1}^k \frac{\|H_j g_j\|}{\|g_j\| \cos \theta_j}, \\
\prod_{j=1}^k \frac{\|H_j g_j\|}{\|g_j\| \cos \theta_j} &\leq \frac{\det(B_{k+1})}{c_5^k \det(B_1)}.
\end{aligned}$$

Using (11) and (13) we get

$$\begin{aligned}
\prod_{j=1}^k \frac{\|H_j g_j\|}{\|g_j\| \cos \theta_j} &\leq \frac{[\text{Tr}(B_{k+1})]^n}{n^n c_5^k \det(B_1)} \leq \frac{[\text{Tr}(B_1) + c_4 k]^n}{n^n \det(B_1) c_5^k} \\
&\leq \frac{[\text{Tr}(B_1) + c_4]^n}{n^n \det(B_1)} \left(\frac{e^n}{c_5}\right)^k \leq c_7^k,
\end{aligned} \tag{15}$$

where $c_7 \geq \frac{e^n}{c_5} \max\{1, \frac{[\text{Tr}(B_1) + c_4]^n}{n^n \det(B_1)}\}$.
(14) times (15), we obtain

$$\begin{aligned}
\prod_{j=1}^k \frac{1}{\cos^2 \theta_j} &\leq [c_7(\text{Tr}(B_1) + c_4)]^k, \\
\prod_{j=1}^k \cos^2 \theta_j &\geq \left[\frac{1}{c_7(\text{Tr}(B_1) + c_4)}\right]^k,
\end{aligned}$$

Select $c_6 = 1/c_7(\text{Tr}(B_1) + c_4)$.

Theorem 3 Assume that (H') holds. Suppose that x_0 is any starting point, B_0 is any symmetric positive definite matrix, and that the sequence $\{x_k\}$ is generated by the BFGS formula (1), in which the stepsize λ_k satisfies the GW linesearch method. Then

$$\sum_{k=1}^{\infty} \|x_k - x^*\| < \infty.$$

Proof Noticing the proof of Lemma 4 and $\gamma_k \rightarrow 0$, we have

$$f(x_{k+1}) \leq f(x_k) - \varepsilon_3 \min\{\gamma_k^2, (\gamma_k)^{(2-p)/(1-p)}\} = f(x_k) - \varepsilon_3 \gamma_k^2. \tag{16}$$

From (16) and Lemma 6 we have for all $k \geq k_1$

$$\begin{aligned}
0 < f(x_{k+1}) - f(x^*) &\leq f(x_k) - f(x^*) - \varepsilon_3 \|g_k\|^2 \cos^2 \theta_k \\
&\leq f(x_k) - f(x^*) - \varepsilon_3 m [f(x_k) - f(x^*)] \cos^2 \theta_k \\
&= (1 - \varepsilon_3 m \cos^2 \theta_k) [f(x_k) - f(x^*)] \\
&\leq \prod_{j=k_1+1}^k (1 - \varepsilon_3 m \cos^2 \theta_j) [f(x_j) - f(x^*)].
\end{aligned} \tag{17}$$

We notice that $1 - \varepsilon_3 m \cos^2 \theta_k > 0$ due to $f(x_k) > f(x^*)$, by geometric-arithmetic mean value formula and Lemma 7 we have

$$\begin{aligned} \prod_{j=1}^k (1 - \varepsilon_3 m \cos^2 \theta_j) &\leq \left(\frac{k - k_1 - \varepsilon_3 m \sum_{j=1}^k \cos^2 \theta_j}{k - k_1} \right)^{k - k_1} \leq \left[\frac{k - \eta_1 m k (\prod_{j=1}^k \cos^2 \theta_j)^{\frac{1}{2}}}{k} \right]^k \\ &= (1 - c_6)^{k - k_1}, \end{aligned}$$

substitute it into (17) we get,

$$f(x_{k+1}) - f(x^*) \leq (1 - c_6)^{k - k_1} (f(x_{k_1+1}) - f(x^*)),$$

where $1 - c_6 > 0$ due to $f(x_k) > f(x^*)$.

Using Lemma 6,

$$\begin{aligned} \frac{m}{2} \|x_{k+1} - x^*\|^2 &\leq (1 - c_6)^{k - k_1} (f(x_{k_1+1}) - f(x^*)) \\ \|x_{k+1} - x^*\| &\leq \sqrt{\frac{2}{m} (1 - c_6)^{k - k_1} (f(x_{k_1+1}) - f(x^*))} \\ \sum_{k=1}^{\infty} \|x_{k+1} - x^*\| &< \infty. \end{aligned}$$

Lemma 9 Let $\{B_k\}$ is generated by the BFGS formula (1), where B_0 is symmetric and positive definite, and where $y_k^T S_k > 0$ for all k . Furthermore assume that (\bar{H}) holds. Then

$$\sum_{k=1}^{\infty} \|x_k - x^*\| < \infty \implies \lim_{k \rightarrow \infty} \frac{\|(B_k - G(x^*))S_k\|}{\|S_k\|} = 0.$$

Proof See Theorem 3.2 in [7].

From Theorem 3 and Lemma 9 we can easily see that the following Theorems is true.

Theorem 4 Let x_0 be a starting point for which f satisfies the assumption (H') , and assume that (\bar{H}) holds. Then for any positive definite B_0 , the BFGS algorithm (1), with the GW linesearch method at each step, gives the Dennis-More condition

$$\lim_{k \rightarrow \infty} \frac{\|(B_k - G(x^*))S_k\|}{\|S_k\|} = 0.$$

Dennis and More^[5] show that when $\frac{\|(B_k - G(x^*))S_k\|}{\|S_k\|}$ and $\|S_k\|$ are sufficiently small then the steplength $\lambda_k = 1$ satisfies the Wolfe conditions, therefore, $\lambda_k = 1$ must satisfy the GW linesearch rule. From Theorem 4 and from the well-known characterization result of Dennis and More^[6], we conclude that the rate of convergence of the BFGS algorithm with the GW linesearch method is Q-superlinear if the unit steplength is always tried first.

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带有广义 Wolfe 线搜索的变尺度算法的收敛性

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摘 要

本文提出一类广义 Wolfe 线搜索模型, 并且把它与著名的 BFGS 方法相结合, 对于所得到的算法证明了: 对于凸函数算法具有全局收敛性和超线性收敛速度. 这推广了参考文献[1]中的结果.