STATE UNIVERSITY OF NEW YORK
AT STONY BROOK

COLLEGE OF
ENGINEERING

Report No. 127

APPLICATIONS OF GENERALIZED INVERSES IN THE SOLUTION OF LINEAR EQUATIONS AND FUNCTION MINIMIZATION

by

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FEBRUARY 15, 1969

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Abstract.

A method is given for deriving the formula for the V-W generalized inverse of a matrix. A similar technique is then used to generalize the method of damped least squares for the solution of linear equations. The V-W generalized inverse is utilized to extend the weak method of steepest descent and to generalize the expression for the basic least squares solution of linear equations. Techniques for improving the computation of V-W generalized inverse and some of the applications to the unconstrained function minimization problem are also given.

1. Introduction.

Let A be an m x n matrix of rank r. Then it is possible to construct [24], [25] an m x r matrix K and an r x n matrix L such that

(1.1) $$A = KL.$$

By direct substitution in the following four defining relations for the generalized inverse of a matrix given by Penrose [19]

(1.2) $$AA^+A = A,\quad A^+AA^+ = A^+,\quad AA^+ = (AA^+)' \text{ and } A^+A = (A^+A)',$$

it can be easily verified that [12]

(1.3) $$A^+ = L^+K^+ = L'(LL')^{-1}(K'K)^{-1}K',$$

where ′ denotes the transpose. It is well known [20] that the solutions of the linear equation

(1.4) $$Ax = b$$

are given by

* This research was supported in part by the National Aeronautics and Space Administration Grant No. NGR-33-015-013.

(1.5) $$x = A^+ b + (I_n - A^+ A)\gamma,$$

where x and b are column vectors with n and m elements respectively, γ is an arbitrary n element column vector and I_n is the identity matrix of order n. Any x given by (1.5) minimizes $\|b-Ax\|_2$ viz., the Euclidean length of the residual, and out of all such x's, $x = A^+b$ has the least Euclidean length viz., $\|x\|_2$ is minimum. In other words, $x = A^+b$ is the unique minimum norm least squares solution of (1.4). Analogus to (1.3) we define [13], [14], [15]

(1.6) $$A^+_{V,W} = WL'(LWL')^{-1}(K'VK)^{-1}K'V,$$

where V and W are nonsingular symmetric matrices of order m and n respctively. It is shown in [15] that if we replace A^+ by $A^+_{V,W}$ in (1.5), then the resulting value of x minimizes $\|b-Ax\|_V$ and out of all such x's, $x = A^+_{V,W}b$ has the least W^{-1} length viz., $\|x\|_{W^{-1}}$ is minimum. The V (or W) length $\|\xi\|_V$, of row vector ξ is defined by $\|\xi\|^2_V = \xi' V \xi$.

In the next section we will give an alternative way of deriving (1.6) from the above mentioned properties of $A^+_{V,W}$, and show that the same technique can be applied to the so called method of damped least squares [16], [27], such that $\|b-Ax\|^2_V + \epsilon\|x\|^2_W$ instead of $\|b-Ax\|^2_2 + \epsilon\|x\|^2_2$ is minimized. We will also show that if W is replaced by I_n then the resulting A^+_{V,I_n} can be used to extend the weak method of steepest descent [26]. If A is of full column rank ($r=n$) than a simple application of $A^+_{V,W}$ to the basic least squares solution of linear equations is also given.

In section 3, we consider the case when A has full row rank ($r=m$) and a method is given to improve the conditioning of $A^+_{V,W}$. In section 4, several applications of the results (obtained in section 3) to the unconstrained optimization of nonlinear functions are given.

2. Alternative derivation of $A^+_{V,W}$ and applications when $r=n$.

It is shown in [20] that for all x the solution $x_0 = A^+b$ of (1.4) satisfies either

$$\|b - Ax\|_2 > \|b - Ax_0\|_2 \quad , \tag{2.1}$$

or

$$\|b - Ax\|_2 = \|b - Ax_0\|_2 \text{ and } \|x\|_2 \geq \|x_0\|_2 \quad . \tag{2.2}$$

Let us consider the solution of the system

$$(EAF)(F^{-1}x) = Eb \tag{2.3}$$

where E and F are nonsingular matrices of order m and n respectively. Then in view of (1.1) and (1.3), the minimum Euclidian length least squares solution of (2.3) is

$$\begin{aligned} F^{-1}x &= (EAF)^+ Eb = (EKLF)^+ Eb \\ &= [(EK)(LF)]^+ Eb = (LF)'[(LF)(LF)']^{-1}[(EK)'(EK)]^{-1}(EK)' Eb \\ &= F'L'(LFF'L')^{-1}(K'E'EK)^{-1}K'E' Eb \ , \end{aligned}$$

or

$$\begin{aligned} \hat{x} &= FF'L'(LFF'L')^{-1}(K'E'EK)^{-1}K'E' Eb \\ &= WL'(LWL')^{-1}(K'VK)^{-1}K'V b, \text{ where } FF' = W \text{ and } E'E = V, \text{ and from} \end{aligned}$$

(1.6), it follows that

$$\hat{x} = A^+_{VW} \ b \quad . \tag{2.4}$$

Since $F^{-1}\hat{x}$ is the least squares solution of (2.3), as in (2.1), for all x, we have $\|Eb - EAFF^{-1}x\|_2 > \|Eb - EAFF^{-1}\hat{x}\|_2$, which implies that

$$\|b - Ax\|_V > \|b - A\hat{x}\|_V \quad . \tag{2.5}$$

Similiarily, the minimum norm condition (2.2) gives

$$\|Eb - EAFF^{-1}x\|_2 = \|Eb - EAFF^{-1}\hat{x}\|_2 \text{ and } \|F^{-1}x\|_2 \geq \|F^{-1}\hat{x}\|_2 \quad ,$$

which yeilds

(2.6) $$\|b - Ax\|_V = \|b - A\hat{x}\|_V \text{ and } \|x\|_{W^{-1}} \geq \|\hat{x}\|_{W^{-1}} .$$

The above results can be stated as

Theorem 2.1. If $\hat{x} = A^+_{V,W}b$ is chosen as the solution of (1.4), then for all x either (2.5) or (2.6) holds.

The above theorem was first given by Greville [13], [14] for either W = I or V = I and was later extended by Herring [15]. Bauer [3] has given an Algol Program for n = r and an especially chosen matrix V. The main advantage of our proof is that a similar technique can be used to extend the method of damped least squares [16], [27], such that the V length of the residual vector and the W length of the solution vector is minimized, instead of the usual Euclidian lengths. We have the following

Theorem 2.2. If in equation (1.4), A has full column rank (n = r) and

(2.7) $$\tilde{x} = (A'VA + \epsilon W)^{-1} A'V b ,$$

then for all x

(2.8) $$\|b - Ax\|^2_V + \epsilon\|x\|^2_W > \|b - A\tilde{x}\|^2_V + \epsilon\|\tilde{x}\|^2_W ,$$

where ϵ is a small positive number.

Proof. Consider the least squares solution of the system

(2.9) $$\begin{pmatrix} EA \\ \tau F \end{pmatrix} x = \begin{pmatrix} Eb \\ 0 \end{pmatrix}, \text{ where } \tau = \sqrt{\epsilon} > 0 .$$

Since A has full column rank (r = n) and E has rank m ≥ n, therefore, in view of (1.1) and (1.3), we have

$$\begin{pmatrix} EA \\ \tau F \end{pmatrix}^+ = \left[(A'E', \tau F')\begin{pmatrix} EA \\ \tau F \end{pmatrix}\right]^{-1} (A'E', \tau F') = (A'E'EA + \tau^2 F'F)^{-1} (A'E', \tau F')$$

$$= (A'VA + \epsilon W)^{-1} (A'E', \tau F'), \text{ since } E'E = V \text{ and } F'F = W ,$$

and

$$\begin{pmatrix} EA \\ \tau F \end{pmatrix}^+ \begin{pmatrix} EA \\ \tau F \end{pmatrix} = (A'VA + \epsilon W)^{-1} (A'E', \tau F')\begin{pmatrix} EA \\ \tau F \end{pmatrix}$$
$$= (A'VA + \epsilon W)^{-1} (A'VA + \epsilon W) = I_n .$$

Thus from (1.5) it follows that the solution of (2.9) is

$$\tilde{x} = (A'VA + \epsilon W)^{-1} (A'E', \tau F') \begin{pmatrix} Eb \\ 0 \end{pmatrix} + (I_n - I_n) \gamma$$
$$= (A'VA + \epsilon W)^{-1} A'V\, b \ ,$$

and $\tilde{x}$ is the unique least squares solution of (2.9) viz., for all x

$$\left\| \begin{pmatrix} Eb \\ 0 \end{pmatrix} - \begin{pmatrix} EA \\ \tau F \end{pmatrix} x \right\|_2^2 > \left\| \begin{pmatrix} Eb \\ 0 \end{pmatrix} - \begin{pmatrix} EA \\ \tau F \end{pmatrix} \tilde{x} \right\|_2^2 ,$$

$$\Rightarrow \| E(b - Ax) \|_2^2 + \tau^2 \| Fx \|_2^2 > \| E(b - A\tilde{x}) \|_2^2 + \tau^2 \| F\tilde{x} \|_2^2$$

$$\Rightarrow \| b - Ax \|_V^2 + \epsilon \| x \|_W^2 > \| b - A\tilde{x} \|_V^2 + \epsilon \| \tilde{x} \|_W^2 ,$$

this completes the proof of the theorem.

For some of the uses and comments on the method of damped least squares as well as the usual least squares method the reader is referred to [4], [5], [6], [11], [16], [27] . We will now show how the $A^+_{V,W}$ can be used in the weak method of steepest descent. To this end, we will need the following theorem, a constructive proof of which is given in [26].

Theorem 2.3. The iterative scheme

(2.10) $$u_{k+1} = (I_n - \mu A'A)\, u_k + \mu A'b$$

with arbitrary u_0 converges to $\bar{u} = A^+ b + (I_n - A^+ A)\, u_0$, if $0 < \mu < 2/\|A'A\|_\infty$.

In the above theorem $\|A'A\|_\infty$ denotes the usual maximum norm [10, p. 63], which is easy to evaluate. Now we can prove the following

Theorem 2.4. The iterative scheme

(2.11) $$u_{k+1} = (I_n - \mu A'VA)\, u_k + \mu A'V\, b$$

converges to $\bar{u} = A^+_{V,I} b$, if $u_0 = A'\gamma$ and $0 < \mu < 2/\|A'VA\|_\infty$, where γ is an arbitrary column vector with m elements.

Proof. Theorem (2.3) is certainly true if the matrix A and the vector b are replaced by EA and Eb respectively, since E is a non-singular matrix. Now

(2.12) $$(EA)'(EA) = A'E'EA = A'VA \text{ , since } V = E'E \text{ .}$$

(2.13) $$(EA)'Eb = A'E'Eb = A'Vb$$

(2.14) $$[I_n - (EA)^+EA]\, A' = A' - (EKL)^+EKL\, L'K' \text{ , using (1.1)}$$
$$= A' - L'(LL')^{-1}(K'E'EK)^{-1}K'E'EK\, LL'K' \text{ , using (1.3)}$$
$$= A' - L'K' = 0 \text{ , using (1.1) .}$$

(2.15) $$(EA)^+Eb = (EKL)^+Eb = L'(LL')^{-1}(K'E'EK)^{-1}K'E'Eb \text{ ,}$$

using (1.1) and (1.3)

$$= L'(LL')^{-1}(K'VK)^{-1}K'Vb = A^+_{V,I}b \text{ .}$$

The theorem follows by replacing A and b by EA and Eb respectively in Theorem (2.3), followed by the use of (2.12), (2.13), (2.14) and (2.15).

From Theorem 2.1, it follows that the iterative scheme (2.11) given above minimizes the V length of the residual instead of the Euclidean length, as is the case if (2.10) is used. Minimizing the V length of the residual is at times desirable due to scaling and round-off considerations.

We will now give an application of $A^+_{V,W}$ to the basic least squares solution $\bar{x}$ of linear equations. Rosen [21] defines $\bar{x}$ as the vector having at most r non-zero components and for all other x

(2.16) $$\|b - Ax\|_2 \geq \|b - A\bar{x}\|_2 \text{ .}$$

Let P be a permutation matrix of order m such that

(2.17) $$AP = (R,\ D) \text{ ,}$$

where R denotes all the linearly independent columns of A and D the dependent ones. Equation (2.17) implies that for any non-singular matrix E, of order m, (2.18) $$EAP = (ER, ED) ,$$

and the columns in ER are linearly independent. Then the basic least squares solution of

$$EAP\, P'x = Eb \quad ,$$

according to Rosen [21], is given by

$$P'\bar{x} = (EAP)^{\#} Eb = \begin{bmatrix} (ER)^{+} \\ 0 \end{bmatrix} Eb \text{ , using (2.18)}$$

$$= \begin{bmatrix} (R'E'ER)^{-1} R'E'Eb \\ 0 \end{bmatrix} ,$$

using (1.3) and the fact that ER is of full column rank. Thus

(2.19) $$\bar{x} = P\begin{pmatrix} (R'VR)^{-1} R'Vb \\ 0 \end{pmatrix} = P\begin{pmatrix} R_V^{+} b \\ 0 \end{pmatrix} ,$$

since $R^{+}_{V,W} = (R'VR)^{-1} R'V$ is independent of W, we denote it by R^{+}_{V}. Furthermore, from (2.16), we have

$$\|Eb - EAPP'x\|_2 \geq \|Eb - EAPP'\bar{x}\|_2 \quad ,$$

which implies that

(2.20) $$\|b - Ax\|_V \geq \|b - A\bar{x}\|_V \quad .$$

Therefore $\bar{x}$ given by (2.19) can be called the V-basic solution of (1.4), since it minimizes the V length of the residual and has at most r non-zero elements. Such V-basic solution may at times be more desirable than the usual basic solution when scaling and round-off errors are taken into consideration.

3. Improving the computation of $A^+_{V,W}$ if $m = r$.

If A has rank m, then by letting $K = I$ and $L \equiv A$ in (1.1), from (1.6) we have

$$A^+_{V,W} = WA'(AWA')^{-1} = A^+_W, \text{ (say)}, \tag{3.1}$$

since the middle expression is independent of V. Also in view of the fact that A has rank m, the system (1.4) has zero residual. Therefore, from Theorem 2.1, it follows that for all x that give zero residual

$$\| x \|_{W^{-1}} \geq \| \bar{x} \|_{W^{-1}} \text{ where } \bar{x} = A^+_W b. \tag{3.2}$$

It is interesting to notice that condition (3.2) does not hold unless W is symmetric (and of course, non-singular). However, if N is a non-singular (not necessarily symmetric) matrix then

$$x = A^+_N b + (I_n - A^+_N A)\, \gamma, \text{ where } A^+_N = NA'(ANA')^{-1}, \tag{3.3}$$

is a solution of (1.4), where $r = m$. This can be easily verified by direct substitution in (1.4). We will have occasion to use (3.3) in section 4.

In case A is such that even AWA is ill-conditioned [27], a simple way of improving the computation of A^+_W is to replace (3.1) by

$$\hat{A}^+_W = WA'(AWA' + \epsilon\, I_m)^{-1}. \tag{3.4}$$

It was proved in [27] that the condition number of $AF(AF)' + \epsilon\, I_m$ is less than or equal to that of $AF(AF)'$, and therefore the computation in (3.4) is, in most cases, better than in (3.1). The following theorem gives an interpretation of the perturbation $\epsilon\, I_m$ suggested in (3.4).

Theorem 3.1. The solution of the system

$$Ax = b - \epsilon\, z, \tag{3.5}$$

where

$$z = (AWA' + \epsilon\, I_m)^{-1} b, \tag{3.6}$$

having the minimum W^{-1} length is given by

(3.7) $$x = \hat{A}^{+}_{W} b.$$

Proof. From (3.5) and (3.6), we have

$$Ax = b - \epsilon\,(AWA' + \epsilon\, I_m)^{-1} b = [(AWA' + \epsilon\, I_m) - \epsilon\, I_m](AWA' + \epsilon\, I_m)^{-1} b$$

$$= AWA'(AWA' + \epsilon\, I_m)^{-1} b.$$

Therefore, in view of (3.1) and (3.2), the solution of (3.5) with the minimum W^{-1} length is

$$x = A^{+}_{W}\, AWA'(AWA' + \epsilon\, I_m)^{-1} b = WA'(AWA')^{-1} AWA'(AWA' + \epsilon\, I_m)^{-1} b$$

$$= WA'(AWA' + \epsilon\, I_m)^{-1} b = \hat{A}^{+}_{W}\, b,$$

which completes the proof of the theorem.

For a given matrix Ω let us define

(3.8) $$\| \Omega \|^{2}_{W^{-1}} = \text{Trace}\,(\Omega'\, W^{-1}\, \Omega).$$

Now, corresponding to Theorem 3.1, we have

Theorem 3.2. In the matrix equation

(3.9) $$AX = B - \epsilon\, Z$$

if X is an n x p matrix, B and Z are both m x p matrices, and

(3.10) $$Z = (AWA' + \epsilon\, I_m)^{-1} B,$$

then

(3.11) $X = \hat{A}^{+}_{W} B$ is the solution that minimizes $\| X \|_{W^{-1}}$.

Proof: Apply Theorem 3.1 to the successive columns of B.

4. Applications of A^{+}_{W} and $\hat{A}^{+}_{W}$ to nonlinear function optimization.

In this section we will use the results obtained in the preceding section to the solution of nonlinear equations. In particular, we give alternative derivations of some of the results of Zeleznik [28] and Pearson [18] and also describe some techniques for making computational improvements in them. Some new methods are also suggested. Generalized inverses have already been utilized in non-linear function optimization by Flecher [8] and Pearson [18]. Let us consider the problem of finding the vector x that minimizes the quadratic function

(4.1) $$f(x) = \tfrac{1}{2} x'Gx + \hat{b}' x + c$$

where G is a positive definite symmetric matrix, $\hat{b}$ is an n element column vector and c a constant [18]. Let x_i denote the i^{th} approximation to the vector which minimizes (4.1). Then it follows that in (4.1), the gradient of f(x) at x_i is given by

$$g_i = Gx_i + \hat{b},$$

which implies that

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

If we let

(4.3) $$y_i = (g_{i+1} - g_i)' \text{ and } s_i = (x_{i+1} - x_i)'$$

then (4.2) can be written as

(4.4) $$y_i = s_i G .$$

We have the following algorithm [18] for the minimization of (4.1).

Algorithm 4.1. Given $Y_i = (y_0', \ldots, y_{i-1}')'$, $S_i = (s_0', \ldots, s'_{i-1})'$ and H_i which satisfies the equation

(4.5) $Y_i H_i = S_i$, where $H_o = R$, a positive definite matrix. 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 (4.5) as follows:

(4.6) $$Y_{i+1} = \begin{bmatrix} Y_i \\ y_i \end{bmatrix}, \quad S_{i+1} = \begin{bmatrix} S_i \\ s_i \end{bmatrix},$$

(4.7) $$Y_{i+1} H_{i+1} = S_{i+1} .$$

It is proved in [18] that the above algorithm terminates for $i \leq n$, if the solution of (4.5) is taken as

$$(4.8) \qquad H_i = (Y_i)^+_W S_i + [I_n - (Y_i)^+_{\bar{W}} (Y_i)]R,$$

where W and $\bar{W}$ are symmetric non-singular matrices. It should perhaps be pointed out here that we have changed the notation in [18] to transposed vectors and matrices, in order to be consistent not only with the results given in section 3 of our paper, but also the current literature in generalized inverses.

The following theorems will be needed in the sequel.

Theorem 4.1. If a non-symmetric matrix N can be found such that $Y_i N y_i' = 0$, and $v_i = N y_i'/y_i N y_i'$, then

$$(4.9) \qquad (Y_{i+1})^+_N = [(I_n - v_i y_i)(Y_i)^+_N , v_i]$$

Proof. Since Y_{i+1} is of full row rank [1], therefore from (3.3) and (4.6), we have

$$\left(Y_{i+1}\right)^+_N = NY'_{i+1}\left(Y_{i+1} NY'_{i+1}\right)^{-1} = NY'_{i+1}\left[\begin{pmatrix} Y_i \\ y_i \end{pmatrix} N(Y_i', y_i')\right]^{-1}$$

$$= NY'_{i-1}\begin{pmatrix} Y_i NY_i' & Y_i Ny_i' \\ y_i NY_i' & y_i Ny_i' \end{pmatrix}^{-1} = NY'_{i+1}\begin{pmatrix} Y_i NY_i' & 0 \\ y_i NY_i' & \alpha \end{pmatrix}, \quad y_i Ny_i' = \alpha \text{ (say)}$$

$$= (NY_i', Ny_i')\begin{pmatrix} (Y_i NY_i')^{-1} & 0 \\ -y_i NY_i'(Y_i NY_i')^{-1}\alpha^{-1} & \alpha^{-1} \end{pmatrix}, \text{ see [10]}$$

$$= \left[NY_i'(Y_i NY_i')^{-1} - Ny_i' y_i (Y_i)^+_N \alpha^{-1}, \ Ny_i'\alpha^{-1}\right]$$

$$= \left[(I_n - v_i y_i)(Y_i)^+_N , \ v_i\right], \text{ since } v_i = Ny_i'/\alpha.$$

Theorem 4.2. If a symmetric matrix N can be found such that $Y_i N y_i' = 0$ and $v_i = Ny_i'/y_i N y_i'$, then

$$(4.10) \qquad (Y_{i+1})_N^+ = \left[(Y_i)_N^+ \ , v_i \right] .$$

Proof: Since $N = N'$, therefore $y_i N Y_i' = Y_i N y_i' = 0$ and $y_i (Y_i)_N^+ = y_i N Y_i'(Y_i N Y_i') = 0$, therefore (4.9) becomes (4.10).

As in [28], let us define

$$(4.11) \qquad H_{i+1} = H_i + C_i .$$

Then from (4.7), (4.11), (4.6) and (4.5), we get

$$(4.12) \qquad Y_{i+1} C_i = S_{i+1} - Y_{i+1} H_i = \begin{pmatrix} S_i \\ s_i \end{pmatrix} - \begin{pmatrix} Y_i \\ y_i \end{pmatrix} H_i$$

$$= \begin{pmatrix} 0 \\ s_i - y_i H_i \end{pmatrix} = \begin{pmatrix} 0 \\ f_i \end{pmatrix}, \text{ where } f_i = s_i - y_i H_i .$$

In view of (3.3), it is easy to see that

$$(4.13) \qquad C_i = \left(Y_{i-1}\right)_N^+ \begin{pmatrix} 0 \\ f_i \end{pmatrix}$$

is a solution of (4.12). In case N is symmetric and positive definite, then from (3.1) and (3.2), it follows that for the C_i given by (4.13), $\|C_i\|_{N^{-1}}$ is minimum. If we substitute the value of $\left(Y_{i-1}\right)_N^+$ from (4.9) or (4.10) in (4.13), then in both cases (symmetric or non-symmetric N)

$$(4.14) \qquad C_i = v_i f_i = \frac{N y_i (s_i - y_i H_i)}{y_i N y_i'} .$$

The equivalence between (4.14) and Algorithm 4.1 can be seen from the following

Theorem 4.3. If (4.8) with $W = N$ and $\bar{W} = \bar{N}$ is chosen as a solution of (4.5) and $Y_i N y_i' = Y_i \bar{N} y_i' = 0$, then the correction matrix C_i in (4.11) is given by either

$$(4.15) \qquad C_i = \bar{v}_i s_i - v_i y_i H_i = \frac{N y_i' s_i}{y_i N y_i'} \quad \frac{\bar{N} y_i' y_i H_i}{y_i \bar{N} y_i'} ,$$

when N and $\bar{N}$ are symmetric but not necessarily equal; or by (4.14) if N and $\bar{N}$ are equal but may be unsymmetric.

Proof: By direct substitution or from (3.3) it can be easily verified that (4.8) is a solution of (4.5) and similarly

$$(4.16) \qquad H_{i+1} = (Y_{i+1})^{+}_{N} S_{i+1} + [I_n - (Y_{i+1})^{+}_{\bar{N}} Y_{i+1}]R$$

is a solution of (4.7) even though N and $\bar{N}$ may not be symmetric. Using (4.10) and (4.6) in the above equation, for symmetric N and $\bar{N}$, we get

$$(4.17) \qquad H_{i+1} = (Y_i)^{+}_{N} S_i + v_i s_i + [I_n - (Y_i)^{+}_{\bar{N}} Y_i - \bar{v}_i y_i] R$$

$$= v_i s_i - \bar{v}_i y_i R + (Y_i)^{+}_{\bar{N}} S_i + \left[I_n - (Y_i)^{+}_{\bar{N}} Y_i\right] R.$$

But

$$(4.18) \qquad H_i = (Y_i)^{+}_{N} S_i + [I_n - (Y_i)^{+}_{\bar{N}} Y_i]R,$$

and $Y_i N y_i' = 0 \Rightarrow y_i N Y_i' = 0$, since $N = N'$. Therefore $y_i (Y_i)^{+}_{N} = y_i N Y_i' (Y_i N Y_i')^{-1}$ and this is also true if N is replaced by $\bar{N}$ which, in view of (4.18), implies that

$$(4.19) \qquad y_i H_i = y_i R.$$

Using (4.19), (4.18) and (4.11) in (4.17), we get (4.15).

In case $N = \bar{N}$, but N is not necessarily symmetric, by using (4.9) and (4.6) in (4.16), we get

$$H_{i+1} = (I_n - v_i y_i)(Y_i)^{+}_{N} S_i + v_i s_i + \left[I_n - (I_n - v_i y_i)(Y_i)^{+}_{N} Y_i - v_i y_i\right] R$$

$$= v_i s_i - v_i y_i \left[(Y_i)^{+}_{N} S_i + (I_n - (Y_i)^{+}_{N})R\right] + (Y_i)^{+}_{N} S_i + \left[I_n - (Y_i)^{+}_{N} Y_i\right] R,$$

which, in view of (4.8) with $W = \bar{W} = N$ and (4.11) gives (4.14). This completes the proof of Theorem 4.3 .

Various choices for N are possible in (4.14) and (4.15), for example:

Case I. If we let $N = H_i$, then in view of (4.5) and (4.4)

$$0 = Y_i N y_i' = Y_i H_i y_i' = S_i G S_i' \Rightarrow s_k G s_j' = 0 \,, \ k \neq j,$$

also (4.14) becomes

$$c_i = \frac{H_i y_i' (s_i - y_i H_i)}{y_i H_i y_i'} \,, \tag{4.20}$$

This is given as Algorithm 3 in [18].

Case II. If in Case I we let $y_i' = M z_i'$, where M is a positive definite symmetric matrix, then the condition

$$s_k G s_j' = 0, \ k \neq j \Rightarrow s_k y_j' = 0 \Rightarrow s_k M z_j' = 0,$$

and (4.20) can be written as

$$c_i = \frac{H_i M z_i' (s_i - y_i H_i)}{y_i H_i M z_i'} \tag{4.21}$$

which is a general case of the Barnes algorithm [2], [28].

Case III. Taking M = I in Case II, we have the Rosen's [22] modification. The z_j's are computed from s_k's such that $s_k z_j' = 0$. This can be done by using the modified Gram-Schmidt orthogonalization [4]. Also (4.21) becomes

$$c_i = \frac{H_i \, z_i' \, (s_i - y_i \, H_i)}{y_i \, H_i \, z_i'} \tag{4.22}$$

Case IV. Taking N = M, $0 = YNy_i' = Y_i M y_i' \Rightarrow y_k M y_j' = 0, \ k \neq j$ and (4.14) becomes

$$c_i = \frac{M y_i' (s_i - y_i \, H_i)}{y_i M y_i'} \,. \tag{4.23}$$

Since M is chosen to be symmetric, the C_i given by (4.23), minimizes $\|C_i\|_{M^{-1}}$. This is the second interation given by Broyden [7].

Case V. Let $N = G^{-1}$. From (4.4) and the definition of Y_i and S_i it follows that

$$(4.24) \qquad Y_i = S_i G,$$

and $0 = Y_i N y_i' = Y_i G^{-1} y_i' = S_i G s_i' \Rightarrow s_k G s_j' = 0 \quad k \neq j$; also (4.14) and (4.4) give

$$(4.25) \qquad C_i = \frac{G^{-1} y_i' (s_i - y_i H_i)}{y_i G^{-1} y_i'} = \frac{s_i' (s_i - y_i H_i)}{y_i s_i'},$$

and $\|C_i\|_G$ is minimized in this case. This is given as Algorithm 2 in [18].

Case VI. In (4.15), let $N = G^{-1}$ and $\overline{N} = H_i$, where for the present we assume that H_i is symmetric. We have

$$0 = Y_i N y_i' = Y_i G^{-1} y_i' = S_i G s_i' \Rightarrow s_k G s_j' = 0, \quad k \neq j, \text{ and}$$

$$0 = Y_i \overline{N} y_i' = Y_i H_i y_i' = S_i G s_i' \Rightarrow s_k G s_j' = 0 \quad k \neq j .$$

Also (4.15) gives

$$(4.26) \qquad C_i = \frac{G^{-1} y_i' s_i}{y_i G^{-1} s_i'} - \frac{H_i y_i' y_i H_i}{y_i H_i y_i'} = \frac{s_i' s_i}{y_i s_i'} - \frac{H_i y_i' y_i H_i}{y_i H_i y_i'} .$$

If H_i is symmetric, then C_i in (4.26) is also symmetric and from (4.11) it follows that H_{i+1} is also symmetric. But $H_0 = R$ is symmetric. Therefore, by induction all the H_i are symmetric. Equation (4.26) is the well-known Fletcher-Powell-Davidon method [9]. It is worth noting that if (4.26) is written as $C_i = \overline{C}_i - \hat{C}_i$, then $\|\overline{C}_i\|_G$ and $\|\hat{C}_i\|_{H_i^{-1}}$ are minimized.

Case VII. If we take $N = \eta G^{-1} + \beta H_i$ in (4.14), then we get

$$0 = Y_i(\eta G^{-1} + \beta H_i)y_i' = \eta Y_i G^{-1} y_i' + \beta Y_i H_i y_i' = (\eta+\beta) S_i G s_i' = 0 \text{ and}$$

$$C_i = \frac{(s_i' + \beta H_i y_i')}{\eta y_i s_i' + \beta y_i H_i y_i'} (S_i - y_i H_i).$$

However α and β should be chosen such that N is always non-singular. One choice could be $\eta = 1$, $\beta = \epsilon$

$$C_i = \frac{(s_i' + \epsilon H_i y_i')}{(y_i S_i' + \epsilon H_i y_i')} (S_i - y_i H_i). \tag{4.27}$$

We shall need the following theorems in order to make use of Theorem 3.2 in order to make improvements in the computation of C_i.

Theorem 4.4. If a non-symmetric matrix N can be found for which $Y_i N y_i' = 0$ and $w_i = N y_i' / (y_i N y_i' + \epsilon)$, then

$$(\hat{Y}_{i+1})_N^+ = [(I_n - w_i y_i)(Y_i)_N^+ , w_i]. \tag{4.28}$$

Proof. As in the proof of Theorem 4.1, from (3.4) and (4.6), we get

$$(\hat{Y}_{i+1})_N^+ = NY_{i+1}'(Y_{i+1} NY_{i+1}' + \epsilon I_{i+1})^{-1} = NY_{i+1}' \begin{pmatrix} Y_i NY_i' + \epsilon I_i & 0 \\ y_i NY_i' & \bar{\alpha} \end{pmatrix}^{-1}, \quad \bar{\alpha} = y_i N y_i' + \epsilon,$$

$$= (NY_i', Ny_i') \begin{bmatrix} (Y_i NY_i' + \epsilon I_i)^{-1} & 0 \\ -y_i NY_i'(Y_i NY_i' + \epsilon I_i)^{-1} \bar{\alpha}^{-1} & \bar{\alpha}^{-1} \end{bmatrix}$$

$= [(I_n - w_i y_i)(\hat{Y}_i)_n^+, w_i]$, since $w_i = N y_i' / \bar{\alpha}$.

Theorem 4.5. If a symmetric matrix N can be found such that $Y_i N y_i' = 0$ and $w_i = N y_i' / (y_i N y_i' + \epsilon)$, then

$$(\hat{Y}_{i+1})_N^+ = [(\hat{Y}_i)_N^+, w_i]. \tag{4.29}$$

Proof.

$$N = N' \Rightarrow y_i NY_i' = 0 \Rightarrow y_i(\hat{Y}_i)_N^+ = y_i NY_i'(Y NY_i' + \epsilon I_i)^{-1} = 0$$

and (4.28) becomes (4.29).

We can now use Theorem 3.2 in the following

Theorem 4.6. For the matrix equation

$$(4.30) \qquad Y_{i+1} C_i = \begin{pmatrix} 0 \\ f_i \end{pmatrix} - \rho \begin{pmatrix} 0 \\ f_i \end{pmatrix} = (1 - \rho) \begin{pmatrix} 0 \\ f_i \end{pmatrix}$$

where $\rho = \epsilon / (y_i N y_i' + \epsilon)$ and $f_i = s_i - y_i H_i$; one of the solutions is given by

$$(4.31) \qquad \hat{C}_i = N y_i' f_i / (y_i N y_i' + \epsilon) \quad .$$

If N is symmetric then for all the other solutions C_i of (4.30)

$$\|C_i\|_{N^{-1}} \geq \|\hat{C}_i\|_{N^{-1}} .$$

Proof: In view of (3.3), if N is not symmetric, and in Theorem 3.2 if we take W = N, then, $X = A_N^+ B$ is still a solution of (3.9) but it does not minimize $\|X\|_{N^{-1}}$. Keeping this fact in view according to (3.11) a solution of (4.30), whether N is symmetric or not is given by

$$\hat{C}_i = (Y_{i+1})_N^+ \begin{pmatrix} 0 \\ f_i \end{pmatrix} .$$

$$= w_i f_i, \text{ using (4.28) or (4.29).}$$

$$= N y_i' f / (y_i N y_i' + \epsilon), \text{ which is (4.31).}$$

If N is symmetric then from (3.11) it follow that $\|C_i\|_{N^{-1}} \geq \|\hat{C}_i\|_{N^{-1}}$.

The above Theorem shows that a small perturbation in the right hand side of (4.12) leads to a corresponding small change in the value of C_i. However, as we mentioned in Section 3, $(\hat{Y}_{i+1})_N^+$ is in general better conditioned than $(Y_{i+1})_N^+$ and therefore the value of C_i computed from (4.31) should generally give better results and keep the numerator $y_i N y_i'$ from getting too small and in some cases negative due to round-off errors. This, to some extent also justifies (4.27). The use of $(\hat{Y}_{i+1})_N^+$ in place of $(Y_{i+1})_N^+$ will be especially advantageous, if in order to improve the computational accuracy, at periodic intervals H_{i+1} is computed directly by the formula (4.18) with $(Y_i)_N^+$ and $(Y_i)_{\bar{N}}^+$ replaced by $(\hat{Y}_i)_N^+$ and $(\hat{Y}_i)_{\bar{N}}^+$ respectively. Such periodic techniques for improvement are being used advantageously in other computational algorithms e.g.., the periodic reinversion of the basis in product form of inverse linear programming codes [14]. McCormick [17] has noted that such periodic improvement techniques improved the performance of the Fletcher-Powell-Davidon algorith [9]. Barnes [1] suggests periodic rescaling of s_i and reinitialization of H_i to improve the computations.

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