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# A New One-Parameter Family of Generalized Variable-Metric Method in Accordance with Fletcher's Duality

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## Abstract

We have developed a new one-parameter family of generalized variable-metric method which is reduced to Fletcher's one-parameter family for certain values of parameters. The process of the development is as follows. First, from the application of the generalized inverse of matrices, we derive the general solution of a matrix equation on which variable-metric methods are based, and we consider only the generalized variable-metric method including the Broyden-Fletcher-Goldfarb-Shanno algorithm. Next, we develop a dual generalized variable-metric method in accordance with both the Sherman and Morrison formula, and Fletcher's idea of *dual*, so that we construct a new one-parameter family which consists of the generalized variable-metric algorithms which are dual with each other. The situation of known variable-metric methods is made more clear by the new one-parameter family of generalized variable-metric method.

## 1. Introduction

There exists a number of variable-metric methods developed by many authors. The superior characteristics of the variable-metric methods are that the methods retain an excellent stability as the steepest-descent methods and use only the first derivatives of the function to be minimized; nevertheless, the variable-metric methods are superior to the steepest-descent methods in a rate of convergence as Newton's methods.

As one of the variable-metric methods, we have already studied a property of Fletcher's one-parameter family of the variable-metric method under linear constraints<sup>1)</sup>. Fletcher's one-parameter family of the variable-metric method<sup>2)</sup> is constructed by taking any linear combination of the Davidon-Fletcher-Powell method<sup>3,4)</sup> and the Broyden-Fletcher-Goldfarb-Shanno method<sup>5,1,6,7)</sup> (referred to as the DFP method and the BFGS method, respectively) in such a way that the coefficients sum is unity. We have shown that Fletcher's one-parameter family of the variable-metric method holds a property represented by the concept of exactness and is stable for the convergence in some range of the parameter even under linear constraints<sup>1)</sup>.

Therefore we consider that it is useful to extend Fletcher's one-parameter family with such excellent properties to a more generalized form. The important

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structural characteristic of Fletcher's one-parameter family is that the DFP method and the BFGS method hold a dual relation with each other in accordance with Fletcher's idea of *dual* (referred to as Fletcher's duality)<sup>3)</sup>. For this reason, we make use of this characteristic and consider the extension of Fletcher's one-parameter family of the variable-metric method.

In this paper, it is our purpose to develop a new one-parameter family which includes Fletcher's one-parameter family as one of the algorithms. The remainder of this paper is arranged as follows. In section 2, we summarize the properties of the variable-metric method and establish a matrix equation on which the variable-metric methods are based. From its general solution, we derive the generalized variable-metric method including the BFGS algorithm<sup>8)</sup>. In section 3, the Sherman and Morrison formula<sup>9)</sup> is applied to the generalized variable-metric method derived in section 2, so that we obtain a dual generalized variable-metric method in accordance with Fletcher's duality. Furthermore, by making use of the results, we construct a new one-parameter family to which Fletcher's one-parameter family is extended. In section 4, discussion about the new one-parameter family is described.

## 2. Generalized Variable-Metric Method

### 2.1 Variable-metric method

We consider the problem to find a local minimum of a function  $f(x)$  of  $n$  variables  $x=(x_1, x_2, \dots, x_n)^T$ , where  $T$  denotes the transpose of a matrix. The gradient of a function  $f(x)$  can be expressed by  $g(x)=(\partial f/\partial x_1, \partial f/\partial x_2, \dots, \partial f/\partial x_n)^T$ , so that the variable-metric method for the problem is to find a sequence of vectors  $(x_0, x_1, \dots, x_n, \dots)$  such that

$$x_{i+1}=x_i+\gamma_i s_i, \quad (2-1)$$

$$s_i=-H_i^T g(x_i), \quad (2-2)$$

and

$$\lim_{i \rightarrow \infty} g(x_i)=0. \quad (2-3)$$

Here, the  $i$ th step size  $\gamma_i$  is determined so that  $f(x_i+\gamma_i s_i)=\min_{\gamma} f(x_i+\gamma s_i)$ , and  $H_i$  is

the  $n \times n$  positive definite matrix and defines the inverse of the metric matrix, so that the direction vectors  $s_i$ ,  $i=0, 1, 2, \dots$ , mean the direction of minimizing the directional derivative of  $f(x_i)$ . Furthermore the matrix  $H_i$  is updated on the basis of a recursive formula. It is shown that if the updating matrix  $H_i$  in eq. (2-2) is replaced by the unit matrix and the inverse for the Hessian matrix, respectively, then the variable-metric method is reduced to the steepest descent method and Newton's method.

For a positive-definite quadratic function  $f(x)=\frac{1}{2}x^T A x - g^T x + a$ , the recursive formula in the variable-metric method has the following properties:

(1) The direction vectors are a set of the  $A$ -conjugate vectors such that  $s_i^T A s_j=0$ ,  $i \neq j$ ,  $i, j=0, 1, \dots, n-1$ , so that the minimum of the function  $f(x)$  is attained at most in  $n$  steps. Then, we obtain the following relations

$$Y_j^T \sigma_j=0 \quad \text{or} \quad S_j^T y_j=0, \quad j=1, \dots, i-1 \quad (2-4)$$

and

$$A^{-1} Y_i = S_i, \quad (2-5)$$

where the  $n \times i$  matrices  $Y_i$  and  $S_i$  are defined by  $Y_i = (y_0, y_1, \dots, y_{i-1})$  and  $S_i = (\sigma_0, \sigma_1, \dots, \sigma_{i-1})$ , respectively. The vectors  $\sigma_i$  and  $y_i$  are defined by  $\sigma_i = x_{i-1} - x_i$  and  $y_i = g_{i+1} - g_i$ , respectively.

(2) The matrix updated by the recursive formula is the positive definite matrix, so that  $H_i$  tends to the inverse matrix  $A^{-1}$  for the Hessian matrix of  $f(x)$  in the vicinity of the extremum point, in which the direction vector is similar to that of Newton's method.

In the next section, we consider a recursive formula which holds the above properties for nonquadratic function.

## 2.2 Generalized variable-metric algorithm

The many variable-metric methods for the problem of minimizing nonquadratic functions are derived on the basis of the following matrix equation

$$H_i Y_i = S_i, \quad (2-6)$$

where the variable-metric matrix  $H_i$  is an unknown matrix and satisfies the second property in section 2.1 because of the similarity to eq. (2-5). If the matrix  $H_i$  satisfies the above equation then the  $A$ -conjugacy condition of  $\sigma_0, \sigma_1, \dots, \sigma_{i-1}$ , is reduced to

$$Y_j^T \sigma_j = 0, \text{ or } \gamma_j Y_j^T H_j^T g_j = \gamma_j S_j^T g_j = 0, \quad j = 1, \dots, i-1 \quad (2-7)$$

A general solution of eq. (2-6) is obtained in accordance with Adachi's derivation<sup>8)</sup> in which a generalized inverse for matrices is applied to eq. (2-6)<sup>10)</sup>, so that the generalized variable-metric method is expressed as follows

$$H_i = S_i Y_i^* + R_i (I_n - Y_i Y_i^*), \quad (2-8)$$

where the  $i \times n$  matrix  $Y_i^*$  is such that  $Y_i Y_i^* Y_i = Y_i$ .

In this paper, we consider only a generalized variable-metric method into which the BFGS algorithm is included. For this reason, the  $n \times n$  matrix  $R_i$  is chosen as  $(S_i Y_i^*)^T$  so that the variable-metric matrix  $H_i$  becomes symmetric. The recursive formula for  $Y_i^*$  used by Adachi<sup>8)</sup> is applied to the solution (2-8), so that the matrix  $H_i$  is expressed recursively as

$$H_{i+1} = H_i - \frac{\eta_i d_i^T}{d_i^T y_i} - \frac{d_i \eta_i^T}{d_i^T y_i} + \frac{y_i^T \eta_i d_i d_i^T}{(d_i^T y_i)^2}, \quad (2-9)$$

where the vectors  $d_i, \eta_i$  and the matrix  $J_i$  are defined by  $(c_i^T J_i)^T, H_i y_i - \sigma_i$  and  $I_n - Y_i Y_i^*$ , respectively. The vector  $c_i$  is any vector such that  $c_i^T J_i Y_i = 0$ . For several values of  $d_i$ , the generalized variable-metric algorithm (2-9) is reduced to the following algorithms:

(1) The BFGS algorithm as  $d_i = \sigma_i^{1,5,6,7)}$

$$H_{i+1} = H_i + \frac{1}{\sigma_i^T y_i} \left[ -\sigma_i y_i^T H_i - H_i y_i \sigma_i^T + \left( 1 + \frac{y_i^T H_i y_i}{\sigma_i^T y_i} \right) \sigma_i \sigma_i^T \right]. \quad (2-10)$$

(2) Broyden's first algorithm as  $d_i = \sigma_i - H_i y_i^{11)}$

$$H_{i+1} = H_i + \frac{(\sigma_i - H_i y_i)(\sigma_i - H_i y_i)^T}{(\sigma_i - H_i y_i)^T y_i}. \quad (2-11)$$

(3) Greenstadt's first algorithm as  $d_i = H_i y_i^{12)}$

$$H_{i+1} = H_i + \frac{1}{y_i^T H_i y_i} \left[ \sigma_i y_i^T H_i + H_i y_i \sigma_i^T - \left( 1 + \frac{y_i^T \sigma_i}{y_i^T H_i y_i} \right) H_i y_i y_i^T H_i \right]. \quad (2-12)$$

(4) Greenstadt's second algorithm as  $d_i = y_i^{13)}$

$$H_{i+1} = H_i + \frac{1}{y_i^T y_i} \left[ \sigma_i y_i^T + y_i \sigma_i^T - H_i y_i y_i^T - y_i y_i^T H_i - \frac{1}{y_i^T y_i} (y_i^T \sigma_i - y_i^T H_i y_i) y_i y_i^T \right]. \quad (2-13)$$

(5) A new algorithm as  $d_i = H_i \sigma_i$ ,

$$H_{i+1} = H_i - \frac{\eta_i \sigma_i^T H_i + H_i \sigma_i \eta_i^T}{\sigma_i^T H_i y_i} + \frac{y_i^T \eta_i}{(\sigma_i^T H_i y_i)^2} H_i \sigma_i \sigma_i^T H_i. \quad (2-14)$$

Thus, we obtained the generalized variable-metric algorithms (2-9) including the BFGS algorithm, so that we next derive a dual generalized variable-metric algorithm in accordance with Fletcher's duality.

### 3. A New One-Parameter Family

#### 3.1 Dual generalized variable-metric algorithm

A simple idea of *dual* was applied to the DFP algorithm of the variable-metric methods<sup>2)</sup>

$$H_{i+1} = H_i + \frac{\sigma_i \sigma_i^T}{\sigma_i^T y_i} - \frac{H_i y_i y_i^T H_i}{y_i^T H_i y_i}, \quad (3-1)$$

so that the BFGS algorithm (2-10) was developed. Fletcher's one-parameter family of the variable-metric method was constructed by taking any linear combination of the right-hand sides of the DFP algorithm (3-1) and the BFGS algorithm (2-10) such that the coefficients sum is unity, i. e.,

$$H_{i+1} = H_i + \frac{\sigma_i \sigma_i^T}{\sigma_i^T y_i} - \frac{H_i y_i y_i^T H_i}{y_i^T H_i y_i} + \phi \nu_i \nu_i^T, \quad (3-2)$$

where

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

In accordance with Fletcher's duality, we consider the extension of Fletcher's one-parameter family (3-2) by making use of the generalized variable-metric algorithm (2-9) which includes the BFGS algorithm. First of all, it is necessary to derive the inverse for the recursive formula (2-9). For this reason, the recursive formula (2-9) is rewritten as follows

$$H_{i+1} = S + \frac{y_i^T \eta_i d_i d_i^T}{(d_i^T y_i)^2}, \quad (3-3 a)$$

$$S = T - \frac{d_i \eta_i^T}{d_i^T y_i}, \quad (3-3 b)$$

$$T = H_i - \frac{\eta_i d_i^T}{d_i^T y_i}. \quad (3-3 c)$$

Then, the following Sherman and Morrison formula<sup>9)</sup> is applied to the recursive formulae (3-3a), (3-3b), and (3-3c), respectively,

$$(B - \sigma u v^T)^{-1} = B^{-1} - \tau B^{-1} u v^T B^{-1}, \quad \tau^{-1} + \sigma^{-1} = v^T B^{-1} u,$$

where  $B$  is nonsingular matrix,  $u$  and  $v$  are any vectors, and  $\sigma$  and  $\tau$  are any scalars. We obtain

$$H_{i+1}^{-1} = S^{-1} - \frac{y_i^T \eta_i}{(d_i^T y_i)^2 + (y_i^T \eta_i) d_i^T S^{-1} d_i} S^{-1} d_i d_i^T S^{-1}, \quad (3-4 a)$$

$$S^{-1} = T^{-1} + \frac{1}{d_i^T y_i - \eta_i^T T^{-1} d_i} T^{-1} d_i \eta_i^T T^{-1}, \quad (3-4 d)$$

$$T^{-1} = H_i^{-1} + \frac{1}{d_i^T y_i - d_i^T H_i^{-1} \eta_i} H_i^{-1} \eta_i d_i^T H_i^{-1}. \quad (3-4 c)$$

The right-hand sides of the eqs. (3-4a), (3-4b) and (3-4c) are expressed in terms of the inverse matrices  $S^{-1}$ ,  $T^{-1}$  and  $H_i^{-1}$ , respectively. The inverse matrix  $S^{-1}$  of eq. (3-4 b) is substituted into eq. (3-4a), so that the inverse matrix  $H_{i+1}^{-1}$  can be written in the form of the inverse matrix  $T^{-1}$ . Since the inverse matrix  $T^{-1}$  can be expressed by the inverse matrix  $H_i^{-1}$  through the eq. (3-4c), the inverse matrix  $H_{i+1}^{-1}$  is expressed by the inverse matrix  $H_i^{-1}$ . As a result, the inverse for the recursive formula (2-9) is given by

$$G_{i+1} = G_i + \frac{1}{(d_i^T G_i \sigma_i)^2 + (\sigma_i^T \mu_i)(d_i^T G_i d_i)} \times [(d_i^T G_i \sigma_i)(\mu_i d_i^T G_i + G_i d_i \mu_i^T) + (d_i^T G_i d_i) \mu_i \mu_i^T - (\sigma_i^T \mu_i) G_i d_i d_i^T G_i], \quad (3-5)$$

where the inverse matrices  $H_{i+1}^{-1}$  and  $H_i^{-1}$  are replaced by  $G_{i+1}$  and  $G_i$ , respectively.

Next, from the recursive formula (3-5), we derive the dual generalized variable-metric algorithm to the eq. (2-9). Since Fletcher's duality is based on the following transformation

$$y_i \leftrightarrow \sigma_i, \quad H_i \leftrightarrow G_i, \quad H_{i+1} \leftrightarrow G_{i+1}, \quad (3-6)$$

the application of the eq. (3-6) to the eq. (3-5) results in

$$H_{i+1} = H_i + \frac{1}{(b_i^T H_i y_i)^2 - (y_i^T \eta_i)(b_i^T H_i b_i)} \times [-(b_i^T H_i y_i)(\eta_i b_i^T H_i + H_i b_i \eta_i^T) + (b_i^T H_i b_i) \eta_i \eta_i^T + (y_i^T \eta_i) H_i b_i b_i^T H_i], \quad (3-7)$$

where a transformation  $d_i \leftrightarrow b_i$  is used. The eq. (3-7) represents the dual recursive formula to the eq. (2-9) on the basis of Fletcher's duality.

Since we have the dual generalized variable-metric algorithm (3-7), we consider dual recursive formulae corresponding to the eqs. (2-10) to (2-14) in section 2. 2. The following dual recursive formulae are derived:

- (1) The DFP algorithm (3-1) as  $b_i = y_i$ ,
- (2) Broyden's first algorithm (2-11) as  $b_i = y_i - G_i \sigma_i$ . This algorithm is identical with dual one, so that it is referred to as *self dual*.
- (3) As  $b_i = G_i \sigma_i$ ,

$$H_{i+1} = H_i + \frac{y_i^T \sigma_i + \sigma_i^T G_i \sigma_i}{y_i^T \sigma_i (y_i^T \sigma_i + \sigma_i^T G_i \sigma_i) - (\sigma_i^T G_i \sigma_i) (y_i^T H_i y_i)} \times \left[ -\sigma_i y_i^T H_i - H_i y_i \sigma_i^T + \left( 1 + \frac{\sigma_i^T G_i \sigma_i}{y_i^T \sigma_i + \sigma_i^T G_i \sigma_i} \right) \sigma_i \sigma_i^T + \frac{\sigma_i^T G_i \sigma_i}{y_i^T \sigma_i + \sigma_i^T G_i \sigma_i} H_i y_i y_i^T H_i \right] \quad (3-8)$$

- (4) As  $b_i = \sigma_i$ ,

$$H_{i+1} = H_i + \frac{1}{(\sigma_i^T H_i y_i)^2 - (y_i^T \eta_i)(\sigma_i^T H_i \sigma_i)} \times [-(\sigma_i^T H_i y_i)(\eta_i \sigma_i^T H_i + H_i \sigma_i \eta_i^T) + (\sigma_i^T H_i \sigma_i) \eta_i \eta_i^T + (y_i^T \eta_i) H_i \sigma_i \sigma_i^T H_i] \quad (3-9)$$

- (5) As  $b_i = G_i y_i$ ,

$$H_{i+1} = H_i + \frac{1}{(y_i^T y_i)^2 - (y_i^T \eta_i)(y_i^T G_i y_i)} \times [-(y_i^T y_i)(\eta_i y_i^T + y_i \eta_i^T) + (y_i^T G_i y_i) \eta_i \eta_i^T + (y_i^T \eta_i) y_i y_i^T]. \quad (3-10)$$

### 3. 2 Extension of Fletcher's one-parameter family

In accordance with Fletcher's duality, Fletcher's one-parameter family is extended to a new one-parameter family which consists of generalized variable-metric algorithms which are dual with each other. We take any linear combination of

eqs. (2-9) and (3-7) in such a way that the coefficients sum is unity, i. e.,

$$H_{i+1} = (1-\phi)H_{i+1}^0 + \phi H_{i+1}^1 = H_i - \frac{\eta_i d_i^T + d_i \eta_i^T}{d_i^T y_i} + \frac{y_i^T \eta_i d_i d_i^T}{(d_i^T y_i)^2} + \phi \tilde{H}_i, \quad (3-11)$$

where

$$\begin{aligned} \tilde{H}_i = \frac{1}{(b_i^T H_i y_i)^2 - (y_i^T \eta_i)(b_i^T H_i b_i)} \{ & (b_i^T H_i y_i)(\eta_i b_i^T H_i + H_i b_i \eta_i^T) - (b_i^T H_i b_i) \eta_i \eta_i^T \\ & - (y_i^T \eta_i) H_i b_i b_i^T H_i \} - \frac{\eta_i d_i^T + d_i \eta_i^T}{d_i^T y_i} + \frac{y_i^T \eta_i d_i d_i^T}{(d_i^T y_i)^2}, \end{aligned}$$

the matrix  $H_{i+1}$  in eqs. (3-7) and (2-9) is denoted by  $H_{i+1}^0$  and  $H_{i+1}^1$ , respectively. The new one-parameter family (3-11) includes the following formulae:

- (1) Fletcher's one-parameter family (3-2) as  $d_i = \sigma_i$  and  $b_i = y_i$ .
- (2) A one-parameter family consisted of Greenstadt's first formula (2-12) and its dual formula (3-8) as  $d_i = H_i y_i$  and  $b_i = G_i \sigma_i$ .
- (3) A one-parameter family consisted of Greenstadt's second formula (2-13) and its dual formula (3-9) as  $d_i = y_i$  and  $b_i = \sigma_i$ .
- (4) A new one-parameter family consisted of eqs. (2-14) and (3-10) as  $d_i = H_i \sigma_i$  and  $b_i = G_i y_i$ .

Furthermore, we can show that Fletcher's one-parameter family derived from the eq. (3-11) includes the following formulae:

- (1) Broyden's first formula (2-11) as  $\phi = \sigma_i^T y_i / (\sigma_i^T y_i - y_i^T H_i y_i)$ .
- (2) Greenstadt's first formula (2-12) as  $\phi = -\sigma_i^T y_i / y_i^T H_i y_i$ .
- (3) Broyden's second formula<sup>11)</sup> as  $\phi = \beta_i \sigma_i^T y_i$ .

$$\begin{aligned} H_{i+1} = H_i - H_i y_i z_i^T + \sigma_i y_i^T, \quad z_i^T = \delta_i y_i^T H_i + \beta_i \sigma_i^T, \quad q_i^T = \alpha_i s_i^T - \beta_i y_i^T H_i, \\ \delta_i = \frac{1 - \beta_i \sigma_i^T y_i}{y_i^T H_i y_i}, \quad \alpha_i = \frac{1 + \beta_i y_i^T H_i y_i}{s_i^T y_i}. \end{aligned} \quad (3-12)$$

- (4) Shanno's formula<sup>7)</sup> as  $\phi = (1-t) \sigma_i^T y_i / ((1-t) \sigma_i^T y_i - y_i^T H_i y_i)$ ,

$$H_{i+1} = H_i + t \frac{\sigma_i \sigma_i^T}{\sigma_i^T y_i} + \frac{[(1-t) \sigma_i - H_i y_i][ (1-t) \sigma_i - H_i y_i ]^T}{[(1-t) \sigma_i - H_i y_i]^T y_i} \quad (3-13)$$

Since we have a new one-parameter family (3-11) of the generalized variable-metric method, we require more theoretical and computational research for the new one-parameter family in order to be regarded as an efficient and practical tool for unconstrained minimization problems. However, in this paper, we do not treat these problems in detail.

#### 4. Discussions

We have the new one-parameter family which consists of the generalized variable-metric methods which are dual with each other. We found that a new one-parameter family was derived from a new one-parameter family generalized variable-metric method. We also showed that the new one-parameter family was the extension of Fletcher's one-parameter family of variable-metric method. However, for the new one-parameter family, we do not study both the property presented by the concept of exactness and the stability for the convergence but Fletcher's one-parameter family has been already investigated for these properties<sup>1)</sup>. In order to guarantee the superiority of the new one-parameter family to other variable-metric methods, it is necessary to study whether or not the new one-

parameter family satisfy the above properties. However, these problems will remain unsolved in this paper. Furthermore, from the computational point of view, it is necessary to test whether or not the new one-parameter family is considered as an efficient and effective method, because of the complicated recursive form for the new one-parameter family. These algorithms will be tested in the near future.

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