A New Derivation of Symmetric Positive Definite Secant Updates

J.E. Dennis, Jr*
Robert B. Schnabel**

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University of Colorado at Boulder
DEPARTMENT OF COMPUTER SCIENCE

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Abstract

In this paper, we introduce a simple new set of techniques for deriving symmetric and positive definite secant updates. We use these techniques to present a simple new derivation of the BFGS update using neither matrix inverses nor weighting matrices. A related derivation is shown to generate a large class of symmetric rank-two update formulas, together with the condition for each to preserve positive definiteness. We apply our techniques to generate a new projected BFGS update, and indicate applications to the efficient implementation of secant algorithms via the Cholesky factorization.
1. Introduction and Background

In 1965, Broyden [2] published two apparently equally reasonable methods for generating Jacobian approximations \( J_+ \in \mathbb{R}^{n\times n} \) in a quasi-Newton method for solving \( F(x) = 0 \) whose basic step is

\[
x_+ = x_c - J_c^{-1} F(x_c),
\]

where \( F : \mathbb{R}^n \to \mathbb{R}^n \), \( x_c \in \mathbb{R}^n \), and \( J_c \in \mathbb{R}^{n\times n} \) is nonsingular. The method which bears his name works very well and consists in taking

\[
J_+ = J_c + \frac{(y - J_c s)s^T}{s^T s}, \tag{1.1}
\]

where \( s = x_+ - x_c \) is the current step, and \( y = F(x_+)-F(x_c) \) is the yield of this step. It is easy to show [7] that \( J_+ \) is nearest \( J_c \) in the Frobenius norm \( \| \cdot \|_F \) among all matrices in

\[
Q(y,s) = \{ J \in \mathbb{R}^{n\times n} : Js = y \},
\]

the generalized quotients of \( y \) by \( s \).

Broyden's other method does not work so well, but it seems just as reasonable, since it is to choose

\[
J_+ = J_c + \frac{(y - J_c s)y^T J_c}{y^T J_c s} \tag{1.2}
\]

or, equivalently,

\[
J_+^{-1} = J_c^{-1} + \frac{(s - J_c^{-1} y)y^T}{y^T y}, \tag{1.3}
\]

the nearest matrix in \( Q(s,y) \) to \( J_c^{-1} \) in the Frobenius norm. These methods have basically the same good theoretical justifications.

Powell [17] and Greenstadt [15] defined symmetric analogs of these methods for the case when \( F \) is the gradient of some nonlinear functional \( f : \mathbb{R}^n \to \mathbb{R} \). Now we are dealing with Hessian matrices, which we will denote by \( H_c \), \( H_+ \), and so it seems desirable to have the
approximation \( H_+ \) inherit symmetry from \( H_\ell \). Again it seems as reasonable to minimize the change from \( Q(s,y) \cap \{ A : A = A^T \} \) to \( H_\ell^{-1} \) as Greenstadt does, as to follow Powell and minimize the change to \( H_\ell \) from candidate approximations in \( Q(y,s) \cap \{ A : A = A^T \} \). Once more, the theoretical justification is similar and good, but numerical experience favors Powell's symmetric form of (1.1).

There are various reasons why it has been thought desirable to maintain positive definiteness as well as symmetry in the sequence of approximate Hessians and this is done, when possible, by the DFP ([4], [10]) update formula

\[
H_+ = H_\ell + \frac{(y-H_\ell s)y^T + y(y-H_\ell s)^T}{y^T s} - \frac{s^T (y-H_\ell s)y}{(y^T s)^2} \quad (1.4)
\]

or

\[
H_+^{-1} = H_\ell^{-1} - \frac{H_\ell^{-1} y y^T H_\ell^{-1}}{y^T H_\ell^{-1} y} + \frac{s s^T}{y^T s},
\]

and also by the BFGS ([3], [9], [13], [19]) formula

\[
H_+^{-1} = H_\ell^{-1} + \frac{(s-H_\ell^{-1} y)s^T + s(s-H_\ell^{-1} y)^T}{s^T y} - \frac{y^T (s-H_\ell^{-1} y)s}{(s^T y)^2} \quad (1.5)
\]

or

\[
H_+ = H_\ell - \frac{H s s^T H_\ell}{s^T H_\ell s} + \frac{y y^T}{y^T s}.
\]

Since \( s^T y = s^T H s \) for any \( H \in Q(y,s) \), it is obvious that a necessary condition for \( Q(y,s) \) to contain a positive definite matrix is \( y^T s > 0 \). It is well-known that if \( H_\ell \) is symmetric and positive definite, then \( y^T s > 0 \) is sufficient to ensure that both (1.4) and (1.5) generate \( H_+ \) that inherit both properties. We will give a very simple short proof of this fact in Section 2.

Dennis and Moré [7] and Dennis and Schnabel [8] show that (1.4)
and (1.5) are again least change updates. In this case, (1.4) defines the minimum change to $H_C$ to obtain $H_+ \in Q(y,s) \cap \{A:A=A^T\}$. The change is measured by $\|W(H_C^{-1} - H_+^{-1})W\|_F$ where $W$ is any nonsingular matrix for which $W^TW = M \in Q(s,y)$. Update (1.5) defines the least change to $H_C^{-1}$ from $Q(s,y) \cap \{A:A=A^T\}$ measured by $\|W^TW^{-1}(H_C^{-1} - H_+^{-1})W^{-1}\|_F$. In this case, unlike the others, computational experience indicates that the BFGS, which makes the least weighted change to the inverse of $H_C$, outperforms the DFP, which makes the least weighted change to $H_C$.

These derivations are unsatisfying because they relate the good Broyden (1.1) to the less successful DFP (1.4) and the bad Broyden (1.3) to the more successful BFGS (1.5). In Section 2, we will give a new derivation of the BFGS directly from the good Broyden. This new derivation is invariably successful in the classroom. We also show how the DFP is derived from the bad Broyden. In Section 3, we show how the new derivation can be used to derive from the rank-one methods a large class of the symmetric rank-two secant updates that inherit positive definiteness. We also use this same technique to obtain a relationship between Oren's [16] sizing of the Hessian and hereditary positive definiteness. It enables us to coerce Powell's symmetric Broyden formula, and all the other rank two updates we derive, into having this desirable property.

Section 4 is devoted to applying our technique to the derivation from projected rank-one updates of the projected rank-two updates of the type introduced by Davidon [5]. In particular, we derive a new projected BFGS update from the projected Broyden update of Gay and Schnabel [11]. In Section 5, we relate our derivations to an algorithm of Goldfarb [14] for updating a Cholesky factorization of $H_C$. 
We hope that specialists will find the entire paper of interest, but we believe that Sections 2 and 5 should be of interest to anyone who teaches this material, since they constitute a quick and simple way to derive the BFGS update from the Broyden update in a form that leads directly to its Cholesky factorization implementation via the update of the LQ factorization. These methods are all the material on updates that really needs to be taught in a general numerical analysis course.
2. The BFGS and DFP from the Good and Bad Broyden Methods

In this section, we will need the following very simple lemma characterizing when a symmetric positive definite matrix exists in $Q(y,s)$ for $y, s \in \mathbb{R}^n$. This lemma is quite easy, and it will form the basis for our subsequent derivations.

**Lemma 2.1:** Let $y, s \in \mathbb{R}^n$, $s$ nonzero, and let $Q(y,s) = \{A \in \mathbb{R}^{n \times n}: As = y\}$. Then $Q(y,s)$ contains a symmetric positive definite matrix if and only if, for some nonzero $v \in \mathbb{R}^n$ and nonsingular $J \in \mathbb{R}^{n \times n}$, $y = Jv$ and $v = J^T s$.

**Proof:** If $v$ and $J$ exist then clearly $y = Jv = JJ^T s$ and $JJ^T$ is the symmetric positive definite matrix we seek.

Now suppose $A$ is a symmetric positive definite matrix with $y = As$. Let $A = LL^T$ be the Cholesky factorization of $A$ and set $J = L$ and $v = L^T s$ to complete the proof.

If we have a symmetric positive definite approximate Hessian $H_C$ and we want to obtain $H_+$, which inherits these properties as well as the property of incorporating the new problem information by being in $Q(y,s)$, then the preceding lemma guides us to a solution. We probably have a Cholesky factorization of $H_C = L_C L_C^T$, and we know from the previous lemma that the sort of $H_+$ we desire exists if and only if we can find a $v$ and $J_+$ such that $y = J_+ v$ and $v = J_+^T s$. It seems quite natural to think of trying to obtain $J_+$ from $L_C$, and in fact, we would hope to do this without making a larger change to $L_C$ than necessary, in order to preserve as much as possible of the information stored in $L_C$ which has been gathered as the iteration has proceeded. This motivates choosing $J_+$ by the following procedure.
BFGS Procedure

1. Assuming we know \( v \in \mathbb{R}^n \), find the \( J_+ \in \mathbb{R}^{n \times n} \) which is nearest \( L_C \) in the Frobenius norm and satisfies \( J_+v = y \).

2. Solve for \( v \) so that \( J_+^Tv = v \).

The proof of the following theorem shows that the solution is the BFGS update.

**Theorem 2.2:** Let \( L_C \in \mathbb{R}^{n \times n} \) be nonsingular, \( H_C = L_CL_C^T \), \( y, s \in \mathbb{R}^n \), \( s \) nonzero. There is a symmetric positive definite matrix \( H_+ \in Q(y,s) \) if and only if \( y^Ts > 0 \). If there is such a matrix, then the BFGS update \( H_+ = J_+J_+^T \) is one such, where

\[
J_+ = L_C + \frac{(y - L_Cv)^T(y - L_Cv)}{v^Tv} \frac{L_C^Ts}{v^Tv} \quad (2.1)
\]

and either the positive or negative square root may be taken.

**Proof:** Recall first from Lemma 2.1 that a necessary condition for the update to exist is that there exist nonzero \( v \in \mathbb{R}^n \), and nonsingular \( J_+ \in \mathbb{R}^{n \times n} \) such that \( J_+v = y \) and \( J_+^Ts = v \). Therefore

\[
v^Tv = (J_+^Ts)^T(J_+^Ts) = s^Ty\]

which shows that \( s^Ty > 0 \) is necessary.

Now we derive the BFGS update via the above procedure. If we knew \( v \), then the nearest matrix to \( L_C \) that sends \( v \) to \( y \) is just the Broyden update (1.1): in this setting,

\[
J_+ = L_C + \frac{(y - L_Cv)^Tv}{v^Tv} \cdot \frac{v^Tv}{v^Tv} \quad (1.1)
\]

Notice that this reduces the problem of determining \( n^2 \) elements of \( J_+ \) to finding the \( n \) components of \( v \). Now we use the condition that

\[
v = J_+^Ts = L_C^Ts + \frac{(y^Ts - v^TL_Cs)}{v^Tv} v.
\]
This implies that \( v = \alpha L_c^T s \) for some scalar \( \alpha \), and so the problem of determining the \( n \) components of \( v \) is reduced to finding the scalar \( \alpha \). Plugging back in, we see that

\[
\alpha = 1 + \frac{(y^T s - \alpha s^T H_c s)}{\alpha^2 s^T H_c s},
\]

or

\[
\alpha^2 = y^T s / s^T H_c s.
\]

Therefore if \( y^T s > 0 \), we have defined a symmetric and positive update in \( Q(y,s) \).

We have now proved everything except the easily verified statement that \( H_+ \) defined by (1.5) is identical to \( J_+ J_+^T \) where \( J_+ \) is given by (2.1), no matter which sign is taken for the square root.

This derivation has the satisfying property of connecting the good Broyden formula (1.1) and the BFGS method. Another alternative in using Lemma 2.1 to derive a symmetric and positive definite \( H_+ \in Q(y,s) \) would be to first chose \( J_+ \) to satisfy

\[
J_+^T s = v
\]

and then solve for \( v \) so that

\[
J_+ v = y.
\]

The proof of Theorem 2.3 shows that if we do this, and choose \( J_+ \) in (2.2) to be the bad Broyden update (1.2) to \( L_c^T \), the solution is the DFP update.
Theorem 2.3: Let $L_{C}$, $H_{C}$, $s$, and $y$ satisfy the hypotheses of Theorem 2.2.  
There is a symmetric positive definite matrix $H_{+} \in Q(y,s)$ if and only if $y^{T}s > 0$. If there is such a matrix, then the DFP update $H_{+} = J_{+}J_{+}^{T}$ is one such, where
\[
J_{+}^{T} = L_{C}^{T} + \frac{\left( y^{T}s \cdot L_{C}^{-1}y - L_{C}^{T}s \right)y^{T}}{y^{T}s}
\]
for either sign of the square root.

Proof: Let us return to the derivational proof of Theorem 2.2. If we decide, given the intermediate vector $v$, that we will obtain $J_{+}^{T}$ from (1.2) via
\[
J_{+}^{T} = L_{C}^{T} + \frac{(v-L_{C}s)^{T}v}{v^{T}L_{C}^{T}s}v L_{C}^{T}
\]  
(2.3)
to satisfy (2.2), then the equation for $y = J_{+}v$ is
\[
y = J_{+}v = L_{C}v+L_{C}(v-L_{C}s)^{T}L_{C}v
\]
so $v = \beta L_{C}^{-1}y$ for some scalar $\beta$ and plugging back in,
\[
\beta = \sqrt{\frac{y^{T}s}{y^{T}H_{C}^{-1}y}}
\]
and
\[
v = \sqrt{\frac{y^{T}s}{y^{T}H_{C}^{-1}y}} L_{C}^{-1}y.
\]  
(2.4)
Again if $y^{T}s > 0$, we have derived a symmetric and positive definite update in $Q(y,s)$. It is easily verified that if $J_{+}$ is defined by (2.3) and (2.4), then $J_{+}J_{+}^{T}$ is the DFP update given by (1.4).
3. Hereditary Positive Definiteness and Oren Sizing For Symmetric Rank-Two Updates

In the last section, we followed two different tacks in our derivations. Assuming that we had \( v \), for the BFGS we updated \( L_C^T \) to \( J_+ \), and for the DFP, \( L_C^T \) to \( J_+ \). Then in each case, we obtained \( v \) from a requirement on the transpose of the updated factor. In this section, we will generalize our derivations to include scaling matrices. The BFGS derivation turns out to be largely invariant to scaling. On the other hand, the generalization of the DFP derivation turns out to yield a large class of symmetric rank two update formulas, including the PSB in the unweighted case, as well as the condition for each to inherit positive definiteness from \( H_C \).

Our second interest in this section is the relationship between Oren's [16] sizing and hereditary positive definiteness of symmetric rank-two updates. Oren's sizing consists of first multiplying \( H_C \) by a constant \( \sigma^2 \) and then updating \( \sigma^2 H_C \) to \( H_+ \). Our generalization of the DFP derivation will lead naturally to a range of sizing factors \( \sigma^2 \) which make the PSB update of a sized positive definite matrix be positive definite. A similar result holds for any update obtained via the DFP derivation.

Let us consider first the "BFGS procedure" from the last section, but with scaling matrices. We want \( H_+ = J_+ J_+^T \) and we assume we have \( H_C = L_C L_C^T \). Given nonsingular \( W_L \) and \( W_R \) in \( \mathbb{R}^{n \times n} \), we consider the procedure

1. Assuming we know \( v \in \mathbb{R}^n \), choose \( J_+ \) to solve
   \[
   \min_{J_+ \in Q(y,v)} \| W_L (J_+ L_C) W_R \|_F \tag{3.1}
   \]

2. Solve for \( v \) so that \( J_+^T s = v \).
The BFGS update came from this procedure with $W_L = W_R = I$. Note that if we are approximating the Hessian, $W_L$ corresponds to a linear transformation of the variable space by $W_L^{-T}$, but $W_R$ has no natural interpretation.

It is well-known ([8], Corr. 2.3) that, for $M = W_R^{-T}W_R^{-1}$,

$$J_+ = L_c + \frac{(y - L_c v)(Mv)^T}{v^T Mv}$$  \hspace{1cm} (3.2)

solves (3.1) independent of $W_L$. Thus, we can say that the BFGS update results from the above procedure with any $W_L$ and $M = I$. Furthermore, $W_R$ can be any unitary matrix without changing the result. It actually turns out that the BFGS results from any $W_L$ and any $W_R$ for which $L_c$ is an eigenvector of $M$. We postpone this and the development for general $W_R$ to the appendix since we can think of no reason to choose any $W_R$ or $M$ other than $I$.

There would have been good choices of $W_L$, e.g., $(W_L^{-T}W_L) \in Q(s,y)$, since this corresponds to scaling $\hat{y} = W_L y$ and $\hat{s} = W_L^{-T}s$ so that $\hat{s} = W_L^{-T}s = W_L^{-T}(W_L^{-T}W_L y) = W_L y = \hat{y}$ and $\hat{s}_+ = I$ is feasible. While our BFGS derivation was invariant under such scalings, the situation reverses when we introduce scaling into the DFP derivation.

The generalization of the "DFP procedure" is to select nonsingular matrices $W_L$ and $W_R$, assume that we know $v = J_+^{-1} y$, choose $J_+^T$ to solve

$$\min_{J_+ \in Q(v,s)} \| W_L (J_+^T - L_c^T) W_R \|_F,$$

and then solve for $v$ from

$$y = J_+ v.$$  \hspace{1cm} (3.4)

Notice that in this case, the role of the scaling matrices is reversed;
$W_R$ corresponds to a transformation of the variable space by $W_R^{-1}$, while $W_L$ has no obvious justification.

As before, we see that for $M = (W_RW_R^T)^{-1}$,

$$J_+^T = L_C^T + \frac{(v-L_C^T)(Ms)^T}{s^TMs}$$  \hspace{1cm} (3.5)

solves (3.3) just as (3.2) solves (3.1). Again the answer is independent of $W_L$, but this time it eliminates the scale matrix that we don't know how to choose. We will finish carrying through the second procedure for general $W_R$ or $M$, but first we state the result.

**Proposition 3.1:** Let $L_C$, $H_+$, $s$ and $y$ satisfy the hypotheses of Theorem 2.2. The result of the procedure outlined by (3.3), (3.4), and (3.5) is

$$H_+ = J_+J_+^T = H_C + \frac{(y-H_Cs)(Ms)^T + (y-H_Cs)^T}{s^TMs} - \frac{s^T(y-H_Cs)Ms^Tm}{(s^TMs)^2},$$  \hspace{1cm} (3.6)

where $J_+$ is given by (3.5) and

$$v = L_C^{-1}(y+\alpha Ms)$$  \hspace{1cm} (3.7)

for either root $\alpha$ of

$$\alpha^2 s^TMH_C^{-1}Ms + 2\alpha s^TMH_C^{-1}y + y^TH_C^{-1}y - s^Ty = 0.$$  \hspace{1cm} (3.8)

If

$$(s^TMH_C^{-1}y)^2 \geq (s^TMH_C^{-1}Ms)(y^TH_C^{-1}y - s^Ty),$$  \hspace{1cm} (3.9)

then $J_+$ is a real matrix and $H_+$ is positive definite.

**Proof:** Again we proceed in a derivational manner beginning with (3.5) and then (3.4),

$$y = J_+v = L_Cv + (Ms)\frac{v^Tv - s^TL_Cv}{s^TMs}.$$  \hspace{1cm} (3.10)
Thus, for some $\alpha$, $y + \alpha M s = L_C v$. Direct substitution into (3.10) shows that (3.4) is satisfied if and only if $\alpha$ is chosen so that

$$y^T s = v^T v = (l^{-1} y + \alpha L^{-1} M s)^T (l^{-1} y + \alpha L^{-1} M s)$$

$$= y^T H^{-1} y + 2 \alpha s^T M H^{-1} y + \alpha^2 s^T M H^{-1} M s.$$

This is equivalent to $\alpha$ being a root of (3.8), which has real roots if and only if (3.9) holds. Clearly, if $v$ and $J_+$ are defined by a real $\alpha$, then $H_+$ is positive definite. It is straightforward to show that $H_+$ is real in any case and is given by (3.6).

It is shown in [18] that the class of matrices (3.6) is equivalent to the set of all symmetric rank-two updates that can be represented as the difference of two symmetric rank-one updates. It should also be noted that the scaling used above corresponds exactly to the scaling used by Dennis and Moré [7] and Dennis and Schnabel [8] in their least change derivations of the same class of updates.

Now we give the relationship of hereditary positive definiteness to Oren's sizing. The proof is obvious.

**Corollary 3.2:** Let $M$ and $H = L_C L_C^T$ be symmetric positive definite matrices and let $s, y \in \mathbb{R}^n$ with $s^T y > 0$. If $\sigma$ is any number for which

$$\sigma^2 > \frac{(s^T M H^{-1} M s) y^T H^{-1} y - (s^T M H^{-1} y)^2}{(s^T M H^{-1} M s) y^T y}$$

then (3.6) applied to $\sigma H = (\sigma L_C)(\sigma L_C^T)$ defines a symmetric positive definite $H_+$, (3.9) is a strict inequality for $\sigma^2 H$, $v$ defined by (3.7) for $\sigma L_C$ is real, and $J_+$ defined by (3.5) is a real matrix with $H_+ = J_+ J_+^T$. 
It is interesting to note that if $\sigma^2 = 1$ satisfies (3.11), then
$H_+$ inherits positive definiteness directly from $H_C$, but that

$$\sigma^2 = \frac{y^T H_C^{-1} y}{y^T s}$$

one of Oren's recommended choices, always satisfies

(3.11) and is independent of $M$ and $W_R$.

We complete the section by specializing Theorem 3.2 to the PSB,
DFP, and BFGS formulas.

Corollary 3.3: Let $L_C$, $H_C$, $s$, $y$ satisfy the hypothesis of Corollary 3.2

and let

$$\sigma^2 > \frac{(s^T H_C^{-1} s)(y^T H_C^{-1} y) - (s^T H_C^{-1} y)^2}{(s^T H_C^{-1} s)(y^T s)}.$$ Then the PSB update of $\sigma^2 H_C$,

$$H_+ = \sigma^2 H_C + \frac{(y - \sigma^2 H_C s)^T s + s(y - \sigma^2 H_C s)}{s^T s} - \frac{s^T (y - \sigma^2 H_C s) ss^T}{(s^T s)^2}$$

is a positive definite matrix, and $H_+ = J_+ J_+^T$, where

$$J_+ = \sigma L_C^T + \frac{(v - \sigma L_C^T s)^T s}{s^T s},$$

$$v = L_C^{-1} (y + \alpha s),$$

$$\alpha = -\frac{s^T H_C^{-1} y \pm \sqrt{(s^T H_C^{-1} y)^2 - (s^T H_C^{-1} s)(y^T H_C^{-1} y - \sigma^2 s^T y)}}{s^T H_C^{-1} s}$$

are all real.

Proof: The proof follows from the quadratic formula and the fact that

(3.6) with $M = I = W_R$ is the PSB update.

As we discussed earlier, other than the identity, the obvious scaling
to try is $M = (W_R W_R^T)^{-1} \in Q(y, s)$. The result is the DFP formula. The
following is straightforward.
Corollary 3.4: Let $L_c, H_c, s, y$ satisfy the hypothesis of Corollary 3.2, and let $\sigma^2$ be any positive number. Then the DFP update $H_+$ of $\sigma^2 H_c$ is positive definite and

$$H_+ = J_+ J_+^T,$$

where

$$J_+^T = \sigma L_c^T + \left( \frac{y^T S - \sqrt{y^T H_c^{-1} y} L_c^T S}{y^T S} \right) y^T S^{-1} S^{-1} y^T S^{-1}.$$

The following corollary is not so obvious, but it is perhaps the most interesting of all. It consists in applying a scaling from [18] to obtain the BFGS update from the same derivation as the DFP and PSB.

Corollary 3.5: Let $L_c, H_c, s, y$ satisfy the hypothesis of Theorem 3.2. Then for any

$$M \in Q(y \sqrt{y^T S^{-1} S^{-1} H_c} s), s)$$

and any scalar $\gamma$, (3.6) defines the BFGS update $H_+$ of $H_c$. The BFGS update of any $\sigma^2 H_c$ is positive definite for any real $\sigma$.

Proof: First notice that (3.6) is independent of scalar multiples of $M$ and then plug and grind. Take (2.1) with its unspecified sign on the radical and equate its transpose to (3.5).

The interesting thing to note here is that, by taking any DFP scaling $\tilde{M} \in Q(y, s)$, the BFGS scaling is

$$M = \frac{1}{1 + \sqrt{y^T S / s^T H_c s}} \tilde{M} + \left(1 - \frac{1}{1 + \sqrt{y^T S / s^T H_c s}}\right) H_c,$$

which is a convex combination of the DFP scaling and the current scaling. In fact, if the conditions of Dennis and Moré [6] for
q-superlinear convergence are met, it is easy to show that \( M \) asymptotically approaches \( (\bar{M} + H_c)/2 \).
4. A Projected BFGS from the Projected Broyden Update

Davidon [5] modified the standard symmetric rank-two update formulas in an attempt to satisfy the current secant condition $H_+ s = y$ without doing more than necessary damage to past secant conditions. We will introduce some notation in order to state the problem. Let \( \{s_1, \ldots, s_m\} \subseteq \mathbb{R}^n \), assume $s$ is linearly independent of the space spanned by the $s_i$'s, and consider the following problem:

Given $H_c = L_c L_c^T$, $s, y \in \mathbb{R}^n$ with $y^T s > 0$ find $H_+ = J_+ J_+^T$ such that

$$H_+ s = y \quad \text{and} \quad H_+ s_i = H_c s_i, \quad i = 1, 1, \ldots, m. \quad (4.1)$$

The $s_i$ can be interpreted as past steps and $s$ as the current step. Schnabel [18] proved that a solution is possible if and only if

$$(y - H_c s)^T s_i = 0, \quad i = 1, 2, \ldots, m. \quad (4.2)$$

Gay and Schnabel [11] gave a projected form of Broyden's update which satisfies (4.1) in the case when $H_c$ and $H_+$ are not required to be symmetric. In this section we will use a form of Gay and Schnabel's update in place of Broyden's update in the BFGS derivation of Section 2. The result will be a new projected BFGS formula which agrees with Davidon's version for quadratic functionals. Our formula will satisfy (4.1) for every $s_i$ that satisfies (4.2), but it will also have a fairly sensible partial version of (4.1) for all the $s_i$.

The procedure we will follow to derive the projected BFGS update is the following. Once again we assume we have $H_c = L_c L_c^T$, and we want $H_+ = J_+ J_+^T$.

**Projected BFGS Procedure**

1) Assuming we know $v \in \mathbb{R}^n$, choose $J_+$ to solve

$$\min \quad ||J_+ - L_c||_F$$

$$J_+ \in Q(y, v)$$

subject to $(J_+ - L_c) L_c^T s_i = 0, \quad i = 1, \ldots, m \quad (4.3)$
2) Solve for \( v \) so that \( J_+^T s = v \)

This procedure is carried out in the proof of Theorem 4.5. It differs from the "BFGS procedure" of Section 2 only in the addition of condition (4.3). In Lemmas 4.1 - 4.4 we justify this condition. Essentially, Lemmas 4.1 and 4.2 show that the condition \( (J_+ - L_c) L_c^T s_i = 0 \) is half of a necessary and sufficient condition for any "reasonable" update to satisfy

\[
(J_+ J_+^T - L_c L_c^T) s_i = 0. \tag{4.4}
\]

The other half is \( (J_+ - L_c)^T s_i = 0 \). Lemma 4.4 shows that the above procedure is guaranteed to produce an \( H_+ = J_+ J_+^T \) which satisfies (4.4) whenever this is consistent with \( H_+ s = y \). We will state the following lemmas in terms of matrices \( J_+ \) and \( L_c \) and vector \( s_i \) for ease in referring to them later, but the lemmas will contain explicit hypotheses and no other assumptions, such as \( L_c \) being lower triangular, are meant to be implied by the notation.

**Lemma 4.1:** Let \( L_c, J_+ \in \mathbb{R}^{n \times n}, s_i \in \mathbb{R}^n \). If

\[
(J_+ - L_c) L_c^T s_i = 0 \tag{4.5}
\]

and

\[
(J_+ - L_c)^T s_i = 0, \tag{4.6}
\]

then

\[
(J_+ J_+^T - L_c L_c^T) s_i = 0. \tag{4.7}
\]

**Proof:** The proof follows from the identity:

\[
J_+ J_+^T - L_c L_c^T = (J_+ - L_c)(J_+ - L_c)^T + L_c (J_+ - L_c)^T + (J_+ - L_c) L_c^T. \tag{4.8}
\]
Lemma 4.2: Let the hypotheses of Lemma 4.1 hold, and assume in addition that $L_c$ is nonsingular. Then (4.7) and

$$\text{rank } (J_+J_+^T - L_cL_c^T) \geq 2 \left( \text{rank}(J_+-L_c) \right) - 1$$

implies that (4.5) and (4.6) hold.

Proof: The proof will consist in showing that if (4.7) holds, then either (4.5) and (4.6) hold or the hypothesized rank condition does not hold. First we regroup terms in (4.8) to obtain

$$(J_+J_+^T - L_cL_c^T) = J_+(J_+-L_c)^T + (J_+-L_c)L_c^T. \quad (4.9)$$

We see immediately that if (4.7) holds, then (4.6) implies (4.5).

Now again from (4.8),

$$s_i^T(J_+J_+^T - L_cL_c^T)s_i = \| (J_+-L_c)^T s_i \|^2 + 2s_i^T(J_+-L_c)L_c^T s_i$$

and so if (4.7) holds, then (4.5) and (4.6) are equivalent.

Now suppose that neither (4.5) nor (4.6) holds. Since $L_c$ is nonsingular, let $k = \text{rank}(J_+-L_c) = \text{rank}(L_c(J_+-L_c)^T)$. Again from (4.8),

$$\text{rank}(J_+J_+^T - L_cL_c^T) = 2k-(a+b),$$

where

$$a = \dim \left( \text{row space of } J_+-L_c \cap \text{row space of } L_c(J_+-L_c)^T \right)$$

$$b = \dim \{ z \in \mathbb{R}^n : (J_+-L_c)^T L_c^T z = 0 \text{ and } (J_+-L_c)^T z \neq 0 \neq (J_+-L_c)L_c^T z \}. $$

Since we are supposing (4.7) but neither (4.5) or (4.6), $b \geq 1$. Now we transpose (4.9) and obtain, from (4.7),

$$0 = L_c^T(J_+-L_c)s_i + (J_+-L_c)^T J_+ s_i.$$

Using this and the fact that $L_c^T(J_+-L_c)s_i \neq 0$ because (4.6) doesn't hold and $L_c$ is nonsingular, we see that $a \geq 1$. Thus, rank
\[(J_+L_C-2k)^T \leq 2k-2.\]

The rank condition in Lemma 4.2 is required to exclude "unreasonable updates" such as \(J_+ = Q \cdot L_C\), Q orthogonal, which satisfy (4.7) without satisfying (4.5) or (4.6). In the case when \(J_+\) is a rank-one update to \(L_C\) we have the following easy corollary.

**Corollary 4.3:** Let \(L_C J_+, s_i\) obey the hypotheses of Lemma 4.2. If \(\text{rank} (J_+L_C) = 1\), and \(J_+L_C^{-1} = L_C^{-1}J_+\), then (4.7) is equivalent to (4.5) and (4.6).

**Proof:** From Lemma 4.2, (4.7) implies (4.5) and (4.6). Lemma 4.1 is the converse.

Now we show that we can expect the result of the **Projected BFGS Procedure** to satisfy (4.6), and hence (4.7), for any \(s_i\) for which (4.2) is true.

**Lemma 4.4:** Let \(L_C \in \mathbb{R}^{n \times n}\) be nonsingular, \(J_+ \in \mathbb{R}^{n \times n}\), \(s, s_i, y \in \mathbb{R}^n\), and let (4.5) hold. Set \(H_C = L_C^{-1}L_C^{-T}\) and \(v = J_+s\). If (4.2) holds for \(s_i\), then \((y-L_Cv)^T s_i = 0\). If \(J_+v = y\), \(\text{rank} (J_+L_C) = 1\), and \(s^Ty = y^TH_C^{-1}y\) also hold, then (4.7) holds.

**Proof:** First we note that

\[
(y-H_C s)^T s_i - (y-L_C v)^T s_i = (L_C v-H_C s)^T s_i
\]

\[
= (L_C J_+s-L_C L_C s)^T s_i
\]

\[
= s^T (J_+L_C)^T L_C^{-1} s_i,
\]

and so (4.2) and (4.5) imply \((y-L_C v)^T s_i = 0\). If we assume that \(J_+v = y\), then

\[
0 = (y-L_C v)^T s_i = v^T (J_+L_C)^T s_i,
\]

(4.10)
but since \( \text{rank } (J_{+} - L_{c}) = 1 \), for some \( w_{1}, w_{2} \in \mathbb{R}^{n}, (J_{+} - L_{c})^{T} = w_{1} w_{2}^{T} \)
and (4.10) becomes
\[
0 = v^{T} w_{1} w_{2} s_{i}.
\]
Thus, either \((J_{+} - L_{c})v = 0\) or \((J_{+} - L_{c})^{T} s_{i} = 0\). If \(0 = (J_{+} - L_{c})v = y - L_{c}v\),
then \(v = L_{c}^{-1}y\) and \(y^{T}s = (J_{+}v)^{T}s = v^{T} J_{+} s = v^{T} v = y^{T} H_{c}^{-1}y\),
which contradicts the hypothesis. This means that (4.6) must hold, and since we have
assumed (4.5), (4.7) must hold by Corollary 4.3.

Now we derive the new projected BFGS update. We let \( \delta_{ij} \) denote
the Kronecker delta.

**Theorem 4.5:** Let \( L_{c} \in \mathbb{R}^{n \times n} \) be nonsingular, \( H_{c} = L_{c} L_{c}^{T} \), and let
\( \{s, y, s_{1}, \ldots, s_{m}\} \subset \mathbb{R}^{n} \), \( s \) linearly independent of the space spanned by
\( \{s_{1}, \ldots, s_{m}\} \). Assume without loss of generality that
\( s_{i}^{T} H_{c} s_{j} = \delta_{ij} \). Define
\[
\overline{s} = s - \sum_{i=1}^{m} s_{i} (s_{i}^{T} H_{c} s_{i})
\]
and
\[
\overline{y} = y - \sum_{i=1}^{m} L_{c} s_{i} (s_{i}^{T} H_{c} s_{i}).
\]
Set
\[
J_{+} = L_{c} + \frac{(\overline{y} - \alpha H_{c} \overline{s})(\alpha L_{c} \overline{s})}{s^{T} \overline{y}} \quad (4.11)
\]
for \( \alpha^{2} = \frac{s^{T} \overline{y}}{s^{T} H_{c} s} \) and define \( H_{+} = J_{+} J_{+}^{T} \). Then
\[
H_{+} = H_{c} + \frac{\overline{y}^{T} \overline{y}}{s^{T} \overline{y} - \frac{H_{c} \overline{s} s^{T} H_{c}}{s^{T} H_{c} s}}, \quad (4.12)
\]
\( H_{+} s = y \), \( (J_{+} - L_{c})^{T} s_{i} = 0, i = 1, 2, \ldots, m \) and \( J_{+} \) is real if \( s^{T} \overline{y} > 0 \).
If \((y - H_{c} s)^{T} s_{i} = 0\) for any \( i = 1, \ldots, m \), then \((H_{+} - H_{c}) s_{i} = 0\).
Proof: The proof consists mainly of the derivation of update (4.12) via the procedure outlined earlier.

From Theorem 2.1 of [11], the solution to step 1 of the projected BFGS procedure is

\[ J^+ = L^+_c + \frac{(y - L^c v)^T}{v^Tv} \v C \]

where

\[ \bar{v} = v - \sum_{i=1}^{m} L^T_{c_i} (v^T L^T_{c_i}) \]

Thus step 2 of the procedure requires that

\[ v = L^T_{c} + \frac{(y^T S - v^T L^T_{c} S)}{v^Tv} \]

which, by (4.14), implies

\[ v = \alpha L^T_{c} + \sum_{i=1}^{m} \beta_i L^T_{c_i} \]

for some scalars \( \alpha, \beta_i, \ldots, \beta_m \). Now from (4.14) and \( s_i^T c_j = \delta_{ij} \), we see that \( \bar{v}^T L^T_{c_i}  = 0 \) for every \( i \), so from (4.15) followed by (4.16), we have for every \( i \),

\[ (L^T_{c} s_i)^T L^T_{c_i} \]

or

\[ \beta_i = (1-\alpha) (L^T_{c} s_i)^T L^T_{c_i} \]

This allows us to rewrite (4.16) as

\[ v = \alpha [L^T_{c} s - \sum_{i=1}^{m} L^T_{c_i} (L^T_{c} s_i)^T L^T_{c_i}] + \sum_{i=1}^{m} L^T_{c_i} (L^T_{c} s_i)^T L^T_{c_i} = \alpha r + z, \]

where \( r \) and \( z \) are defined in the obvious way and \( r = L^T_{c} s \). Notice that \( \bar{v} = v-z \), so \( \bar{v} = \alpha r \) and we only need find \( \alpha \) to have \( \bar{v} \) and hence \( v \). Note also that

\[ r^T z = \frac{v^T z}{\alpha} = 0, \]

since \( v^T L^T_{c_i} s_i = 0 \) for all \( i \).
To find $\alpha$, direct substitution shows that as in the proof of Proposition 3.1, (4.15) is satisfied if and only if
\[
T_y = \alpha T = \alpha^2 r^T r + 2\alpha r^T z + z^T z = \alpha^2 r^T r + z^T z.
\]

Thus
\[
T_y - z^T z = \alpha^2 \sum_{i=1}^{m} (s_i^T H_s i) = \alpha^2 \sum_{i=1}^{m} s_i^T H_s i,
\]
\[
T_y - z^T z = \alpha^2 \sum_{i=1}^{m} (s_i^T H_s i)^2 = \alpha^2 \sum_{i=1}^{m} s_i^T H_s i.
\]
\[
T_y - z^T z = \alpha^2 \sum_{i=1}^{m} s_i^T H_s i,
\]

and
\[
\alpha^2 = \frac{T_y - z^T z}{\sum_{i=1}^{m} s_i^T H_s i}.
\]

Next we show that (4.13) reduces to (4.11). Using $v = \alpha r$, $r^T z = 0$, $r^T r = s^T H_s i$, and the value we have just found for $\alpha^2$, $v^T v = \alpha r^T v = \alpha r^T (\alpha r + z) = \alpha^2 r^T r = s^T y$. Also, by the definition of $v$, $\bar{y}$, and $z$, and $r = L_c T_s$, $y - L_c v = y - \alpha L_c r - L_c z$,
\[
y - L_c v = y - \alpha H_c s - \sum_{i=1}^{m} s_i^T H_s i = \bar{y} - \alpha H_c s.
\]

and so (4.13) becomes
\[
J_+ = L_c + \frac{(y - \alpha H_c s)(s^T H_s i)^T}{s^T y},
\]

which is (4.11). Notice that $\alpha$ and $J_+$ are real if $\bar{y}^T s > 0$. Equation (4.12) is obtained by algebra from $J_+ J_+^T$.

To complete the proof, notice that if $0 = (y - H_c s)^T s_i$ holds for any $s_i$, then $(H_+ - H_c) s_i = 0$ from Lemma 4.4.
It is straightforward to confirm that (4.12) agrees with Davidon's projected BFGS formula when $f$ is a positive definite quadratic function, but not necessarily otherwise. Schnabel is currently testing an algorithm using the above projected BFGS update; the results will be reported elsewhere. Finally, we note that in analogy to the weighted DFP derivation of Chapter 3, an entire class of projected rank-two updates can be derived using the procedure (3.3) - (3.4) with the condition

$$(J^+ - L_C)^T S_i = 0, \ i = 1, \ldots, m$$

added to (3.3).
5. Updating Cholesky Factors

Finally we discuss the efficient sequencing of Cholesky factorizations in algorithms that use the update formulas derived in this paper. All the algorithms of this section have already been suggested by Goldfarb [14] using the Brodlie, Gourlay, and Greenstadt [1] factored form of the BFGS and DFP updates and the orthogonal decompositon update ideas of Gill, Golub, Murray, and Saunders [12]. Our purpose is to point out that they follow very naturally from the preceding derivations.

We will focus on the BFGS formula since the development for the others is similar. We assume we have $L_c$, the lower triangular Cholesky factor of the current Hessian approximation, and that

$$J_+ = L_c + \frac{(y - s^T H_c s + H_c s^T L_c)}{\sqrt{s^T H_c s}} = L_c + w z^T \quad (5.1)$$

from (2.1). Now we want the Cholesky factorization $L_+ L_+^T$ of $H_+ = J_+ J_+^T$. However, (5.1) is an especially handy form for the algorithms of [12] in which we are given

$$J_+ = L_c Q_c + w z^T$$

or

$$J_+ = L_c D_c V_c + w z^T$$

and find

$$J_+ = L_+ Q_+ \quad (5.2)$$

or

$$J_+ = L_+ D_+ V_+ \quad (5.3)$$
respectively, in a small multiple of \( n^2 \) operations. (Here \( Q \) and \( V \) denote matrices with orthogonal columns and \( D \) a diagonal matrix.) Equation (5.1) is handy because since \( Q_c = V_c = I \), the \( n^2 \) work ordinarily necessary to obtain \( Q_c^Tz \) or \( V_c^Tz \) as a first step to obtaining \( L_+ \) is not needed.

It is also unnecessary to accumulate \( Q_+ \) or \( V_+ \). From (5.2) or (5.3)

\[
H_+ = J_+J_+^T - L_+Q_+Q_+^TL_+ - L_+L_+^T
\]

or

\[
H_+ = J_+J_+^T = L_+D_+V_+V_+^TD_+L_+^T = L_+D_+L_+^T,
\]

and so we have a cheap stable computation for the Cholesky or LDL^T factorization of \( H_+ \) from the corresponding factorization of \( H_c \).
References


Appendix: The scaled BFGS derivation

If we carry through the first derivation of Section 2 with scaling matrices, then we consider:

1. Assuming we know \( v \), choose \( J_+ \) to solve
\[
\min_{J_+ \in \mathcal{Q}(y,v)} \| W_L (J_+ - L_C) W_R \|_F
\]

2. Solve for \( v \) so that \( J_+^T s = v \).

The solution is independent of \( W_L \) and depends on \( W_R \) through
\[
M = W_R^{-T} W_R^{-1}
\]
As noted in Section 3, step 1 gives
\[
J_+ = L_C + \frac{(y - L_C v)(Mv)^T}{v^T Mv} \tag{A.1}
\]
and step 2 gives
\[
v = J_+^T s = L_C^T s + M v \left( \frac{y^T s - v^T L_C^T s}{v^T M v} \right) \tag{A.2}
\]
From (A.2),
\[
M v = \alpha (v - L_C^T s) \tag{A.3}
\]
for some scalar \( \alpha \), and substituting this into (A.2)
\[
v = L_C^T s + (v - L_C^T s) \left( \frac{y^T s - v^T L_C^T s}{v^T v - v^T L_C^T s} \right),
\]
which is satisfied if and only if
\[
v^T v = y^T s = v^T L_C^T s. \tag{A.4}
\]
Substituting (A.3) into (A.1),
\[
J_+ = L_C + \frac{(y - L_C v)(v - L_C^T s)}{(v - L_C^T s)^T v}
\]
and so using (A.4) and doing some rearranging of terms, we find that the solution to our procedure is
\[
H_+ = J_+ J_+^T = H_C + \frac{(y - H_C s)^T w^T + w (y - H_C s)}{w^T s} - \frac{(y - H_C s)^T s w w^T}{(w^T s)^2}, \tag{A.5}
\]
where
\[ w = y - L_C v \]  \hspace{1cm} (A.6)

and \( v \) satisfies
\[ v = (I - (1/\alpha)M)^{-1} L_C^T s \]  \hspace{1cm} (A.7)

for some scalar \( \alpha \) such that
\[ v^T v = y^T s. \]  \hspace{1cm} (A.8)

If \( L_C^T s \) is an eigenvector of \( M \), we have that
\[ v = \left( \frac{y^T s}{s^T H_C s} \right)^{1/2} L_C^T s \]

and the solution is again the BFGS update. The reader can also verify that if
\[ M = \beta \left[ I + \left( \frac{y^T H_C^{-1} y}{y^T s} \right)^{1/2} L_C^T H^{-1} L_C \right] \]

for any positive definite \( H \in Q(y,s) \) and any positive scalar \( \beta \), then \( M \) is positive definite and the DFP update results from (A.5-8). In fact, if \( M \) is any matrix of the form
\[ M = \beta_1 I + \beta_2 L_C^T H^{-1} L_C, \]

where \( H \) is defined as above, and \( \beta_1, \beta_2 \) are positive scalars, then \( M \) is positive definite and an update from the Broyden class results.

In general, if \( y^T s > y^T H_C^{-1} y \), it can be seen from (A.6-8) that \( w \) can have any direction, and we have the same class of updates as we derived with the DFP derivation with scaling matrices. If \( y^T s < y^T H_C^{-1} y \), we have a subset of this class.