N 71 10539
CR 111129

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COLLEGE OF ENGINEERING

FACILITY FORM 602

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|---|---|
| N71-10539 (ACCESSION NUMBER) | — (THRU) |
| 14 (PAGES) | G1 (CODE) |
| NASA-CR-111129 (NASA CR OR TMX OR AD NUMBER) | 19 (CATEGORY) |

Report No. 140

## ON THE DAVIDON-FLETCHER-POWELL METHOD FOR FUNCTION MINIMIZATION

by

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July 1, 1969

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# On the Davidon-Fletcher-Powell Method for Function Minimization[1]

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Abstract. A method for improving the computations in the Davidon-Fletcher-Powell method for function minimization is suggested. It utilizes the doubly relaxed generalized inverse of the matrix which is usually obtained from the gradient vectors. The method consists of simple perturbations in the scalar terms of the correction matrix.

## 1. Introduction

The Davidon-Fletcher-Powell (DFP) method (Refs. 1, 2) for function minimization is one of the most popular methods. However, it has been observed that the DFP method does not always proceed smoothly. For example: Broyden (Ref. 3) remarked that occasionally negative steps had to be taken. McCormick (Ref. 4) observed that periodic reinitialization of the matrix lead to significant improvement. Wolfe (Ref. 5) has reported cases where convergence to non-stationary points had taken place. Bard (Ref. 6) had encountered similar behavior which, he observed, was invariably the result of the matrix turning singular.

In this paper we shall make use of the generalized inverses to give a technique for improving the DFP method. In Section 2 we will introduce the doubly relaxed W-generalized inverse, where W is a positive definite matrix.

[1] Paper received July , 1969. This research was supported in part by the National Aeronautics and Space Administration, Grant No. NGR-33-015-013.

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In Section 3, we will describe a modification in the DFP method and prove that the associated matrices are positive definite.

## 2. The doubly relaxed W-generalized inverse

Let B be an m x n matrix of rank r ($r \le m \le n$). If X is a matrix satisfying each of the equations

$$B\,X\,B = B, \quad X\,B\,X = X, \quad (BX)^T = BX \text{ and } (XB)^T = XB, \tag{2.1}$$

(where T denotes the transpose), then X is unique and is called the generalized inverse of B, viz., $X = B^+$, (Ref. 7). If

$$\Delta = BB^T + \varepsilon\, I_m, \tag{2.2}$$

where $I_m$ is the identity matrix of order m and $\varepsilon$ is a small positive number, then $B(\varepsilon)^+$, the doubly relaxed generalized inverse of B, is defined by Rutishauser (Ref. 8) as

$$B(\varepsilon)^+ = B^T(\Delta + \varepsilon\, \Delta^{-1})^{-1}. \tag{2.3}$$

Let $D = \{d_i\}$ be a non-singular diagonal matrix of order r with $d_i > 0$ as its ith diagonal element, then we have

Lemma 2.1.

$$\lim_{\varepsilon \to 0} D(D^2 + \varepsilon\, I_r + \varepsilon\, (D^2 + \varepsilon\, I_r)^{-1})^{-1} = D^{-1}. \tag{2.4}$$

Proof. Since $D = \{d_i\}$, $d_i > 0$, we have

$$\lim_{\varepsilon \to 0} D(D^2 + \varepsilon\, I_r + \varepsilon(D^2 + \varepsilon\, I_r)^{-1})^{-1} = \lim_{\varepsilon \to 0} \left\{ \frac{d_i}{d_i^2 + \varepsilon + \dfrac{\varepsilon}{d_i^2 + \varepsilon}} \right\} = \left\{\frac{1}{d_i}\right\} = D^{-1}.$$

The following Theorem shows the relation between $B^+$ and $B(\varepsilon)^+$.

Theorem 2.1 (Rutishauser, Ref. 8).

$$B^+ = \lim_{\varepsilon \to 0} B(\varepsilon)^+. \tag{2.5}$$

We give a proof of the above theorem since, in Ref. 8 it is omitted.

Proof. There exist matrices Q and S such that (Ref. 9, p. 10)

$$Q^TQ = QQ^T = I_m \ , \quad S^TS = SS^T = I_n \tag{2.6}$$

and

$$QBS = \begin{bmatrix} D & 0 \\ 0 & 0 \end{bmatrix}, \tag{2.7}$$

where D is a non-singular, diagonal matrix of rank r. The diagonal elements of D are greater than zero and are the non-zero singular values of B. In view of (2.7), (2.2) and (2.6), we have

$$B = Q^T \begin{bmatrix} D & 0 \\ 0 & 0 \end{bmatrix} S^T \tag{2.8}$$

$$\Rightarrow \ \Delta = Q^T \begin{bmatrix} D^2 & 0 \\ 0 & 0 \end{bmatrix} Q + \epsilon \, Q^TQ \ ,$$

$$\Rightarrow \ \Delta = Q^T \begin{bmatrix} D^2 + \epsilon I_r & 0 \\ 0 & \epsilon \, I_{m-r} \end{bmatrix} Q. \tag{2.9}$$

From (2.9) it follows that

$$(\Delta + \epsilon \, \Delta^{-1})^{-1} = Q^T \begin{bmatrix} \left(D^2 + \epsilon I_r + \epsilon \, (D^2 + \epsilon I_r)^{-1}\right)^{-1} & 0 \\ 0 & (1 + \epsilon)^{-1} I_{m-r} \end{bmatrix} Q$$

and from (2.3), (2.8) and Lemma 2.1, we have

$$B(\epsilon)^+ = B^T(\Delta + \epsilon \, \Delta^{-1})^{-1} = S \begin{bmatrix} D\left(D^2 + \epsilon \, I_r + \epsilon \, (D^2 + \epsilon \, I_r)^{-1}\right)^{-1} & 0 \\ 0 & 0 \end{bmatrix} Q \ ,$$

$$\lim_{\epsilon \to 0} B(\epsilon)^+ = S \begin{bmatrix} D^{-1} & 0 \\ 0 & 0 \end{bmatrix} Q = B^+,$$

the last equality follows from direct substitution in (2.1) and using (2.8) and (2.6) (Ref. 10). This completes the proof of the theorem.

Rutishauser (Ref. 8) has shown theoretically and also by one numerical example that the doubly relaxed generalized inverse $B(\epsilon)^+$ leads to better results on a computer than the direct computation of $B^+$, if the non-singular part of B is ill-conditioned. In order to make use of the above fact in the DFP method, we will need the following.

Since W is a positive definite matrix, there exists a non-singular lower triangular matrix R, such that

$$RR^T = W. \tag{2.10}$$

This is known as the Choleskey decomposition of W (Ref. 11, p. 229). Let A be an m x n matrix of rank r, such that

$$B = AR . \tag{2.11}$$

Then the unique solution X of the equations

$$AXA = A,\ XAX = X,\ (AX)^T = AX \text{ and } (XAW)^T = XAW, \tag{2.12}$$

is called the W-generalized inverse of A and is denoted by $A^+_W$. This definition of $A^+_W$ was given by Herring (Ref. 12) in a slightly more general form. For our pusposes the above definition will suffice. Let the $W^{-1}$ norm of X be defined by

$$\|X\|_{W^{-1}} = \text{trace } X^T W^{-1} X, \tag{2.13}$$

then Herring (Ref. 12) has proved the following theorem.

Theorem 2.2 (Herring). If F is a matrix with m rows, then

$$X = A^+_W F \tag{2.14}$$

is the least squares solution of the matrix equation

$$AX = F . \tag{2.15}$$

having the minimum $W^{-1}$ norm.

We will also need the following theorem.

Theorem 2.3. If $A^+_W$ and $B^+$ are the solutions of (2.12) and (2.1) respectively, then

$$A^+_W = RB^+. \tag{2.16}$$

Proof. By direct substitution in (2.1) and using (2.8) and (2.6), it is easy to verify that (Ref. 10)

$$B^+ = S\begin{bmatrix} D^{-1} & 0 \\ 0 & 0 \end{bmatrix} Q. \tag{2.17}$$

Also, from (2.11) and (2.8), it follows that

$$A = BR^{-1} = Q^T \begin{bmatrix} 0 & 0 \\ 0 & 0 \end{bmatrix} S^T R^{-1}. \tag{2.18}$$

In view of (2.17), (2.18), (2.6) and (2.10), it is easy to check that $RB^+$ satisfies (2.12) and therefore (2.16) holds.

We conclude this section with the definition of $A(\epsilon)^+_W$ as follows.

$$A(\epsilon)^+_W = RB(\epsilon)^+ , \tag{2.19}$$

which, in view of (2.3), (2.11), (2.10) and (2.2), implies that

$$A(\epsilon)^+_W = RB^T(\Delta + \epsilon\, \Delta^{-1})^{-1} = RR^TA^T(\Delta + \epsilon\, \Delta^{-1})^{-1} = WA^T(\Delta + \epsilon\, \Delta^{-1})^{-1}, \tag{2.20}$$

where

$$\Delta = BB^T + \epsilon\, I_m = ARR^TA^T + \epsilon\, I_m = AWA^T + \epsilon\, I_m . \tag{2.21}$$

## 3. A Modification in the DFP Method.

Let us consider the problem of finding the n element column vector x that minimizes the quadratic function

$$f(x) = \tfrac{1}{2}\, x^TGx + b^Tx + c, \tag{3.1}$$

where G is a positive definite matrix, b is an n element column vector and c a constant (Ref. 13, Chap. 3 and Ref. 14).

Let the $i^{th}$ approximation to the vector which minimizes (3.1) be denoted by $x_i$. Then in (3.1), the gradient of $f(x)$ at $x_i$ is given by

$$g_i = Gx_i + b, \tag{3.2}$$

which implies that

$$g_{i+1} - g_i = G(x_{i+1} - x_i) . \tag{3.3}$$

If we let

$$g_{i+1} - g_i = y_i^T \text{ and } x_{i+1} - x_i = s_i^T , \tag{3.4}$$

then (3.3) can be written as

$$y_i^T = G\, s_i^T \Rightarrow y_i = s_i\, G. \tag{3.5}$$

Let

$$Y_i = \begin{bmatrix} y_o \\ \cdot \\ \cdot \\ \cdot \\ y_{i-1} \end{bmatrix} \text{and } S_i = \begin{bmatrix} s_o \\ \cdot \\ \cdot \\ \cdot \\ s_{i-1} \end{bmatrix} . \tag{3.6}$$

Pearson (Ref. 14) gives the following algorithm for the minimization of (3.1).

Algorithm 3.1. Let P be a positive definite matrix. Given $x_o$ and $H_o = P$. Solve for $H_i$, the equation

$$Y_i\, H_i = S_i \tag{3.7}$$

and determine $x_{i+1}$ from the relation

$$f(x_{i+1}) = \min_{\alpha_i} f(x_i + \alpha_i H_i g_i) .$$

Compute $g_{i+1}$ and using $x_{i+1}$, update $Y_i$ and $S_i$ and (3.7) as follows

$$Y_{i+1} = \begin{bmatrix} Y_i \\ y_i \end{bmatrix} \text{and } S_{i+1} = \begin{bmatrix} S_i \\ s_i \end{bmatrix}, \tag{3.8}$$

$$Y_{i+1} H_{i+1} = S_{i+1} . \tag{3.9}$$

It is proved in Ref. 14, that the above algorithm terminates for $i \le n$, if the solution of (3.7) is taken as

$$H_i = (Y_i)^+_W S_i + (I_n - (Y_i)^+_{\hat{W}} Y_i)^{-1} P \tag{3.10}$$

and $W = P$ or $G^{-1}$ and $\hat{W} = P$ or $G^{-1}$. In case $W = G^{-1}$ and $\hat{W} = P$, we get the Davidon-Fletcher-Powell method.

We are now in a position to describe a modification to the DFP method. To this end, let

$$H_{i+1} = H_i + C_i \,. \tag{3.11}$$

In view of (3.9), (3.11), (3.8) and (3.7), we have

$$Y_{i+1} C_i = S_{i+1} Y_{i+1} H_i = \begin{bmatrix} S_i \\ s_i \end{bmatrix} - \begin{bmatrix} Y_i \\ y_i \end{bmatrix} H_i = \begin{bmatrix} S_i - Y_i H_i \\ s_i - y_i H_i \end{bmatrix}$$

$$= \begin{bmatrix} 0 \\ s_i - y_i H_i \end{bmatrix}. \tag{3.12}$$

Let

$$Y_{i+1} \bar{C}_i = \begin{bmatrix} 0 \\ s_i \end{bmatrix} \text{ and } Y_{i+1} \hat{C}_i = \begin{bmatrix} 0 \\ y_i H_i \end{bmatrix}, \tag{3.13}$$

then from (3.12), it follows that

$$C_i = \bar{C}_i - \hat{C}_i. \tag{3.14}$$

Also, in view of Theorem 2.2, (3.13) implies that

$$\bar{C}_i = (Y_{i+1})^+_W \begin{bmatrix} 0 \\ s_i \end{bmatrix} \text{ and } \hat{C}_i = (Y_{i+1})^+_{\hat{W}} \begin{bmatrix} 0 \\ y_i H_i \end{bmatrix} \tag{3.15}$$

are the least squares solutions of the two equations in (3.13) with the minimum $W^{-1}$ and $\hat{W}^{-1}$ norms respectively. We will need the following theorem.

Theorem 3.1. If in (3.15), $(Y_{i+1})^T_W$ and $(Y_{i+1})^+_{\hat{W}}$ are replaced by $Y_{i+1}(\epsilon)^+_W$ and $Y_{i+1}(\epsilon)^+_{\hat{W}}$ respectively and

$$y_i W Y_i^T = 0 \text{ and } y_i \hat{W} Y_i^T = 0 , \tag{3.16}$$

then

$$\bar{C}_i = W y_i^T s_i (\alpha + \epsilon \alpha^{-1})^{-1} \text{ and } \hat{C}_i = \hat{W} y_i^T y_i H_i (\hat{\alpha} + \epsilon \hat{\alpha}^{-1})^{-1}, \tag{3.17}$$

where

$$\alpha = y_i W y_i^T + \epsilon \text{ and } \hat{\alpha} = y_i \hat{W} y_i^T + \epsilon \tag{3.18}$$

Proof. From (2.20), (2.21), (3.8) and (3.16), we have

$$Y_{i+1}(\epsilon)^+_W = W Y_{i+1}^T (\Delta_{i+1} + \epsilon \Delta_{i+1}^{-1})^{-1}, \tag{3.19}$$

where

$$\Delta_{i+1} = Y_{i+1} W Y_{i+1}^T + \epsilon I_{i+1} = \begin{bmatrix} Y_i \\ y_i \end{bmatrix} W \begin{bmatrix} Y_i^T , y_i^T \end{bmatrix} + \epsilon I_{i+1}$$

$$= \begin{bmatrix} Y_i W Y_i^T & Y_i W y_i^T \\ y_i W Y_i^T & y_i W y_i^T \end{bmatrix} + \epsilon I_{i+1} = \begin{bmatrix} Y_i W Y_i^T + \epsilon I_i & 0 \\ 0 & y_i W y_i^T + \epsilon \end{bmatrix},$$

and using (3.18), we get

$$\Delta_{i+1} = \begin{bmatrix} \Delta_i & 0 \\ 0 & \alpha \end{bmatrix}, \tag{3.20}$$

where $\Delta_i = Y_i W Y_i^T + \epsilon I_i$ . Now, in view of (3.8), equations (3.19) and (3.20) give

$$Y_{i+1}(\epsilon)^+_W = W Y_{i+1}^T \left[ \begin{bmatrix} \Delta_i & 0 \\ 0 & \alpha^{-1} \end{bmatrix} + \epsilon \begin{bmatrix} \Delta_i^{-1} & 0 \\ 0 & \alpha^{-1} \end{bmatrix} \right]^{-1}$$

$$= W(Y_i^T, y_i^T) \begin{bmatrix} (\Delta_i + \epsilon \Delta_i^{-1})^{-1} & 0 \\ 0 & (\alpha + \epsilon \alpha^{-1})^{-1} \end{bmatrix}$$

$$= W\left( Y_i^T (\Delta_i + \epsilon \Delta_i^{-1})^{-1}, y_i^T (\alpha + \epsilon \alpha^{-1})^{-1} \right) . \tag{3.21}$$

Now, from the hypothesis of theorem, (3.15) and (3.21), it follows that

$$\bar{C}_i = Wy_i^T s_i(\alpha + \epsilon\,\alpha^{-1})^{-1}.$$

Replacing W by $\hat{W}$ in (3.21), we get the value of $\hat{C}$ given by (3.17). This completes the proof of the theorem.

The following corollary to the above theorem gives the desired resired result.

Corollary 3.1. If, in Theorem 3.1, $W = G^{-1}$ and $\hat{W} = H_i$, then

$$H_{i+1} = H_i + \frac{s_i^T s_i}{y_i s_i^T + \epsilon + \epsilon(y_i s_i^T + \epsilon)^{-1}} - \frac{H_i y_i^T y_i H_i}{y_i H_i y_i^T + \epsilon + \epsilon(y_i H_i y_i^T + \epsilon)^{-1}}. \quad (3.22)$$

Proof: Since, in view of (3.5), $Wy_i^T = G^{-1}y_i^T = s_i^T$, and $\hat{W}y_i^T = H_i y_i^T$; equation (3.22) follows from (3.17), (3.18), (3.14) and (3.11).

It is easy to see that (3.16) is satisfied if $\hat{W} = G^{-1}$ and $\hat{W} = H_i$, because in view of (3.5) and (3.7), we have $y_i G^{-1} Y_i^T = s_i G S_i^T$ and $y_i H_i Y_i^T = s_i G S_i^T$. Therefore, in this case (3.16) implies that $s_i G s_i^T = 0$, $j < i$, which is known to be satisfied (Ref. 13, Chap. 3).

The choice of $H_i$ for $\hat{W}$ in Corollary 3.1 is justified provided that $H_i$ given by (3.22) is positive definite. It is easy to see that for $\epsilon = 0$, equation (3.22) is the usual updating formula for the DFP method and $H_i$ is known to be positive definite (Ref. 13, Chap. 3). For $\epsilon > 0$, we have

Theorem 3.3. If $H_o = P$, then the $H_i$ given by (3.22) are positive definite for all i.

Proof. Since $H_o = P$ is positive definite, we will show that whenever $H_i$ is positive definite $H_{i+1}$ is also positive definite; then by induction the theorem is proved. Let $H_i$ be positive definite, then

$$\delta = \epsilon + \frac{\epsilon}{y_i H_i y_i^T + \epsilon} > 0 .$$

By the Cauchy-Schwartz inequality for an arbitrary n dimensional row vector u with $u^T u \neq 0$, we have

$$(y_i H_i u^T)^2 \leq (y_i H_i y_i^T)(u H_i u^T) < (y_i H_i y_i^T + \delta)(u H_i u^T),$$

which implies that

$$\frac{(y_i H_i u^T)^2}{y_i H_i y_i^T + \delta} < u H_i u^T. \tag{3.23}$$

But, from (3.22) and (3.23) it follows that

$$u H_{i+1} u^T = \frac{(s_i u^T)^2}{y_i s_i^T + \epsilon + \epsilon(y_i s_i^T + \epsilon)^{-1}} + u H_i u^T - \frac{(y_i H_i u^T)^2}{y_i H_i y_i^T + \delta}.$$

$$> 0, \text{ if } y_i s_i^T + \epsilon > 0.$$

Since $\epsilon > 0$ and in view of (3.5) and the fact that G is positive definite $y_i s_i^T = s_i G s_i^T > 0$; therefore $y_i s_i^T + \epsilon > 0$, and thus we have proved that if $H_i$ is positive definite, then $H_{i+1}$ is also positive definite and this completes the proof of the theorem.

## 4. Concluding Remarks.

In this paper we have given a technique (3.22) for improving the computation of the $H_i$ matrix in the DFP method. In the derivation of (3.22), we made use of the doubly relaxed W-generalized inverse $Y_{i+1}(\epsilon)^+_W$. Since R is a non-singular matrix from Ref. 8, (2.16) and (2.19), it follows that, in general, $Y_{i+1}(\epsilon)^+_W$ will give better results than $(Y_{i+1})^+_W$. This is especially true, if due to round-off errors etc., the rows of $Y_{i+1}$ are not linearly independent (Ref. 6). Rutishauser (Ref. 8) observes that the choice $10^{-5} \le \epsilon \le 10^{-10}$ lead to good results in a computer with 35 bit mantissa when he computed the boubly relaxed generalized inverse. The proper value for $\epsilon$ will have to be determined on the basis of large scale numerical experimentation.

We can also use the doubly relaxed W-generalized inverse in the periodic computation of $H_i$ directly from (3.10). It is known that such periodic direct computation of $H_i$ improves the performance of the DFP method (Ref. 4). Thus in (3.10), replacing $(Y_i)^+_W$ and $(Y_i)^+_{\hat{W}}$ by $Y_i(\epsilon)^+_W$ and $Y_i(\epsilon)^+_{\hat{W}}$ respectively and in view of the fact that $W = G^{-1}$ and $\hat{W} = P$ for the DFP method, we get

$$H_i = Y_i(\epsilon)^+_{G^{-1}} S_i + (I_n - Y_i(\epsilon)^+_P Y_i) P \quad , \tag{3.24}$$

where, in view of (3.19) and (3.5), we have

$$Y_i(\epsilon)^+_{G^{-1}} = S_i^T(\Delta_i + \epsilon \Delta_i^{-1})^{-1} \quad , \tag{3.25}$$

$$\Delta_i = S_i Y_i^T + \epsilon I_i \quad , \tag{3.26}$$

$$Y_i(\epsilon)^+_P = PY_i^T(\hat{\Delta}_i + \epsilon \hat{\Delta}_i^{-1})^{-1} \tag{3.27}$$

and

$$\hat{\Delta}_i = Y_i \, P \, Y_i^T + \epsilon \, I_i \quad . \tag{3.28}$$

Note that (3.24) can be computed even if $Y_i$ does not have full row rank, which would not be possible in Ref. 14. In view of the theoretical results in Ref. 8, equations (3.24)-(3.28) should in general, lead to better $H_i$.

We conclude this paper with the following remarks on $H_i$ which is given by (3.22). The $H_i$ for the DFP method is

$$H_{i+1} = H_i + \frac{s_i^T \, s_i}{y_i \, s_i^T} - \frac{H_i \, y_i^T \, y_i \, H_i}{y_i \, H_i \, y_i^T} \tag{3.29}$$

If $y_i \, s_i^T$ is small then evidently $\frac{s_i^T \, s_i^T}{y_i \, s_i^T}$ dominates $\frac{H_i \, y_i^T \, y_i \, H_i}{y_i \, H_i \, y_i^T}$, this leads to inaccuracy in $H_{i+1}$ (Ref. 6). Let $y_i \, s_i^T = o(\epsilon) = \lambda \, \epsilon$, where $\lambda$ is a constant, then

$$\lim_{\epsilon \to 0} \frac{s_i^T \, s_i}{y_i \, s_i^T} = \infty \quad .$$

On the other hand

$$\lim_{\epsilon \to 0} (y_i \, s_i^T + \epsilon + \epsilon(y_i \, s_i^T + \epsilon)^{-1}) = \lim_{\epsilon \to 0} ((\lambda + 1) \, \epsilon + (\lambda + 1)^{-1}) = (\lambda + 1)^{-1} .$$

The perturbation in $y_i \, H_i \, y_i^T$ can be similarly justified.

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