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Title	Extension of Fletcher's One-Parameter Family of Variable-Metric Method to Minimization under Linear Constraints
Author(s)	Honma, Toshihisa; Kaji, Ikuo
Citation	北海道大學工學部研究報告, 87, 175-182
Issue Date	1978-06-05
Doc URL	https://hdl.handle.net/2115/41467
Type	departmental bulletin paper
File Information	87_175-182.pdf

Hokkaido University Collection of Scholarly and Academic Papers : HUSCAP

Bulletin of the Faculty of Engineering,
Hokkaido University, No. 87 (1978)

Extension of Fletcher's One-Parameter Family of Variable-Metric Method to Minimization under Linear Constraints

Toshihisa HONMA* Ikuo KAJI**

(Received September 30, 1977)

Abstract

A property of Fletcher's one-parameter family of the variable-metric method in the linear constraint manifold is examined. We can find that if linear constraints remain unchanged for successive iterations then the method has an important property represented by the concept of exactness and is stable for the convergence in the range of the parameter $\phi > -a/b$, where $a=g_i^T H_q^i g_i$, $b=g_{i+1}^T H_q^i g_{i+1}$, g_i is the gradient vector of the objective function at x_i and H_q^i is the updating matrix. Since a proper choice of the parameter ϕ is derived as $\phi=1$, we can obtain the Broyden-Fletcher-Goldfarb-Shanno algorithm in the constraint manifold.

1. Introduction

A number of methods for nonlinear programming with linear constraints have been investigated. One of the efficient and well-known methods is Rosen's gradient projection method[1]. The method is an extension of the steepest-descent technique to minimization under linear constraints.

The steepest-descent method has an excellent stability and requires only the first derivatives of the function to be minimized, but convergence is often very slow. On the other hand, Newton's method is superior to the steepest-descent method in a rate of convergence, but the method may not converge at all and requires the second derivatives of the function to be minimized.

From the point of practical computation, the use of second derivatives is undesirable. Therefore, methods which retain the good characteristics of the steepest-descent method and use only first derivatives have been developed. The methods are called variable-metric[2], quasi-Newton[3], or conjugate-gradient methods[4].

An extension of the variable-metric method to minimization under linear constraints was tried by Goldfarb[5]. Step 5 of the algorithm is used to update a matrix H_q^i in a manner similar to Davidon's[2], as modified by Fletcher and Powell[6] (referred to as DFP method). However, Fletcher[7] pointed out that the updating matrix by using the DFP method became singular for one example of unconstrained problems. For this reason, he developed a new updating formula, based upon a very simple idea. That is Fletcher's one-parameter family of the variable-metric method.

* Division of Information Engineering, Graduate School of Engineering, University of Hokkaido, Sapporo 060
** Department of Electricity, Faculty of Engineering, University of Hokkaido, Sapporo 060.

In this paper, we try to extend the method of Fletcher's one-parameter family to minimization under linear constraints in accordance with Goldfarb's algorithm. Namely, only the updating DFP formula in Step 5 is replaced by Fletcher's one-parameter formula, and Steps except for Step 5 remain unchanged. We formulate the minimization problem with linear constraints in the section 2. Fletcher's one-parameter family is discussed in section 3. The exactness and stability for method is examined in section 4 and 5, respectively. In section 6, the conclusions are described.

2. Formulation of the problem

The general nonlinear programming problem subject to linear constraints can be expressed as

$$\text{Minimize} \qquad f(x)=f(x_1, \cdots, x_m)\,, \tag{2-1}$$

subject to linear equalities and inequalities of the form

$$n_i^T x-b_i=0\,, \qquad i=1, \cdots, k, \tag{2-2}$$

$$n_i^T x-b_i \geqq 0\,, \qquad i=k+1, \cdots, p\,, \tag{2-3}$$

where the n_i are unit normals, the b_i are scalars and the superscript T is used to denote transposition.

These equality and inequality constraints represent k hyperplanes, and $p-k$ closed half-spaces. The hyerplane corresponding to a strict equality for a particular i in eq. (2-3) is called the "defining hyperplane" for the associated half-space. The convex polyhedral region R in E^m formed by these constraints (2-2) and (2-3) is assumed to be bounded. For this to be true, it is necessary that $p \geqq m+1$. The region R is called feasible and any point x such that $x \in R$ is called a feasible solution. The boundary B of R is itself a bounded region and is the intersection of R with the union of these $p-k$ defining hyperplanes.

A set of hyperplanes is linearly independent if the set of unit normals to these hyperplanes is linearly independent. The term "constraint basis" refers to the set of linearly independent defining hyperplanes. When the movement is restricted in the intersection of q linearly independent hyperplanes, this intersection is called by the term "linear constraint manifold", M_q.

3. Fletcher's one-parameter family

We consider the problem of finding the point at which a strictly convex quadratic function

$$f(x)=f_0+a^T x+\frac{1}{2}\,x^T G x\,, \tag{3-1}$$

is minimized in the constraint manifold M_q, starting from a point x_i in this manifold. Here, the matrix G is constant positive definite. Then the iterative method for this problem can be expressed as

$$x_{i+1}=x_i-\hat{P}_q G^{-1} g_i \tag{3-2}$$

where $\hat{P}_q=I-G^{-1}N_q(N_q^T G^{-1}N_q)^{-1}N_q$, $N_q=(n_1, \cdots, n_q)$, and g_i denotes the gradient vector

of $f(x)$ at x_i. The operator $\hat{P}_q$ is a non-Euclidean projection operator weighted by G^{-1} that projects E^m onto the constraint manifold M_q.

In most actual problems, $f(x)$ is nonquadratic and the inverse matrix G^{-1} is variable for successive iterations. For this reason, Goldfarb[5] introduced the approximating matrix H_q^i to $\hat{P}_q G^{-1}$ and used the DFP formula in Step 5 of his algorithm, i.e.,

$$H_q^{i+1} = H_q^i + \frac{\sigma_i \sigma_i^T}{\sigma_i^T y_i} - \frac{H_q^i y_i y_i^T H_q^i}{y_i^T H_q^i y_i}, \tag{3-3}$$

where $\sigma_i = x_{i+1} - x_i$ and $y_i = g_{i+1} - g_i$. The correction σ_i is taken as multiple γ_i of a "direction of search" $s_i = -H_q^i g_i$, i.e.,

$$\sigma_i = \gamma_i s_i = -\gamma_i H_q^i g_i . \tag{3-4}$$

However, Fletcher[7] pointed out that one expample was found in which failure occurred because the matrix H_q^i became singular. Therefore, he set forth a new updating formula, based upon an idea of *dual*,

$$H_q^{i+1} = H_q^i + \frac{1}{\sigma_i^T y_i}\left\{-\sigma_i y_i^T H_q^i - H_q^i y_i \sigma_i^T + \left(1 + \frac{y_i^T H_q^i y_i}{\sigma_i^T y_i}\right)\sigma_i \sigma_i^T\right\}. \tag{3-5}$$

We note that this formula coincides with Goldfarb's formula derived from the variational method.[8] Furthermore, Fletcher derived a one-parameter family of the variable-metric method by taking any linear combination of the right-hand sides of (3-3) and (3-5) such that the coefficients sum to unity, i.e.,

$$\begin{aligned} H_q^{i+1} &= (1-\phi)\, H_{q0}^{i+1} + \phi H_{q1}^{i+1} \\ &= H_{q0}^{i+1} + \phi \nu_i \nu_i^T , \end{aligned} \tag{3-6}$$

where

$$\nu_i = (y_i^T H_q^i y_i)^{1/2}\left(\frac{\sigma_i}{\sigma_i^T y_i} - \frac{H_q^i y_i}{y_i^T H_q^i y_i}\right),$$

and H_q^{i+1} in eqs. (3-3) and (3-5) is denoted by H_{q0}^{i+1} and H_{q1}^{i+1}, respectively.

We can show that the one-parameter family (3-6) includes the following formulae:

i) Broyden's first formula[3] as $\phi = \sigma_i^T y_i / (\sigma_i^T y_i - y_i^T H_q^i y_i)$,

$$H_q^{i+1} = H_q^i + \frac{(\sigma_i - H_q^i y_i)(\sigma_i - H_q^i y_i)^T}{(\sigma_i - H_q^i y_i)^T y_i} . \tag{3-7}$$

ii) Broyden's second formula[3] as $\phi = \beta_i \sigma_i^T y_i$,

$$\begin{aligned} H_q^{i+1} &= H_q^i - H_q^i y_i z_i^T + \sigma_i y_i^T , \\ z_i^T &= \delta_i y_i^T H_q^i + \beta_i \sigma_i^T , \qquad q_i^T = \alpha_i s_i^T - \beta_i y_i^T H_q^i , \\ \delta_i &= \frac{1 - \beta_i \sigma_i^T y_i}{y_i^T H_q^i y_i} , \qquad \alpha_i = \frac{1 + \beta_i y_i^T H_q^i y_i}{s_i^T y_i} . \end{aligned} \tag{3-8}$$

iii) Shanno's formula[9] as $\phi = (1-t)\sigma_i^T y_i / [(1-t)\sigma_i^T y_i - y_i^T H_q^i y_i]$,

$$H_q^{i+1} = H_q^i + t\frac{\sigma_i \sigma_i^T}{\sigma_i^T y_i} + \frac{[(1-t)\,\sigma_i - H_q^i y_i]\,[(1-t)\,\sigma_i - H_q^i y_i]^T}{[(1-t)\,\sigma_i - H_q^i y_i]^T y_i} . \tag{3-9}$$

iv) Greenstadt's first formula[10] as $\phi=-\sigma_i^T y_i/y_i^T H_q^i y_i$

$$H_q^{i+1}=H_q^i+\frac{1}{y_i^T H_q^i y_i}\left\{\sigma_i y_i^T H_q^i+H_q^i y_i\sigma_i^T-\left(1+\frac{y_i^T\sigma_i}{y_i^T H_q^i y_i}\right)H_q^i y_i y_i^T H_q^i\right\}. \quad (3\text{-}10)$$

v) The formulae (3-3) and (3-5) are derived by taking a linear combination of the formulae (3-7) and (3-10), i. e.,

$$H_{q0}^{i+1}=(1-\alpha)\,H_{B1}^{i+1}+\alpha H_{G1}^{i+1}, \quad (3\text{-}11)$$

$$H_{q1}^{i+1}=(1-\alpha^2)\,H_{B1}^{i+1}+\alpha^2 H_{G1}^{i+1}, \quad (3\text{-}12)$$

where $\alpha=y_i^T H_q^i y_i/\sigma_i^T y_i$ and H_q^{i+1} in eqs. (3-7) and (3-10) is denoted by H_{B1}^{i+1} and H_{G1}^{i+1}, respectively.

In what follows, we use the formula (3-6) by which the formula (3-3) in Step 5 of Goldfarb's algorithm is replaced.

4. Exactness

In this section, we prove a property represented by the concept of exactness. That is, if the linear constraint manifold M_q remains unchanged for successive iterations and the objective function is given by eq (3-1), then the algorithm (3-6) terminates within $m-q$ steps and the variable-metric matrix H_q^{m-q} is equal to the matrix $\hat{P}_q G^{-1}$.

We introduce the following theorem without proof because the proof is identical to that of Goldfarb's theorem 4.[5]

THEOREM 1. *A minimization method in an unconstrained n-dimensional space which performs successive univariate minimization along mutually conjugate directions terminates within n iterations.*

In this proof, we use the G-conjugacy condition of $s_0, \cdots, s_{n-1}$, i. e., $s_j^T G s_i=0$, for $i\neq j$, and the relation $g_{i+1}^T s_i=0$ and $y_i=G\sigma_i$. If the constraint basis remains unchanged for n successive steps and the formula (3-6) is used to update H_q^i, then the following theorem can be proved.

THEOREM 2. *If the $(m-q)$-dimensional linear constraint manifold M_q remains unchanged for n successive iterations $(n\leqq m-q)$ of the formula* (3-6), *then the directions of search determined by these iterations satisfy the proper equation $H_q^{k+i}G\sigma_k=\sigma_k$ and the G-conjugacy condition of σ_{k+j}, σ_k, i.e., $\sigma_{k+j}^T G\sigma_k=0$ for $0<j\leqq i$, $1\leqq i$ and $0\leqq k$.*

Proof. The proof proceeds by induction on i. The proper equation is obviously true for $i=1$ and all $k\geqq 0$ since then the formula (3-6) yields.

$$\begin{aligned}H_q^{k+1}G\sigma_k &= H_q^{k+1}y_k\\ &= H_{q0}^{k+1}y_k+\phi\nu_k\nu_k^T y_k\\ &= H_q^k y_k+\frac{\sigma_k\sigma_k^T y_k}{\sigma_k^T y_k}-\frac{H_q^k y_k y_k^T H_q^k y_k}{y_k^T H_q^k y_k}+\phi\nu_k(y_k^T H_q^k y_k)^{1/2}\left(\frac{\sigma_k^T y_k}{\sigma_k^T y_k}-\frac{y_k^T H_q^k y_k}{y_k^T H_q^k y_k}\right)\\ &= \sigma_k.\end{aligned}$$

Since $g_{k+1}^T\sigma_k=0$, the G-conjugacy condition for $i=1$ and all $k\geqq 0$ follows when both

sides of the above equation are premultiplied by $\gamma_{k+1}g_{k+1}^T$.

Assuming for all $k\geqq 0$ that the proper equation and the G-conjugacy condition are true for i, we now show that they are also true for $i+1$. From the formula (3-6), we obtain

$$\begin{aligned}
H_q^{k+i+1}G\sigma_k &= H_{q0}^{k+i+1}G\sigma_k+\phi\nu_{k+i}\nu_{k+i}^TG\sigma_k \\
&= H_q^{k+i}G\sigma_k+\frac{\sigma_{k+i}\sigma_{k+i}^TG\sigma_k}{\sigma_{k+i}^Ty_{k+i}}-\frac{H_q^{k+i}y_{k+i}y_{k+i}^TH_q^{k+i}G\sigma_k}{y_{k+i}^TH_q^{k+i}y_{k+i}} \\
&\qquad +\phi\nu_{k+i}(y_{k+i}^TH_q^{k+i}y_{k+i})^{1/2}\left(\frac{\sigma_{k+i}^TG\sigma_i}{\sigma_{k+i}^Ty_{k+i}}-\frac{y_{k+i}^TH_q^{k+i}G\sigma_k}{y_{k+i}^TH_q^{k+i}y_{k+i}}\right) \\
&= \sigma_k-\frac{H_q^{k+i}y_{k+i}y_{k+i}^T\sigma_k}{y_{k+i}^TH_q^{k+i}y_{k+i}}+\phi\nu_{k+i}(y_{k+i}^TH_q^{k+i}y_{k+i})^{1/2}\left(-\frac{y_{k+i}^T\sigma_k}{y_{k+i}^TH_q^{k+i}y_{k+i}}\right) \\
&= \sigma_k\,.
\end{aligned}$$

Finally, from the above proper equation and a relation

$$g_{k+i+1}=g_{k+1}+\sum_{j=1}^{i}G\sigma_{k+j}\,,$$

we obtain

$$\begin{aligned}
\sigma_{k+i+1}^TG\sigma_k &= -\gamma_{k+i+1}g_{k+i+1}^TH_q^{k+i+1}G\sigma_k \\
&= -\gamma_{k+i+1}(g_{k+1}^T\sigma_k+\sum_{j=1}^{i}\sigma_{k+j}^TG\sigma_k) \\
&= 0\,.
\end{aligned}$$

This completes the induction.

From Theorem 1 and 2, we can find that the algorithm (3-6) is terminated within $(m-q)$ steps if the linear manifold M_q remains unchanged for n successive iterations.

We can prove the following corollary by using the G-conjugacy condition in Theorem 1.

COROLLARY. *If $f(x)$ is a quadratic function given by* (3-1), *then*

$$\hat{P}_qG^{-1}=\sum_{i=0}^{m-q-1}\frac{\sigma_i\sigma_i^T}{\sigma_i^Ty_i}\,.$$

Proof. The G-conjugacy condition in Theorem 1 implies that $S^TGS=\Lambda$, where S is the $m\times q$ matrix $S=\{\sigma_0,\cdots,\sigma_{m-q-1}\}$ and Λ is a diagonal $q\times q$ matrix with elements $\sigma_i^TG\sigma_i$. If we define the partitioned $m\times m$ matrix $\underset{\sim}{S}$ by $\underset{\sim}{S}=[S|G^{-1}N_q]$, then S is invertible and $\underset{\sim}{S}^TG\underset{\sim}{S}=\underset{\sim}{\Lambda}$
where

$$\underset{\sim}{\Lambda}=\begin{bmatrix}\Lambda & 0\\ 0 & N_q^TG^{-1}N_q\end{bmatrix}.$$

Therefore, the invertible matrix G^{-1} is derived as follows

$$G^{-1}=S\Lambda^{-1}S^T+G^{-1}N_q(N_q^TG^{-1}N_q)^{-1}N_q^TG^{-1}\,,$$

and we obtain

$$\hat{P}_q G^{-1} = S\Lambda^{-1}S^T = \sum_{i=0}^{m-q-1} (\Lambda^{-1})_{ii}\sigma_i\sigma_i^T = \sum_{i=0}^{m-q-1} \frac{\sigma_i\sigma_i^T}{\sigma_i^T y_i} .$$

The corollary is proved.

The following theorem is introduced without proof because the proof is given in Goldfarb's Theorem 6.[5]

THEOREM 3. *If $f(x)$ is a quadratic function given by* (3-1), *and the linear constraint manifold M_q remains unchanged for $(m-q)$ successive iterations of the formula* (3-6), *then $H_q^{m-q}g(x^{m-q})=0$ and $H_q^{m-q}=\hat{P}_q G^{-1}$.*

We can find from the corollary that it is the term $\sigma_i\sigma_i^T/\sigma_i^T y_i$ in the formula (3-6) which makes the variable-metric matrix H_q^i tend to $\hat{P}_q G^{-1}$. Theorem 3 shows that the matrix H_q^{m-q} is equal to the matrix $\hat{P}_q G^{-1}$. Therefore, the formula (3-6) has the property of exactness.

5. Stability

In this section, stability for the convergence is proved by showing that the direction of search $s_i=-H_q^i g_i$ is downhill at each step. Since $s_i^T g_i=-g_i^T H_q^i g_i$, the direction s_i is downhill if and only if $g_i^T H_q^i g_i>0$ for all g_i other than g_i at a constrained stationary point. Therefore, when the linear constraint manifold M_q remains unchanged for successive iterations, we investigate whether or not the matrix H_q^i is positive definite. The proof proceeds by induction on i. If a initial matrix H_q^i is positive definite, then s_0 is downhill. Assuming for i that the matrix H_q^i is positive definite, we show that the matrix is also positive definite for $i+1$.

First of all, we prove the following theorem.

THEOREM 4. *Let $a=g_i^T H_q^i g_i$, $b=g_{i+1}^T H_q^i g_{i+1}$. Then*

$$H_q^{i+1}g_{i+1} = \phi(\phi)[aH_q^i g_{i+1} + bH_q^i g_i] ,$$

where $\phi(\phi)=(a+b\phi)/[a(a+b)]$.

Proof. Since $y_i=g_{i+1}-g_i$ and $g_{i+1}^T\sigma_i=0$, we have $y_i^T H_q^i y_i=a+b$, $y_i^T H_q^i g_{i+1}=b$ and $\sigma_i^T y_i=\gamma_i a$. Then the formula (3-6) postmultiplied by g_{i+1} yields

$$\begin{aligned} H_q^{i+1}g_{i+1} &= H_q^i g_{i+1} - \frac{H_q^i y_i y_i^T H_q^i g_{i+1}}{y_i^T H_q^i y_i} + \phi(y_i^T H_q^i y_i)\left(\frac{\sigma_i}{\sigma_i^T y_i} - \frac{H_q^i y_i}{y_i^T H_q^i y_i}\right)\left(-\frac{y_i^T H_q^i g_{i+1}}{y_i^T H_q^i y_i}\right) \\ &= \left(1 - \frac{b}{a+b} + \frac{b}{a+b}\phi\right) H_q^i g_{i+1} + \left(\frac{b}{a+b} + \frac{b}{a}\phi - \frac{b}{a+b}\phi\right) H_q^i g_i \\ &= \frac{a+b\phi}{a+b}(H_q^i g_{i+1} - H_q^i g_i) + \frac{a+b\phi}{a} H_q^i g_i \\ &= \frac{a+b\phi}{a+b}(aH_q^i g_{i+1} + bH_q^i g_i) , \end{aligned}$$

If we define $\phi(\phi)$ by $(a+b\phi)/(a+b)$, then the theorem is proved.

We now consider the following lemma and theorem.

LEMMA. *H_q^i positive definite implies $g_{i+1}^T H_q^{i+1} g_{i+1}>0$ if and only if $\phi(\phi)>0$.*

Proof. From $H_q^{i+1}y_i=\sigma_i$, we obtain $g_{i+1}^T H_q^{i+1} g_{i+1}=g_{i+1}^T H_q^{i+1} g_i$. Applying this relation to Theorem 4 yields

$$g_{i+1}^T H_q^{i+1} g_{i+1} = ab\psi(\phi) .$$

Now since H_q^i is assumed to be positive definite, a and b is positive if both g_i and g_{i+1} is not the gradient at a constrained stationary point, so the lemma is proved.

THEOREM 5. *If the matrix H_q^i is positive definite, then H_q^{i+1} is positive definite if and only if $\psi(\phi)>0$.*

Proof. Since the matrix H_q^i is positive definite, any set of $(m-q)$ vectors which satisfy the H_q^i-conjugacy condition span E^{m-q}. Furthermore, since $g_i^T H_q^i g_{i+1}=0$ and g_{i+1}, $g_i \in M_q$, let g_i, g_{i+1} and any $(m-q-2)$ vectors $z_1, \cdots, z_{m-q-2}$ which satisfy the H_q^i-conjugacy condition, be a basis for E^{m-q}. Therefore, any arbitrary vector ξ can be expressed as

$$\xi = \sum_{i=1}^{m-q-2} a_i z_i + a_{m-q-1} g_i + a_{m-q} g_{i+1} . \tag{5-1}$$

From eq. (5-1) and the formula (3-6) it is shown that the H_q^i-conjugacy condition guarantees that $z_i^T H_q^{i+1} z_j=0$, for $i \neq j$, $z_i^T H_q^{i+1} g_i=0$ and $z_i^T H_q^{i+1} g_{i+1}=0$. Then, we obtain

$$\begin{aligned} \xi^T H_q^{i+1} \xi = & \sum_{j=1}^{m-q-2} a_j^2 z_j^T H_q^i z_j + a_{m-q-1}^2 g_i^T H_q^{i+1} g_i \\ & + (2a_{m-q-1} a_{m-q} + a_{m-q}^2)\, g_{i+1}^T H_q^{i+1} g_{i+1} . \end{aligned} \tag{5-2}$$

Furthermore, since we can show that from $H_q^{i+1} y_i = \sigma_i$,

$$g_i^T H_q^{i+1} g_i = \gamma_i g_i^T H_q^i g_i + g_{i+1}^T H_q^{i+1} g_{i+1} ,$$

eq. (5-2) becomes

$$\begin{aligned} \xi^T H_q^{i+1} \xi = & \sum_{j=1}^{m-q-2} a_j^2 z_j^T H_q^i z_j + a_{m-q-1}^2 \gamma_i g_i^T H_q^i g_i \\ & + (a_{m-q-1} + a_{m-q})^2\, g_{i+1}^T H_q^{i+1} g_{i+1} . \end{aligned} \tag{5-3}$$

Applying Lemma to eq. (5-3) gives the desired result.

From Theorem 5, we can find that the stability for convergence is guaranteed for $\psi(\phi)>0$, i. e., $\phi > -a/b$. Thus, the choice of the parameter ϕ in this range maintains stability.

Finally, we consider the choice of the parameter ϕ in the above range. According to Shanno's computational experience[11], the proper choice of ϕ is to keep the eigenvalues of H_q^{i+1} in the direction of g_{i+1} as close to that of H_q^i in the direction of g_{i+1} as possible. From Lemma, we have

$$g_{i+1}^T H_q^{i+1} g_{i+1} = g_i^T H_q^{i+1} g_{i+1} = g_{i+1}^T H_q^i g_{i+1} \frac{g_i^T H_q^i g_i + g_{i+1}^T H_q^i g_{i+1} \phi}{g_i^T H_q^i g_i + g_{i+1}^T H_q^i g_{i+1}} .$$

If the parameter ϕ tend to one, then

$$\lim_{\phi \to 1} g_{i+1}^T H_q^{i+1} g_{i+1} = g_{i+1}^T H_q^i g_{i+1} .$$

This choice of the parameter ϕ coincides with Shanno's experience, so we obtain $\phi=1$. Furthermore, we can find that the choice of $\phi=1$ yields the Broyden-Fletcher-Shanno-Goldfarb algorithm (referred to as BFSG algorithm) in the linear constraint manifold.

6. Conclusions

We discuss the property of Fletcher's one-parameter family of the variable-metric method in the linear constraint manifold. As the important property of the method, we can find that the algorithm for the positive-definite quadratic function is terminated within the finite steps and the matrix H_q^{n-q} is equal to the matrix $\hat{P}_q G^{-1}$ if the constraint manifold remains unchanged for successive iterations. That is, this method has the property represented by the concept of exactness. Furthermore, we can find that if the parameter $\phi > -a/b$, then this method is stable for the convergence and the choice of $\phi=1$ yields the BFSG algorithm.

We require more theoretical and experimental research for the nonquadratic case in order to regard this algortihm as efficient and practical tools for the linear constrained minimization.

Acknowlegment

The authors wish to thank Dr. T. Oohori of this Laboratory for his useful discussions.

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