

**A Family of Optimally Conditioned Quasi-Newton
Updates for Unconstrained Optimization**

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Mathematics Report Number A151
April 1991. Revised December 1991.

Abstract. In this paper a general optimal conditioning problem for updates which satisfy the quasi-Newton condition is solved. The new solution is comprised of a family of updates which contains other known optimally conditioned updates but also includes new formulae of increased rank. Ways of implementing the new updates are discussed and some numerical results are given.

Keywords.

Unconstrained optimization, quasi-Newton updates, optimal conditioning, rank n family.

AMS (MOS) subject classifications: 65K10, 15A23.

1. Introduction

Consider the unconstrained optimization problem,

$$\min_{x \in \mathbb{R}^n} f(x).$$

Quasi-Newton methods (see, e.g., Fletcher, 1987) decide the new search direction d^+ , at each iteration, by

$$d^+ = -H^+ g^+,$$

where x^+ is the current point, $g^+ = \nabla f(x^+)$ and H^+ is an approximation to $\{\nabla^2 f(x^+)\}^{-1}$. H^+ satisfies the quasi-Newton condition

$$H^+ \gamma = \delta,$$

where $\gamma = g^+ - g$, $\delta = x^+ - x$, x is the previous point and $g = \nabla f(x)$. There is, of course, much freedom in the selection of H^+ , even though the quasi-Newton condition is satisfied, and other desirable properties such as symmetry and positive definiteness can be imposed on H^+ .

An important family of formulae for deriving H^+ from the previous matrix H (H is said to be “updated” to H^+) is the self scaling Broyden family of updates, which has the form

$$H_B^+(\phi, \xi) = \xi \left(H - \frac{H\gamma\gamma^T H}{\gamma^T H \gamma} + \phi \gamma^T H \gamma v v^T \right) + \frac{\delta\delta^T}{\delta^T \gamma}, \quad (1.1)$$

where

$$v = \frac{\delta}{\delta^T \gamma} - \frac{H\gamma}{\gamma^T H \gamma},$$

ξ is the scaling factor and ϕ a free parameter. Clearly $H_B^+(\phi, \xi)$ is symmetric if H is symmetric and, writing

$$b = \frac{\gamma^T H \gamma}{\delta^T \gamma}, \quad h = \frac{\delta^T H^{-1} \delta}{\delta^T \gamma},$$

then, provided $\delta^T \gamma > 0$ and H is positive definite, $H^+(\phi, \xi)$ is positive definite *iff*

$$\phi > \bar{\phi} = \frac{1}{1 - bh}.$$

Three well-known members of the family are the *BFGS*, *DFP* and symmetric rank one updates, which are given by $\phi = 1$, $\phi = 0$ and $\phi = 1/(1 - b\xi)$ respectively. When $\phi = \bar{\phi}$, $H_B^+(\phi, \xi)$ becomes singular.

Recent interest in quasi-Newton methods has concentrated on updates with $\phi > 1$ following the extension of global convergence results for *BFGS* (Powell, 1976) to all updates with $\phi \in (0, 1]$, $\xi = 1$ (Byrd, Nocedal and Yuan, 1988). Optimal conditioning of $H^{-\frac{1}{2}} H_B^+ H^{-\frac{1}{2}}$ by suitable choice of ξ and ϕ was studied by several authors (Oren and Luenberger, 1974, Davidon, 1975 and Oren and Spedicato, 1976) but they confined their discussion to either $\phi \in [0, 1]$ or $\xi = 1$. More recently optimal conditioning, without these restrictions, has been studied by Al-Baali (1990), Lukšan (1990), and Hu and Storey (1991). It was found that the spectral condition number K of $H^{-\frac{1}{2}} H_B^+ H^{-\frac{1}{2}}$ is minimized on the curve

$$\phi^*(\xi) = \frac{\frac{h}{\xi} - 1}{bh - 1}, \quad \xi_- \leq \xi \leq \xi_+,$$

where

$$\xi_{\pm} = h \left(1 \pm \sqrt{1 - \frac{1}{bh}} \right), \quad (1.2)$$

and that,

$$K^* = \min_{\phi, \xi} K \left(H^{-\frac{1}{2}} H_B^+ H^{-\frac{1}{2}} \right) = bh \left(1 + \sqrt{1 - \frac{1}{bh}} \right)^2.$$

In this paper we solve the more general problem

$$\min_{H^+} K (Z^{-1} H^+ Z^{-T}), \quad (1.3)$$

$$\text{subject to } \begin{cases} H^+ \gamma = \delta, \\ H^+ = H^{+T}, \quad H^+ > 0, \end{cases}$$

with Z non-singular and $ZZ^T = H$. We establish that the solutions of (1.3) form a family of updates, containing those updates in the Broyden family defined by ϕ^* , but allowing the rank of $H^+ - \xi H$ to extend up to n .

2. Preliminary Results.

We first consider the connections between the condition number of a positive definite matrix and those of its principal submatrices and have the following lemmas.

Lemma 2.1

The eigenvalues of the leading principal submatrix of order $\ell - 1$ of a symmetric $\ell \times \ell$ matrix A separate the eigenvalues of A .

Proof

See Wilkinson (1965), page 103.

Corollary 2.1

If B is a leading principal submatrix of any order of a positive definite symmetric matrix A then $K(B) \leq K(A)$.

Proof

This follows directly (by induction) from Lemma 2.1 and the positive definiteness of A .

Lemma 2.2

Let $A \in R^{(\ell+1) \times (\ell+1)}$, $\ell \geq 1$, be a positive definite symmetric matrix such that

$$A = \begin{pmatrix} B & u \\ u^T & \alpha \end{pmatrix}$$

with $u \in R^\ell$, $\alpha \in R$ and $B = \text{diag}(\alpha_1, \dots, \alpha_\ell)$, then a necessary condition for $K(A) = K(B)$ is that all u_i corresponding to α_{\max} and α_{\min} , the greatest and least eigenvalues of B , are zero and $\alpha_{\min} \leq \alpha \leq \alpha_{\max}$.

Proof

If $\alpha_{\min} = \alpha_{\max}$ then $K(B) = 1$ and, since A is positive definite, $K(A) = K(B)$ only if $A = \alpha_{\min}I$, giving $u = 0$ and $\alpha = \alpha_{\min}$ as required.

Now assume $\alpha_{\min} < \alpha_{\max}$ and consider a 3×3 principal submatrix of A

$$C = \begin{pmatrix} \alpha_i & 0 & u_i \\ 0 & \alpha_j & u_j \\ u_i & u_j & \alpha \end{pmatrix}$$

where $\alpha_i = \alpha_{\min}$, $\alpha_j = \alpha_{\max}$. By Corollary 2.1 $K(C) \leq K(A)$ and so

$$K(C) \leq K(A) = K(B) = \frac{\alpha_{\max}}{\alpha_{\min}}. \quad (2.1)$$

Assume that the eigenvalues of C are $\beta_1 \leq \beta_2 \leq \beta_3$, then by Lemma 2.1,

$$0 < \beta_1 \leq \alpha_i \leq \beta_2 \leq \alpha_j \leq \beta_3. \quad (2.2)$$

Consider the determinant

$$|\lambda I - C| = (\lambda - \alpha_i) (\lambda - \alpha_j) p(\lambda),$$

with

$$p(\lambda) = \lambda - \alpha - \frac{u_i^2}{\lambda - \alpha_i} - \frac{u_j^2}{\lambda - \alpha_j},$$

so that any root of $p(\lambda)$ is an eigenvalue of C . If $u_i \neq 0$ then, as $p(\lambda) \rightarrow -\infty$ when $\lambda \rightarrow -\infty$ and $p(\lambda) \rightarrow +\infty$ when $\lambda \rightarrow \alpha_i^-$, there must be a root in $(-\infty, \alpha_i)$. Thus from (2.2), $0 < \beta_1 < \alpha_i$ and so

$$K(C) = \frac{\beta_3}{\beta_1} > \frac{\alpha_j}{\alpha_i} = \frac{\alpha_{\max}}{\alpha_{\min}} = K(B), \quad (2.3)$$

which contradicts (2.1). If $u_j \neq 0$, a similar argument leads to (2.3) again and contradicts (2.1). It follows that all elements of u corresponding to the greatest and least eigenvalues of B must be zero. But C is then diagonal and so satisfies (2.1) only if $\alpha_{\min} \leq \alpha \leq \alpha_{\max}$. \square

Lemma 2.3

Let $A \in R^{n \times n}$ be symmetric, positive definite and

$$A = \begin{pmatrix} B & U \\ U^T & D \end{pmatrix}$$

with $B \in R^{m \times m}$, $U \in R^{m \times (n-m)}$, $D \in R^{(n-m) \times (n-m)}$, with $m \geq 1$. Then $K(A) \geq K(B)$ and if $m = 2$ equality holds iff $U = 0$ and the eigenvalues of D lie between those of B .

Proof

Since B is a principal submatrix of A we have $K(A) \geq K(B)$ in general. Now let $m = 2$. Since B and D are symmetric we can let $B = Q^T \bar{B} Q$, $D = \Omega^T \bar{D} \Omega$ where \bar{B} , \bar{D} are diagonal and $Q \in R^{m \times m}$, $\Omega \in R^{(n-m) \times (n-m)}$ are orthogonal. Let $\bar{U} = Q U \Omega^T$ then the eigenvalues of A are equal to those of

$$C = \begin{pmatrix} \bar{B} & \bar{U} \\ \bar{U}^T & \bar{D} \end{pmatrix}$$

and so $K(A) = K(B)$ iff $K(C) = K(\bar{B})$. Thus any of the principal submatrices of C containing \bar{B} has the same condition number as \bar{B} . Since \bar{B} is 2×2 and diagonal its two eigenvalues are the greatest and least respectively and so by using Lemma 2.2 inductively on a series of bordered diagonal matrices, containing \bar{B} and of order $3, 4, \dots, n$, we find that $K(C) = K(\bar{B})$ only if $\bar{U} = 0$ and the eigenvalues of \bar{D} lie between the greatest and least eigenvalues of \bar{B} . This proves the “only if” part of the lemma. The proof of the “if” part is immediate. \square

Note 2.1 The conditions for $K(A) = K(B)$ in Lemma 2.2 are necessary only. The conditions for $K(A) = K(B)$ in Lemma 2.3 do not necessarily hold for $m > 2$.

We now give a result concerning the minimum value of the condition number of a 2×2 matrix.

Lemma 2.4

Let $A = \begin{pmatrix} t & s \\ s & r \end{pmatrix}$ be positive definite with t and s fixed real numbers and r a parameter. Then $K(A)$ is minimized if $r = (t^2 + 2s^2)/t$ and, at this minimum the eigenvalues of A are

$$\lambda_{\pm} = \frac{t^2 + s^2 \pm s\sqrt{t^2 + s^2}}{t},$$

with

$$\min_r K(A) = \frac{\lambda_+}{\lambda_-} = \frac{\sqrt{(t/s)^2 + 1} + 1}{\sqrt{(t/s)^2 + 1} - 1}.$$

Proof

It is easily seen that $\frac{dK(A)}{dr} = 0$ iff $r = (t^2 + 2s^2)/t$ and the rest of the proof follows. \square

3. A Family of Optimally Conditioned Updates

A technique used by Ip (1987) is now adapted to solve problem (1.3) by using an orthogonal transformation to reduce the vectors γ and δ to their simplest possible forms as follows. Let Ω be any orthogonal matrix that satisfies

$$\Omega^T(Z^T\gamma, Z^{-1}\delta) = \begin{pmatrix} \alpha & 0 & 0 & \dots & 0 \\ \beta & \rho & 0 & \dots & 0 \end{pmatrix}^T, \quad (3.1)$$

then if q_i , $i = 1, \dots, n$, are the columns of Ω we see that

$$\alpha = \sqrt{\gamma^T H \gamma}, \quad (3.2)$$

$$q_1 = \frac{Z^T \gamma}{\sqrt{\gamma^T H \gamma}}, \quad (3.3)$$

$$\beta = (Z^{-1}\delta)^T q_1 = \frac{\delta^T \gamma}{\sqrt{\gamma^T H \gamma}}, \quad (3.4)$$

$$\rho = \sqrt{\delta^T H^{-1} \delta - \frac{(\delta^T \gamma)^2}{\gamma^T H \gamma}} \quad (3.5)$$

and

$$q_2 = \frac{Z^{-1} \delta - \frac{\delta^T \gamma}{\gamma^T H \gamma} Z^T \gamma}{\sqrt{\delta^T H^{-1} \delta - \frac{(\delta^T \gamma)^2}{\gamma^T H \gamma}}}. \quad (3.6)$$

If now we let

$$\tilde{H}^+ = \Omega^T Z^{-1} H^+ Z^{-T} \Omega \quad (3.7)$$

then, since the spectral condition number is invariant under orthogonal transformation, (3.1) implies that (1.3) is equivalent to

$$\min_{\tilde{H}^+} K(\tilde{H}^+) \quad (3.8)$$

$$\text{subject to } \begin{cases} \tilde{H}^+(\alpha, 0, \dots, 0)^T = (\beta, \rho, 0, \dots, 0)^T \\ \tilde{H}^+ = \tilde{H}^{+T}, \quad \tilde{H}^+ > 0. \end{cases}$$

Our main theorem follows.

Theorem 3.1

The minimum value of the condition number in (1.3) is K^* and the solution of problem (1.3) is the family of updates

$$H^+ = H_B^+(\phi^*(\xi), \xi) + \sum_{i=3}^n (\xi_i - \xi) \bar{z}_i \bar{z}_i^T, \quad (3.9)$$

where,

$$\xi_- \leq \xi_i \leq \xi_+, \quad i = 3, \dots, n,$$

and

$$\xi_{\pm} = h \left(1 \pm \sqrt{1 - \frac{1}{bh}} \right).$$

In (3.9) the \bar{z}_i , $i = 3, \dots, n$, are the columns of $\bar{Z} = Z\Omega$ where Ω is any orthogonal matrix satisfying (3.1).

Proof

Let $\tilde{H}^+ = (h_{ij})$, $i, j = 1, \dots, n$, then

$$h_{11} = \frac{\beta}{\alpha}, \quad h_{21} = h_{12} = \frac{\rho}{\alpha}, \quad h_{i1} = h_{1i} = 0, \quad i = 3, \dots, n. \quad (3.10)$$

Write

$$\tilde{H}_{22}^+ = \begin{pmatrix} h_{11} & h_{12} \\ h_{12} & h_{22} \end{pmatrix},$$

then, by Lemma 2.2,

$$K(\tilde{H}^+) \geq K(\tilde{H}_{22}^+),$$

so that for any \tilde{H}^+ satisfying the constraints in (3.8) and any \tilde{H}_{22}^+ satisfying (3.10) we have

$$K(\tilde{H}^+) \geq \min_{h_{22}} K(\tilde{H}_{22}^+). \quad (3.11)$$

By Lemma 2.4 $K(\tilde{H}_{22}^+)$ is minimized if

$$h_{22} = \frac{h_{11}^2 + 2h_{12}^2}{h_{11}} = \frac{\beta^2 + 2\rho^2}{\alpha\beta} \quad (3.12)$$

and the eigenvalues of \tilde{H}_{22}^+ are then, by Lemma 2.4, (3.2), (3.4) and (3.5),

$$\begin{aligned} \xi_{\pm} &= \frac{h_{11}^2 + h_{12}^2 \pm h_{12}\sqrt{h_{11}^2 + h_{12}^2}}{h_{11}} \\ &= h \left(1 \pm \sqrt{1 - \frac{1}{bh}} \right). \end{aligned}$$

Again, from Lemma 2.4, by using (3.2), (3.4) and (3.5) it is seen that $\min_{h_{22}} K(\tilde{H}_{22}^+) = K^*$.

By Lemma 2.3, (3.11) holds with equality *iff* (3.12) holds and \tilde{H}^+ is of the form

$$\tilde{H}^+ = \begin{pmatrix} \tilde{H}_{22}^+ & 0 \\ 0 & D \end{pmatrix}$$

with the eigenvalues of D lying between ξ_- and ξ_+ . Let $D = Q^T \text{diag}(\xi_3, \dots, \xi_n)Q$ where Q is orthogonal and

$$\xi_- \leq \xi_i \leq \xi_+, \quad i = 3, \dots, n.$$

Let $R = \begin{pmatrix} I_2 & 0 \\ 0 & Q^T \end{pmatrix}$ and set $\Omega_1 = \Omega R$ and $\tilde{H}_1^+ = R^T \tilde{H}^+ R = \Omega_1 Z^{-1} H^+ Z^{-T} \Omega_1$. Then Ω_1 is again orthogonal and satisfies (3.1). Hence we have

$$\tilde{H}_1^+ = \begin{pmatrix} \beta/\alpha & \rho/\alpha & & & \mathbf{0} \\ \rho/\alpha & (\beta^2 + 2\rho^2)/\alpha\beta & & & \\ & & \xi_3 & & \\ & \mathbf{0} & & \ddots & \\ & & & & \xi_n \end{pmatrix}, \quad (3.13)$$

and now

$$H^+ = Z \Omega_1 \tilde{H}_1^+ \Omega_1^T Z^T.$$

Let $\bar{Z} = Z \Omega_1 = (\bar{z}_1, \dots, \bar{z}_n)$ then as Ω_1 is orthogonal, we have

$$\bar{Z}\bar{Z}^T = ZZ^T = H \quad (3.14)$$

and

$$\bar{Z}^T(\gamma, H^{-1}\delta) = \begin{pmatrix} \alpha & 0 & 0 & \dots & 0 \\ \beta & \rho & 0 & \dots & 0 \end{pmatrix}^T. \quad (3.15)$$

Thus from (3.3) and (3.6)

$$\bar{z}_1 = Zq_1 = \frac{H\gamma}{\sqrt{\gamma^T H \gamma}}, \quad (3.19)$$

$$\bar{z}_2 = Zq_2 = \frac{\delta - \frac{\delta^T \gamma}{\gamma^T H \gamma} H \gamma}{\sqrt{\delta^T H^{-1} \delta - \frac{(\delta^T \gamma)^2}{\gamma^T H \gamma}}}. \quad (3.17)$$

In terms of \bar{Z} we have

$$\begin{aligned} H^+ &= \bar{Z} \tilde{H}_1^+ \bar{Z}^T \\ &= (\bar{z}_1 \ \bar{z}_2) \begin{pmatrix} \beta/\alpha & \rho/\alpha \\ \rho/\alpha & (\beta^2 + 2\rho^2)/\alpha\beta \end{pmatrix} \begin{pmatrix} \bar{z}_1^T \\ \bar{z}_2^T \end{pmatrix} + \sum_{i=3}^n \xi_i \bar{z}_i \bar{z}_i^T. \end{aligned}$$

and since $\bar{Z}\bar{Z}^T = H$ it follows that

$$\begin{aligned} H^+ &= \xi H + (\bar{z}_1 \ \bar{z}_2) \begin{pmatrix} \beta/\alpha - \xi & \rho/\alpha \\ \rho/\alpha & (\beta^2 + 2\rho^2)/\alpha\beta - \xi \end{pmatrix} \begin{pmatrix} \bar{z}_1^T \\ \bar{z}_2^T \end{pmatrix} + \sum_{i=3}^n (\xi_i - \xi) \bar{z}_i \bar{z}_i^T \\ &= H_1 + H_2 \end{aligned} \quad (3.18)$$

where H_1 denotes the first two terms of H^+ and H_2 the remaining term.

By (3.15) we know $H_2\gamma = 0$ and therefore $H_1\gamma = \delta$. We now examine H_1 . It is easily seen that

$$\begin{pmatrix} \beta/\alpha - \xi & \rho/\alpha \\ \rho/\alpha & (\beta^2 + 2\rho^2)/\alpha\beta - \xi \end{pmatrix} = \begin{pmatrix} \frac{1}{b} - \xi & \frac{1}{b} \sqrt{bh-1} \\ \frac{1}{b} \sqrt{bh-1} & 2h - \frac{1}{b} - \xi \end{pmatrix}.$$

Assume $\xi > 0$, denote $H_0 = \xi H$, $\bar{b} = \frac{\gamma^T H_0 \gamma}{\delta^T \gamma} = \xi b$ and $\bar{h} = \frac{\delta^T H_0^{-1} \delta}{\delta^T \gamma} = \frac{h}{\xi}$, then $\bar{b} \bar{h} = b h$ and

$$\begin{aligned} H_1 &= \xi H + (\bar{z}_1 \ \bar{z}_2) \begin{pmatrix} \frac{1}{b} - \xi & \frac{1}{b} \sqrt{bh-1} \\ \frac{1}{b} \sqrt{bh-1} & 2h - \frac{1}{b} - \xi \end{pmatrix} \begin{pmatrix} \bar{z}_1^T \\ \bar{z}_2^T \end{pmatrix} \\ &= H_0 + \begin{pmatrix} \frac{H_0 \gamma}{\sqrt{\gamma^T H_0 \gamma}} & \frac{\delta - \frac{\delta^T \gamma}{\gamma^T H_0 \gamma} H_0 \gamma}{\sqrt{\delta^T H_0^{-1} \delta - (\delta^T \gamma)^2 / \gamma^T H_0 \gamma}} \end{pmatrix} \begin{pmatrix} \frac{1}{\bar{b}} - 1 & \frac{1}{\bar{b}} \sqrt{\bar{b}\bar{h} - 1} \\ \frac{1}{\bar{b}} \sqrt{\bar{b}\bar{h} - 1} & 2\bar{h} - \frac{1}{\bar{b}} - 1 \end{pmatrix} \\ &\quad \times \begin{pmatrix} \frac{H_0 \gamma}{\sqrt{\gamma^T H_0 \gamma}} & \frac{\delta - \frac{\delta^T \gamma}{\gamma^T H_0 \gamma} H_0 \gamma}{\sqrt{\delta^T H_0^{-1} \delta - (\delta^T \gamma)^2 / \gamma^T H_0 \gamma}} \end{pmatrix}^T. \end{aligned} \quad (3.19)$$

Thus, H_1 can be written as

$$H_1 = H_0 + a_1 \delta \delta^T + a_2 (H_0 \gamma \delta^T + \delta \gamma^T H_0) + a_3 H_0 \gamma \gamma^T H_0$$

and satisfies $H_1 \gamma = \delta$, so it must be of the form (see, Fletcher, 1987, p.62),

$$\begin{aligned} H_1 &= H_0 - \frac{H_0 \gamma \gamma^T H_0}{\gamma^T H_0 \gamma} + \frac{\delta \delta^T}{\delta^T \gamma} + \phi \gamma^T H_0 \gamma \left(\frac{\delta}{\delta^T \gamma} - \frac{H_0 \gamma}{\gamma^T H_0 \gamma} \right) \left(\frac{\delta}{\delta^T \gamma} - \frac{H_0 \gamma}{\gamma^T H_0 \gamma} \right)^T \\ &= H_B^+(\phi, \xi). \end{aligned} \tag{3.20}$$

The parameter ϕ can be found by matching the coefficient of any term in (3.20) with the corresponding term in (3.19). Taking the coefficient of $\delta \delta^T$ we obtain,

$$\frac{2\bar{h} - \frac{1}{\bar{b}} - 1}{\delta^T H_0^{-1} \delta - \frac{(\delta^T \gamma)^2}{\gamma^T H_0 \gamma}} = \frac{1}{\delta^T \gamma} + \phi \frac{\gamma^T H_0 \gamma}{(\delta^T \gamma)^2},$$

so that

$$2\bar{h} - \frac{1}{\bar{b}} - 1 = \bar{h} - \frac{1}{\bar{b}} + \phi(\bar{b}\bar{h} - 1)$$

or

$$\phi = \frac{\bar{h} - 1}{\bar{b}\bar{h} - 1} = \frac{\frac{h}{\xi} - 1}{\frac{h}{b\xi} - 1} = \phi^*(\xi).$$

Therefore (3.20) becomes

$$H_1 = H_B^+(\phi^*(\xi), \xi). \tag{3.21}$$

Obvious changes show that (3.21) is also true when $\xi < 0$. Its validity for $\xi = 0$ follows by continuity.

Therefore by (3.18) and (3.21) we have proved that the minimum value of K is K^* and that any solutions of (1.3) must be of the form (3.9). Conversely, Let H^+ be any member of (3.9), that is,

$$H^+ = H_B^+(\phi^*(\xi), \xi) + \sum_{i=3}^n (\xi_i - \xi) \bar{z}_i \bar{z}_i^T,$$

where $\xi_- \leq \xi_i \leq \xi_+$, $1 \leq i \leq n$, and \bar{z}_i , $1 \leq i \leq n$, are the columns of $\bar{Z} = Z\Omega$ with Ω an orthogonal matrix satisfying (3.1). Then \bar{Z} satisfies (3.14) and (3.15), thus $H^+ \gamma = \delta$ and \bar{z}_1, \bar{z}_2 are given by (3.16) and (3.17).

Therefore from the previous part of the proof

$$H_B^+(\phi^*(\xi), \xi) = \xi H + (\bar{z}_1 \bar{z}_2) \begin{pmatrix} \frac{1}{b} - \xi & \frac{1}{b} \sqrt{bh-1} \\ \frac{1}{b} \sqrt{bh-1} & 2h - \frac{1}{b} - \xi \end{pmatrix} \begin{pmatrix} \bar{z}_1^T \\ \bar{z}_2^T \end{pmatrix}$$

and so

$$\begin{aligned}
H^+ &= H_B^+(\phi^*(\xi), \xi) + \sum_{i=3}^n (\xi_i - \xi) \bar{z}_i \bar{z}_i^T \\
&= \bar{Z} \begin{pmatrix} \frac{1}{b} & \frac{1}{b}\sqrt{bh-1} & \mathbf{O} \\ \frac{1}{b}\sqrt{bh-1} & 2h - \frac{1}{b} & \\ \mathbf{O} & & \xi_3 \\ & & \ddots \\ & & & \xi_n \end{pmatrix} \bar{Z}^T \\
&= Z\Omega\tilde{H}^+\Omega^T Z^T.
\end{aligned}$$

Thus H^+ is symmetric positive definite, satisfies $H^+\gamma = \delta$ and $K(Z^{-1}H^+Z^{-T}) = K(\tilde{H}^+) = K^*$, so it is the solution of (1.3). \square

4. Factorizations of Quasi-Newton Updates

From the proof of Theorem 3.1 it is clear that any update in (3.9) can be written as

$$H^+ = Z\Omega\tilde{H}^+\Omega^T Z^T, \quad (4.1)$$

where $ZZ^T = H$, Ω is an orthogonal matrix satisfying (3.1) and

$$\tilde{H}^+ = \begin{pmatrix} \frac{1}{b} & \frac{1}{b}\sqrt{bh-1} & \mathbf{O} \\ \frac{1}{b}\sqrt{bh-1} & 2h - \frac{1}{b} & \\ \mathbf{O} & & \xi_3 \\ & & \ddots \\ & & & \xi_n \end{pmatrix}, \quad \xi_- \leq \xi_i \leq \xi_+, \quad i = 3, \dots, n. \quad (4.2)$$

In fact, any member of the self-scaling Broyden family (1.1) can also be written in the form (4.1) with Z and Ω defined as before and

$$\tilde{H}^+ = \begin{pmatrix} \frac{1}{b} & \frac{1}{b}\sqrt{bh-1} & \mathbf{O} \\ \frac{1}{b}\sqrt{bh-1} & 2h - \frac{1}{b} + (\phi - \phi^*)\xi (bh-1) & \\ \mathbf{O} & & \xi \\ & & \ddots \\ & & & \xi \end{pmatrix}, \quad (4.3)$$

or equivalently,

$$\tilde{H}^+ = \begin{pmatrix} \frac{1}{b} & \frac{1}{b}\sqrt{bh-1} & \mathbf{O} \\ \frac{1}{b}\sqrt{bh-1} & h - \frac{1}{b} + \xi + \phi \xi (bh-1) & \\ \mathbf{O} & & \xi \\ & & \ddots \\ & & & \xi \end{pmatrix}. \quad (4.4)$$

Both (4.2) and (4.3) are clearly contained in the more general expression

$$\tilde{H}^+ = \begin{pmatrix} \frac{1}{b} & \frac{1}{b}\sqrt{bh-1} & \mathbf{O} \\ \frac{1}{b}\sqrt{bh-1} & h - \frac{1}{b} + \xi + \phi\xi(bh-1) & \\ & \mathbf{O} & \xi_3 \\ & & \ddots \\ & & & \xi_n \end{pmatrix} \quad (4.5)$$

The right-hand side of (4.5) can be factorized, provided $\xi > 0$, $\phi > \bar{\phi}$ and $\xi_i > 0$ for $3 \leq i \leq n$, as $\tilde{H}^+ = LL^T$ with

$$L = \begin{pmatrix} \frac{1}{\sqrt{b}} & \mathbf{O} \\ \frac{\sqrt{bh-1}}{\sqrt{b}} & \sqrt{\xi}\sqrt{1+\phi(bh-1)} \\ & \mathbf{O} \\ & & \sqrt{\xi_3} \\ & & & \ddots \\ & & & & \sqrt{\xi_n} \end{pmatrix}$$

and thus $H^+ = \bar{Z}\tilde{H}^+\bar{Z}^T = Z^+Z^{+T}$ with $Z^+ = \bar{Z}L$. Because of (3.16) and (3.17), we have

$$Z^+ = \left(\frac{\delta}{\sqrt{\delta^T\gamma}}, \sqrt{\xi}\sqrt{1+\phi(bh-1)}\bar{z}_2, \sqrt{\xi_3}\bar{z}_3, \dots, \sqrt{\xi_n}\bar{z}_n \right). \quad (4.6)$$

Formula (4.6) is a useful factorization for quasi-Newton updates. If $\xi_i = \xi$ for $3 \leq i \leq n$, it gives a factorization of the self-scaling Broyden family (1.1). If $\phi = \phi^*(\xi)$ and $\xi_- \leq \xi_i \leq \xi_+$ for $3 \leq i \leq n$, it gives a factorization of the family of optimally conditioned updates (3.9). In general it gives an update formula which allows the rank of $H^+ - \xi H$ to be up to n .

It is interesting to notice that a very similar factorization of the Broyden family was proposed by Siegal (1991) using a different approach. He considered orthogonal matrices Ω satisfying

$$\Omega^T(Z^{-1}\delta, Z^T\gamma) = \begin{pmatrix} a_1 & 0 & 0 & \dots & 0 \\ a_2 & a_3 & 0 & \dots & 0 \end{pmatrix}^T \quad (4.7)$$

instead of (3.1), and found that (1.1) can be factorized as $H^+ = Z^+Z^{+T}$ with

$$Z^+ = \left(\frac{\delta}{\sqrt{\delta^T\gamma}}, \sqrt{\xi}\sqrt{\frac{1+\phi(bh-1)}{bh}} \left(I - \frac{\delta\gamma^T}{\delta^T\gamma} \right) \bar{z}_2, \sqrt{\xi}\bar{z}_3, \dots, \sqrt{\xi}\bar{z}_n \right), \quad (4.8)$$

where \bar{z}_i are columns of the matrix $\bar{Z} = Z\Omega$.

We have seen that factorization (4.6) results from an LL^T factorization, with L lower-triangular. We now show that (4.8) results from a UU^T factorization, where U is upper-triangular. Let $\bar{Z} = Z\Omega$ with Ω satisfying (4.7). Then the Broyden family (1.1) can be written as $H_B^+ = \bar{Z}\tilde{H}^+\bar{Z}^T$ with

$$\begin{aligned} \tilde{H}^+ &= \Omega^T Z^{-1} H_B^+ Z^{-T} \Omega \\ &= \xi \left(I - \frac{\bar{\gamma}\bar{\gamma}^T}{\bar{\gamma}^T\bar{\gamma}} + \phi\bar{\gamma}\bar{\gamma}^T \bar{v}\bar{v}^T \right) + \frac{\bar{\delta}\bar{\delta}^T}{\bar{\delta}^T\bar{\gamma}} \end{aligned} \quad (4.9)$$

where $\bar{\delta} = \Omega^T Z^{-1}\delta = (a_1, 0, \dots, 0)^T$, $\bar{\gamma} = \Omega^T Z^T\gamma = (a_2, a_3, 0, \dots, 0)^T$ and $\bar{v} = \bar{\delta}/\bar{\delta}^T\bar{\gamma} - \bar{\gamma}/\bar{\gamma}^T\bar{\gamma}$.

Basic calculations show that $a_1 = (\delta^T H^{-1} \delta)^{\frac{1}{2}}$, $a_2 = \delta^T \gamma / (\delta^T H^{-1} \delta)^{\frac{1}{2}}$, $a_3 = (\gamma^T H \gamma - (\delta^T \gamma)^2 / \delta^T H^{-1} \delta)^{\frac{1}{2}}$ and the first two columns of the matrix \bar{Z}

$$\bar{z}_1 = \frac{\delta}{\sqrt{\delta^T H^{-1} \delta}}, \quad (4.10)$$

$$\bar{z}_2 = \frac{H\gamma - \frac{\delta^T \gamma}{\delta^T H^{-1} \delta} \delta}{\sqrt{\gamma^T H \gamma - \frac{(\delta^T \gamma)^2}{\delta^T H^{-1} \delta}}}. \quad (4.11)$$

Substituting a_1, a_2, a_3 into (4.9) gives

$$\tilde{H}^+ = \begin{pmatrix} h + \frac{1+\phi(bh-1)}{bh} (bh-1)\xi & -\frac{1+\phi(bh-1)}{bh} \sqrt{bh-1} \xi & & & & \\ -\frac{1+\phi(bh-1)}{bh} \sqrt{bh-1} \xi & \frac{1+\phi(bh-1)}{bh} \xi & & & \mathbf{O} & \\ & & \mathbf{O} & & \xi & \\ & & & & & \ddots & \\ & & & & & & \xi \end{pmatrix}.$$

If we factorize \tilde{H}^+ into UU^T with U upper-triangular, then

$$U = \begin{pmatrix} \sqrt{h} & -\sqrt{\xi} \sqrt{\frac{1+\phi(bh-1)}{bh} (bh-1)} & & & & \\ & \sqrt{\xi} \sqrt{\frac{1+\phi(bh-1)}{bh}} & & & \mathbf{O} & \\ & & \sqrt{\xi} & & & \\ & & & \mathbf{O} & & \ddots & \\ & & & & & & \sqrt{\xi} \end{pmatrix}. \quad (4.12)$$

Thus $H^+ = Z^+ Z^{+T}$ with $Z^+ = \bar{Z}U$. Combining (4.10), (4.11) and (4.12) we get (4.8).

5. Numerical Implementation

In this section we discuss a way of implementing the quasi-Newton methods given by (4.6). For this purpose we need to find an orthogonal matrix Ω satisfying (3.1). Since $H^{-1} \delta = \lambda g$ where λ is the step length, (3.1) can also be written as

$$\Omega^T Z^T(\gamma, g) = \begin{pmatrix} * & 0 & 0 & \dots & 0 \\ * & * & 0 & \dots & 0 \end{pmatrix}^T, \quad (5.1)$$

where “*” is used to denote those elements of matrices that may not necessarily be zero.

Following Powell (1987), we will form the matrix Ω using multiplication by a series of Givens rotations. We shall denote $\Omega_{i,i+1}(1 \leq i \leq n-1)$ as the Givens rotation matrix that differs from the unit matrix only in its i -th and $(i+1)$ -th row.

Our implementation is similar to Algorithm 1 of Siegel (1991a). Let $\bar{Z} = Z\Omega$. At $x^{(k+1)}$, (5.1) shows that the last $n-2$ elements of $\bar{Z}^{(k)T} g^{(k+1)}$ are zero, so that by (4.6) the last $n-2$ elements of $Z^{(k+1)T} g^{(k+1)}$ are also zero. Let $\Gamma^{(k+1)} = \Omega_{1,2}$ be the Givens rotation which makes the 2nd and 1st elements of $\Gamma^{(k+1)T} Z^{(k+1)T} g^{(k+1)}$ zero and positive respectively. Let $\tilde{Z}^{(k+1)} = Z^{(k+1)} \Gamma^{(k+1)}$, then clearly the new search direction is

$$d^{(k+1)} = -Z^{(k+1)} Z^{(k+1)T} g^{(k+1)} = -\tilde{z}_1^{(k+1)} \tilde{z}_1^{(k+1)T} g^{(k+1)},$$

where $\tilde{z}_1^{(k+1)}$ denotes the first column of $\tilde{Z}^{(k+1)}$. At $x^{(k+2)}$ we have

$$\tilde{Z}^{(k+1)T} g^{(k+1)} \parallel e_1, \quad (5.2)$$

where $e_1 = (1, 0, \dots, 0)^T$. Let $\Omega^{(k+1)} = \Omega_{n-1,n}\Omega_{n-2,n-1}\dots\Omega_{1,2}$, with $\Omega_{i,i+1}$ the Givens rotation that makes the $(i+1)$ -th and i -th elements of the vector $\Omega_{i,i+1}^T\Omega_{i+1,i+2}^T\dots\Omega_{n-1,n}\tilde{Z}^{(k+1)T}\gamma^{(k+1)}$ zero and positive respectively. We know $\Omega^{(k+1)}$ is lower-Hessenberg and thus using (5.2) we have $\Omega^{(k+1)T}\tilde{Z}^{(k+1)T}g^{(k+1)} = (*, *, 0, \dots, 0)^T$, therefore

$$\Omega^{(k+1)T}\tilde{Z}^{(k+1)T}(\gamma^{(k+1)}, g^{(k+1)}) = \begin{pmatrix} * & 0 & 0 & \dots & 0 \\ * & * & 0 & \dots & 0 \end{pmatrix}^T$$

Let $\bar{Z}^{(k+1)} = \tilde{Z}^{(k+1)}\Omega^{(k+1)}$, we can form $Z^{(k+2)}$ as in (4.6), and the process can now be repeated.

The complete algorithm is given as follows:

Algorithm

step 1 Let $x^{(1)}$ be a starting point and $\tilde{Z}^{(1)}$ be a nonsingular matrix (see later for a possible choice of $\tilde{Z}^{(1)}$) satisfying

$$\tilde{Z}^{(1)T}g^{(1)} = (*, 0, \dots, 0)^T.$$

Let $k = 1$. If $\|g^{(1)}\| = 0$ then stop.

step 2 Form search direction $d^{(k)} = -\tilde{z}_1^{(k)}\tilde{z}_1^{(k)T}g^{(k)}$.

step 3 Line search to get $x^{(k+1)} = x^{(k)} + \lambda^{(k)}d^{(k)}$, if $\|g^{(k+1)}\| = 0$ then stop.

step 4 Let $\delta^{(k)} = x^{(k+1)} - x^{(k)}$, $\gamma^{(k)} = g^{(k+1)} - g^{(k)}$, $s^{(k)} = \tilde{Z}^{(k)T}\gamma^{(k)}$,
 $b^{(k)} = s^{(k)T}s^{(k)}/\delta^{(k)T}\gamma^{(k)}$ and $h^{(k)} = -\lambda^{(k)}\delta^{(k)T}g^{(k)}/\delta^{(k)T}\gamma^{(k)}$.

step 5 Let $\Omega^{(k)}$ be the product of Givens rotations such that

$$\Omega^{(k)T}s^{(k)} = (*, 0, \dots, 0)^T.$$

Now we actually have

$$\Omega^{(k)T}\tilde{Z}^{(k)T}(\gamma^{(k)}, g^{(k)}) = \begin{pmatrix} * & 0 & 0 & \dots & 0 \\ * & * & 0 & \dots & 0 \end{pmatrix}^T$$

step 6 Let $\bar{Z}^{(k)} = \tilde{Z}^{(k)}\Omega^{(k)}$

step 7 Let

$$Z^{(k+1)} = \begin{pmatrix} \frac{\delta^{(k)}}{\sqrt{\delta^{(k)T}\gamma^{(k)}}}, \sqrt{\xi^{(k)}}\sqrt{1 + \phi^{(k)}(b^{(k)}h^{(k)} - 1)}\bar{z}_2^{(k)}, \sqrt{\xi_3^{(k)}}\bar{z}_3^{(k)}, \\ \dots, \sqrt{\xi_n^{(k)}}\bar{z}_n^{(k)} \end{pmatrix}. \quad (5.3)$$

step 8 Let $\Gamma^{(k+1)}$ be the Givens rotation such that $\Gamma^{(k+1)T}Z^{(k+1)T}g^{(k+1)} \parallel e_1$. Here $Z^{(k+1)T}g^{(k+1)} = (z_1^{(k+1)T}g^{(k+1)}, z_2^{(k+1)T}g^{(k+1)}, 0, \dots, 0)^T$. Let $\tilde{Z}^{(k+1)} = Z^{(k+1)}\Gamma^{(k+1)}$, $k := k + 1$, go to step 2.

The main operational costs of the algorithm come from step 4, the calculation of $s^{(k)} = \tilde{Z}^{(k)T}\gamma^{(k)}$, which needs n^2 multiplications, and from step 6, the multiplication of $\tilde{Z}^{(k)}$ by a sequence of Givens rotations $\Omega_{n-1,n}, \Omega_{n-2,n-1}, \dots, \Omega_{1,2}$, which can be done in about $3n^2$ multiplications (see Powell, 1987). The scaling of the columns of $Z^{(k+1)}$ by $\sqrt{\xi_i^{(k)}}$ in step 7 can be combined with step 6. Thus the whole algorithm needs about $4n^2$ multiplications per iteration.

Like the BFGS algorithm of Powell (1987), the algorithm has an interesting property, namely, when working on quadratics with exact arithmetic, the second to the $(k+1)$ -th columns of the matrix $\tilde{Z}^{(k+1)}$

are parallel to the k past search directions, and all search directions are conjugate to each other, thus the algorithm has the quadratic termination property. This is proved in the following theorem.

Theorem 5.1 Suppose the Algorithm is applied to a quadratic function with positive definite Hessian $G \in R^{n \times n}$. If the line searches are exact, $\phi^{(k)} > \bar{\phi}^{(k)}$, $\xi^{(k)} > 0$ and $\xi_i^{(k)} > 0$ ($3 \leq i \leq n$), then the algorithm will terminate within n steps.

Proof

We prove by induction on k the following results. At the iterative point $x^{(k+1)}$ ($k \geq 1$), if $\|g^{(k+1)}\| \neq 0$, then

$$\delta^{(1)}, \delta^{(2)}, \dots, \delta^{(k)} \text{ are mutually conjugate,} \quad (5.4)$$

$$\tilde{z}_i^{(k+1)} = \pm \sqrt{\prod_{j=3}^i \xi_j^{(k-i+j)}} \delta^{(k+2-i)} / \sqrt{\delta^{(k+2-i)^T} \gamma^{(k+2-i)}}, \quad 2 \leq i \leq k+1, \quad (5.5)$$

$$\tilde{z}_i^{(k+1)^T} G \tilde{z}_j^{(k+1)} = 0, \quad 2 \leq i \leq k+1, \quad j = 1 \text{ or } k+2 \leq j \leq n, \quad (5.6)$$

and

$$\tilde{Z}^{(k+1)} \text{ is non-singular.} \quad (5.7)$$

At $x^{(2)}$ ($k = 1$), (5.4) is vacuous.

Because $\bar{Z}^{(1)} = \tilde{Z}^{(1)}\Omega^{(1)}$ is non-singular, and by step 5 $\delta^{(1)}$ is conjugate to $\bar{z}_i^{(1)}$, $i = 2, 3, \dots, n$, so from (4.6) the first column of $Z^{(2)}$ is conjugate to the rest of the columns (which are multiples of $\bar{z}_i^{(1)}$, $i = 2, 3, \dots, n$), thus $Z^{(2)}$ is non-singular and so is $\tilde{Z}^{(2)} = Z^{(2)}\Gamma^{(2)}$. Therefore (5.7) is valid for $k = 1$.

Since

$$Z^{(2)} = \left(\frac{\delta^{(1)}}{\sqrt{\delta^{(1)^T} \gamma^{(1)}}}, \sqrt{\xi^{(1)}} \sqrt{1 + \phi^{(1)}(b^{(1)}h^{(1)} - 1)} \bar{z}_2^{(1)}, \sqrt{\xi_3^{(1)}} \bar{z}_3^{(1)}, \dots, \sqrt{\xi_n^{(1)}} \bar{z}_n^{(1)} \right),$$

because of exact line search, in step 8 we have

$$Z^{(2)^T} g^{(2)} = \left(0, \sqrt{\xi^{(1)}} \sqrt{1 + \phi^{(1)}(b^{(1)}h^{(1)} - 1)} \bar{z}_2^{(1)^T} g^{(2)}, 0, \dots, 0 \right)^T.$$

Thus the Givens rotation $\Gamma^{(2)}$ differs from the unit matrix only in its leading principal 2×2 matrix, with $\Gamma_{11}^{(2)} = \Gamma_{22}^{(2)} = 0$ and $|\Gamma_{12}^{(2)}| = |\Gamma_{21}^{(2)}| = 1$. Therefore $\tilde{Z}^{(2)} = Z^{(2)}\Gamma^{(2)}$ is the matrix derived from exchanging the first and second columns of $Z^{(2)}$, with possible sign changes in the two columns and so $\tilde{z}_2^{(2)} = \pm \delta^{(1)} / (\delta^{(1)^T} \gamma^{(1)})^{\frac{1}{2}}$. Hence (5.5) is valid for $k = 1$, and (5.6) is also valid for $k = 1$ since $\delta^{(1)}$ is conjugate to $\bar{z}_i^{(1)}$, $i = 2, 3, \dots, n$.

Now assume (5.4), (5.5), (5.6) and (5.7) are valid for some $k \geq 1$ and assume $\|g^{(k+2)}\| \neq 0$ so the algorithm does not terminate at $x^{(k+2)}$. Then $\bar{Z}^{(k+1)} = \tilde{Z}^{(k+1)}\Omega^{(k+1)}$ is non-singular, and so is $Z^{(k+2)}$ since $\delta^{(k+1)}$ is conjugate to the linearly independent vectors $\bar{z}_i^{(k+1)}$ ($2 \leq i \leq n$) by step 5 of the algorithm. Thus $\tilde{Z}^{(k+2)} = Z^{(k+2)}\Gamma^{(k+2)}$ is non-singular. Hence (5.7) is valid with k replaced by $k+1$.

Since (5.6) shows that $\tilde{z}_1^{(k+1)}$ is conjugate to $\bar{z}_i^{(k+1)}$ ($2 \leq i \leq k+1$), by (5.5) it is conjugate to the previous k search directions. Therefore by step 2, $d^{(k+1)}$ is conjugate to the previous k search directions and so (5.4) is valid with k replaced by $k+1$.

At $x^{(k+2)}$, because by (5.5), the 2nd to the $(k+1)$ -th columns of $\tilde{Z}^{(k+1)}$ contain the first k search directions, and since $\delta^{(k+1)}$ is conjugate to these directions the vector $s^{(k+1)} = \tilde{Z}^{(k+1)T} \gamma^{(k+1)}$ is of the form $(s_1^{(k+1)}, 0, \dots, 0, s_{k+2}^{(k+1)}, \dots, s_n^{(k+1)})^T$. So during step 5, we have

$$\Omega_{k+2, k+3}^T \dots \Omega_{n-1, n}^T s^{(k+1)} = (s_1^{(k+1)}, \overbrace{0, \dots, 0}^k, a^{(k+1)}, 0, \dots, 0)^T,$$

where $a^{(k+1)} = \left(\sum_{i=k+2}^n (s_i^{(k+1)})^2 \right)^{\frac{1}{2}}$. Notice that $a^{(k+1)} \neq 0$, for otherwise $s_i^{(k+1)} = \tilde{z}_i^{(k+1)T} \gamma^{(k+1)} = 0$ ($2 \leq i \leq n$), and $\tilde{z}_i^{(k+1)T} g^{(k+1)} = 0$ ($2 \leq i \leq n$) because of step 8 of the algorithm, so we have $\tilde{z}_i^{(k+1)T} g^{(k+2)} = 0$ ($2 \leq i \leq n$). Since $d^{(k+1)} \parallel \tilde{z}_1^{(k+1)}$, exact line search gives $\tilde{z}_1^{(k+1)T} g^{(k+2)} = 0$. So $\tilde{Z}^{(k+1)T} g^{(k+2)} = 0$, which is contradictory to the non-singularity of $\tilde{Z}^{(k+1)}$ and the assumption that $\|g^{(k+2)}\| \neq 0$. Hence $\Omega_{k+1, k+2}, \dots, \Omega_{2, 3}$ are all Givens rotations that are derived from exchanging the i -th and $(i+1)$ -th ($2 \leq i \leq k+1$) columns of the unit matrix, with possible sign changes in the columns. So $\Omega^{(k+1)}$ is of the form

$$\Omega^{(k+1)} = \begin{pmatrix} * & * & 0 & \cdots & 0 & 0 & \cdots & 0 \\ 0 & 0 & \pm 1 & \ddots & \vdots & \vdots & & \vdots \\ \vdots & \vdots & 0 & \ddots & 0 & \vdots & & \vdots \\ 0 & 0 & \vdots & \ddots & \pm 1 & 0 & & \vdots \\ * & * & \vdots & & 0 & * & \ddots & \vdots \\ \vdots & \vdots & \vdots & & \vdots & * & \ddots & 0 \\ \vdots & \vdots & \vdots & & \vdots & \vdots & \ddots & * \\ * & * & 0 & \cdots & 0 & * & \cdots & * \end{pmatrix}.$$

A 7×7 example of $\Omega^{(k+1)}$ would be as follows (assume $n = 7$ and $k = 3$)

$$\Omega^{(k+1)} = \begin{pmatrix} * & * & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & \pm 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & \pm 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & \pm 1 & 0 & 0 \\ * & * & 0 & 0 & 0 & * & 0 \\ * & * & 0 & 0 & 0 & * & * \\ * & * & 0 & 0 & 0 & * & * \end{pmatrix}.$$

Therefore $\bar{Z}^{(k+1)} = \tilde{Z}^{(k+1)} \Omega^{(k+1)}$ has the property that

$$\bar{z}_i^{(k+1)} = \tilde{z}_{i-1}^{(k+1)} = \pm \sqrt{\prod_{j=3}^{i-1} \xi_j^{(k+1-i+j)}} \delta^{(k+3-i)} / \sqrt{\delta^{(k+3-i)T} \gamma^{(k+3-i)}}, \quad 3 \leq i \leq k+2, \quad (5.8)$$

and these k columns are by (5.6) conjugate to the rest of the columns of $\bar{Z}^{(k+1)}$, which are linear combinations of $\tilde{z}_1^{(k+1)}$ and $\tilde{z}_j^{(k+1)}$ ($k+2 \leq j \leq n$).

Now at step 7 of the algorithm, we have

$$Z^{(k+2)} = \left(\frac{\delta^{(k+1)}}{\sqrt{\delta^{(k+1)T} \gamma^{(k+1)}}}, \sqrt{\xi^{(k+1)}} \sqrt{1 + \phi^{(k+1)}(b^{(k+1)} h^{(k+1)} - 1)} \bar{z}_2^{(k+1)}, \right. \\ \left. \sqrt{\xi_3^{(k+1)}} \bar{z}_3^{(k+1)}, \dots, \sqrt{\xi_n^{(k+1)}} \bar{z}_n^{(k+1)} \right).$$

So the 3rd to the $(k+2)$ -th columns of $Z^{(k+2)}$ are by (5.8)

$$\begin{aligned} z_i^{(k+2)} &= \sqrt{\xi_i^{(k+1)}} \bar{z}_i^{(k+1)} \\ &= \pm \sqrt{\prod_{j=3}^i \xi_j^{(k+1-i+j)}} \delta^{(k+3-i)} / \sqrt{\delta^{(k+3-i)^T} \gamma^{(k+3-i)}}, \\ & \quad 3 \leq i \leq k+2, \end{aligned} \tag{5.9}$$

and we know that these k columns are conjugate to the rest of the columns. The first column is conjugate to all the other columns because of step 5.

Because of exact line searches, $Z^{(k+2)^T} g^{(k+2)} = (0, z_2^{(k+2)^T} g^{(k+2)}, 0, \dots, 0)^T$, so using the same reasoning as before the matrix $\tilde{Z}^{(k+2)}$ is derived by exchanging the first and second columns of $Z^{(k+2)}$, with possible sign changes in the two columns. Therefore

$$\tilde{z}_2^{(k+2)} = \pm \delta^{(k+1)} / \sqrt{\delta^{(k+1)^T} \gamma^{(k+1)}}$$

and

$$\tilde{z}_i^{(k+2)} = z_i^{(k+2)}, \quad 3 \leq i \leq k+2,$$

which together with (5.9) shows that (5.5) is valid with k replaced by $k+1$. The fact that the 2nd to the $(k+2)$ -th columns of $\tilde{Z}^{(k+2)}$ are conjugate to the rest of the columns shows that (5.6) is also valid with k replaced by $k+1$.

By induction (5.4), (5.5), (5.6) and (5.7) are true for all k such that $\|g^{(k+1)}\| \neq 0$, so (5.4) and exact line searches show that the algorithm will terminate in at most n steps. \square

Theorem 5.1 shows that even with arbitrary scaling factors $\xi_i^{(k)} \geq 0$ ($3 \leq i \leq n$), our algorithm still has the quadratic termination property theoretically (It is also possible to prove this result for Algorithm 1 of Siegel (1991)). However in practice using small scaling factors (smaller than 1) at every iteration can cause the algorithms to lose the quadratic termination property. The reason is seen as follows. In the proof of theorem 5.1 we have shown that the vector $s^{(k+1)} = \tilde{Z}^{(k+1)} \gamma^{(k+1)}$ is of the form $(s_1^{(k+1)}, 0, \dots, 0, s_{k+2}^{(k+1)}, \dots, s_n^{(k+1)})^T$, and $a^{(k+1)} = \left(\sum_{i=k+2}^n (s_i^{(k+1)})^2 \right)^{\frac{1}{2}} \neq 0$. But with finite arithmetic, the zero elements of $s^{(k+1)}$ can be nonzero numbers of small magnitude and because of small scaling factors in the current and previous iterations, the columns of $\tilde{Z}^{(k+1)}$ can also be of small magnitude. Thus $a^{(k+1)}$ can be of the same magnitude as $s_i^{(k+1)}$, $i = 2, \dots, k+1$. This causes the proof of the theorem to break down and the algorithm can take more than n iterations to converge, if it converges at all. Our numerical experience however indicates that large scaling factors do not cause so many problems.

We now discuss the scaling factors $\xi_i^{(k)}$, $i = 3, \dots, n$. If the optimally conditioned family (3.9) is to be used, then since $\phi^{(k)} = (h^{(k)}/\xi^{(k)} - 1)/(b^{(k)}h^{(k)} - 1)$, we see that

$$Z^{(k+1)} = \left(\frac{\delta^{(k)}}{\sqrt{\delta^{(k)^T} \gamma^{(k)}}}, \sqrt{h^{(k)}} \bar{z}_2^{(k)}, \sqrt{\xi_3^{(k)}} \bar{z}_3^{(k)}, \dots, \sqrt{\xi_n^{(k)}} \bar{z}_n^{(k)} \right), \tag{5.10}$$

where $\xi_-^{(k)} \leq \xi_i^{(k)} \leq \xi_+^{(k)}$ ($3 \leq i \leq n$) and $\xi_-^{(k)}$ and $\xi_+^{(k)}$ are given by (1.2). There is still a lot of freedom in choosing the $\xi_i^{(k)}$ and so we investigate ways of specifying them. Incidentally, noticing that the first and second columns of $Z^{(k+1)}$ are independent of the scaling factors $\xi_i^{(k)}$, this together with step 8 of the algorithm shows that the search direction $d^{(k+1)}$ is also independent of the current scaling factors $\xi_i^{(k)}$.

One possibility is to find the least change update

$$\begin{aligned} & \min \|W^{-1}(H^{(k+1)} - H^{(k)})W^{-T}\|_F \\ & \text{subject to } \xi_-^{(k)} \leq \xi_i^{(k)} \leq \xi_+^{(k)}, \quad 3 \leq i \leq n \end{aligned}$$

where $H^{(i)} = Z^{(i)}Z^{(i)T}$ and $Z^{(i)}$ is given by (5.10). If we take $W = Z^{(k)}$, in view of (4.2), the solution is obviously to take $\xi_i^{(k)}$ to be the number in the interval $[\xi_-^{(k)}, \xi_+^{(k)}]$ that is nearest to 1. The resulting algorithm will be denoted as [LCHANG].

Since, as previously mentioned, small scaling factors can cause problems on quadratics, and in their implementations of the BFGS method, Powell (1987) and Siegel (1991 b) found that scaling columns up can be efficient when the Hessian of the function to be minimized is nearly singular at the minimum, we will also try to use the freedom in $\xi_i^{(k)}$ to scale the columns of $Z^{(k+1)}$ up if their magnitudes are small compared with that of the first column.

So we let $\xi_i^{(k)}$ ($3 \leq i \leq n$) be the number in the interval $[\xi_-^{(k)}, \xi_+^{(k)}]$ that is nearest to $\max\{1, \|z_1^{(k+1)}\|^2 / \|\bar{z}_i^{(k)}\|^2\}$. The resulting algorithm is denoted by [SCAUP].

We compare these two optimally conditioned algorithms with five other algorithms as follows.

1. The BFGS algorithm [BFGS], that is (5.3) with $\xi^{(k)} = 1$, $\xi_i^{(k)} = 1$ and $\phi^{(k)} = 1$.
2. The optimally conditioned BFGS algorithm [OCBFGS], that is (5.10) with $\xi_i^{(k)} = 1/b^{(k)}$.
3. The BFGS algorithm with initial scaling [INIBFGS], that is (5.3) with $\xi^{(k)} = 1/b^{(k)}$, $\xi_i^{(k)} = 1/b^{(k)}$, $\phi^{(k)} = 1$ for $k = 1$, and $\xi^{(k)} = 1$, $\xi_i^{(k)} = 1$ and $\phi^{(k)} = 1$ for $k \geq 2$.
4. Davidon's (1975) optimally conditioned algorithm [DAV], that is (5.3) with $\xi^{(k)} = 1$ and $\xi_i^{(k)} = 1$. Then $\phi^{(k)} = (h^{(k)} - 1)/(b^{(k)}h^{(k)} - 1)$ if $\xi^{-^{(k)}} \leq 1 \leq \xi^{+(k)}$ and $\phi^{(k)} = 1/(1 - b^{(k)})$ otherwise.

It was found, by Hu and Storey (1991), that if K denotes the condition number of $H^{-\frac{1}{2}}H^+H^{-\frac{1}{2}}$ with H^+ Davidon's (1975) optimally conditioned update, then

$$K/K^* \leq \max \left\{ \frac{1}{\min\{b, h\}}, \quad 1 \right\}.$$

Furthermore, K/K^* can be arbitrarily large if $\min\{b, h\}$ is sufficiently small. Thus we will try a modified Davidon algorithm [MDAV] given by the following choice of parameters.

5. If $b^{(k)} > 0.1$ and $h^{(k)} > 0.1$ then [DAV], otherwise set $\xi^{(k)}$ and $\xi_i^{(k)}$ equal to the number in the interval $[\xi_-^{(k)}, \xi_+^{(k)}]$ that is nearest to 1 and $\phi^{(k)} = (h^{(k)}/\xi^{(k)} - 1)/(b^{(k)}h^{(k)} - 1)$. This scheme ensures that $K/K^* < 10$.

We implemented the seven algorithms on a HP 9000/870 computer with double precision in FORTRAN. The algorithms only differ from each other in the choice of parameters $\xi^{(k)}$, $\xi_i^{(k)}$ ($3 \leq i \leq n$) and $\phi^{(k)}$. The initial matrix $\tilde{Z}^{(1)}$ is taken to be the product of Givens rotations such that $\tilde{Z}^{(1)}g^{(1)} = (*, 0, \dots, 0)^T$, so the initial H -matrix is the unit matrix ($H^{(1)} = \tilde{Z}^{(1)}\tilde{Z}^{(1)T} = I$). The line search routine we use finds a step length $\lambda^{(k)}$ satisfying

$$f(\mathbf{x}^{(k)} + \lambda^{(k)}\mathbf{d}^{(k)}) \leq f(\mathbf{x}^{(k)}) + 10^{-4}\lambda^{(k)}\mathbf{g}^{(k)T}\mathbf{d}^{(k)}$$

and

$$|\mathbf{g}(\mathbf{x}^{(k)} + \lambda^{(k)}\mathbf{d}^{(k)})^T\mathbf{d}^{(k)}| \leq 0.9 |\mathbf{g}^{(k)T}\mathbf{d}^{(k)}|$$

If during the line search the length of the interval in which the final step length is predicted to lie becomes less than 10^{-15} , then the line search is assumed to fail. The initial step length is always taken as

one except when $k = 1$, in which case we take it as $\max\{2, (\text{EST} - f^{(k)})/g^{(k)T}d^{(k)}\}$ where we set EST equal to zero.

To test the algorithms, we use the first 31 test functions of Moré et al. (1981). These are all sums of squares with the number of square terms either as given, if a number is recommended in their paper, or is set to 100. Standard starting points are used. The stopping criterion is $\|g^{(k+1)}\| \leq 10^{-5} \max\{1, \|x^{(k+1)}\|\}$ for all the algorithms.

Table 5.1 contains the number of iterations (the number of function evaluations) for the seven algorithms on the 31 test functions. We use “F2” to denote failures due to the line search, “F3” to denote failure due to overflow of functions (gradients). To summarize the results we add the number of iterations (the number of function evaluations) of the seven algorithms on 28 function and list the totals in the last row of the table. In doing so we do not count functions 6, 10 and 17 on which some algorithms failed.

From the table we can see that [LCHANG] and [MDAV] perform very well. The simple BFGS algorithm with initial scaling [INIBFGS] also does very well. [OCBFGS], [DAV] and [SCAUP] all improve a little over [BFGS] although they are not so good as [LCHANG], [MDAV] and [INIBFGS]. On function 10 although [BFGS], [DAV] find a point satisfying the stopping criterion, the point is actually not the minimum.

Overall we also see that algorithms with some kind of optimal conditioning tend to be more reliable.

It is slightly disappointing that the algorithm [SCAUP] that attempts to scale up small columns does not work very well. But we expect that such an algorithm will be more useful when the initial matrix or the Hessian at the solution is nearly singular.

The success of [INIBFGS] and [LCHANG] seem to indicate that although optimal conditioning is important, it is also important to force the scaling factors to be close to unity.

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Table 5.1 Number of iterations (number of function evaluations) for the seven algorithms

K	N	BFGS	OCBFGS	INIBFGS	DAV	MDAV	LCHANG	SCAUP
1	2	34 (43)	43 (63)	35 (56)	41 (51)	41 (56)	43 (63)	43 (63)
2	2	9 (10)	16 (17)	19 (20)	9 (10)	18 (19)	16 (17)	16 (17)
3	2	143 (186)	187 (270)	145 (195)	168 (201)	167 (205)	187 (270)	187 (270)
4	2	11 (37)	15 (18)	12 (16)	12 (15)	13 (17)	15 (18)	15 (18)
5	2	14 (18)	17 (19)	18 (19)	12 (16)	15 (16)	17 (19)	17 (19)
6	2	F3 (F3)	18 (19)	20 (21)	F3 (F3)	19 (21)	18 (19)	18 (19)
7	3	27 (36)	32 (45)	26 (29)	27 (36)	30 (34)	30 (33)	32 (37)
8	3	19 (21)	22 (23)	28 (29)	18 (20)	25 (26)	22 (23)	19 (22)
9	3	2 (3)	3 (5)	3 (5)	2 (3)	2 (3)	3 (5)	3 (5)
10	3	2 (14)	F2 (F2)	F2 (F2)	2 (14)	432 (544)	F2 (F2)	F2 (F2)
11	3	14 (23)	22 (35)	17 (22)	9 (20)	14 (18)	23 (29)	8 (22)
12	3	23 (27)	38 (43)	36 (42)	22 (26)	38 (43)	38 (43)	33 (39)
13	4	35 (44)	32 (33)	51 (52)	29 (39)	42 (43)	40 (41)	41 (47)
14	4	76 (118)	154 (177)	36 (52)	78 (122)	55 (85)	108 (132)	103 (121)
15	4	21 (26)	35 (36)	32 (35)	23 (27)	23 (27)	33 (35)	26 (33)
16	4	25 (51)	24 (25)	35 (36)	20 (46)	27 (28)	24 (25)	19 (20)
17	5	F3 (F3)	140 (151)	97 (104)	F3 (F3)	93 (101)	94 (102)	86 (101)
18	6	33 (39)	51 (54)	44 (46)	32 (34)	41 (45)	39 (43)	101 (124)
19	11	49 (71)	110 (116)	74 (79)	52 (68)	64 (67)	68 (71)	72 (91)
20	12	43 (54)	103 (112)	86 (94)	41 (52)	84 (86)	81 (90)	132 (168)
21	12	121 (170)	42 (62)	35 (56)	133 (150)	41 (56)	44 (64)	87 (112)
22	12	60 (81)	36 (38)	51 (52)	69 (81)	42 (43)	42 (44)	66 (79)
23	12	174 (242)	59 (84)	51 (63)	105 (127)	66 (80)	59 (84)	60 (85)
24	12	249 (363)	92 (111)	136 (171)	177 (238)	141 (171)	24 (26)	96 (114)
25	12	23 (25)	21 (22)	21 (22)	22 (24)	21 (22)	21 (22)	21 (22)
26	12	29 (37)	52 (54)	27 (33)	26 (32)	26 (32)	41 (43)	29 (32)
27	12	11 (12)	11 (15)	12 (16)	11 (12)	10 (14)	11 (15)	12 (17)
28	12	17 (29)	31 (33)	34 (36)	20 (26)	27 (29)	27 (29)	41 (52)
29	12	8 (11)	6 (7)	7 (8)	7 (9)	7 (9)	6 (7)	6 (7)
30	12	22 (48)	18 (19)	22 (23)	21 (38)	18 (19)	18 (19)	18 (22)
31	12	50 (113)	15 (16)	39 (40)	31 (52)	32 (33)	15 (16)	15 (16)
TOTALS		1342(1938)	1287(1552)	1132(1347)	1217(1575)	1130(1326)	1095(1326)	1318(1674)