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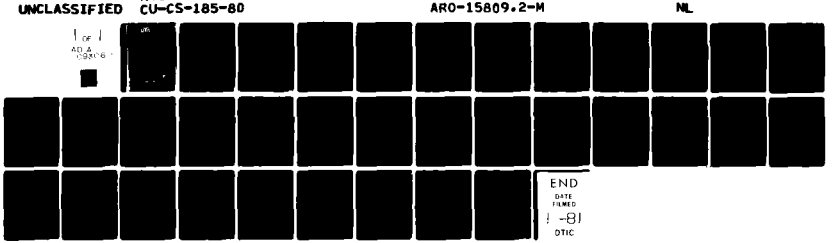

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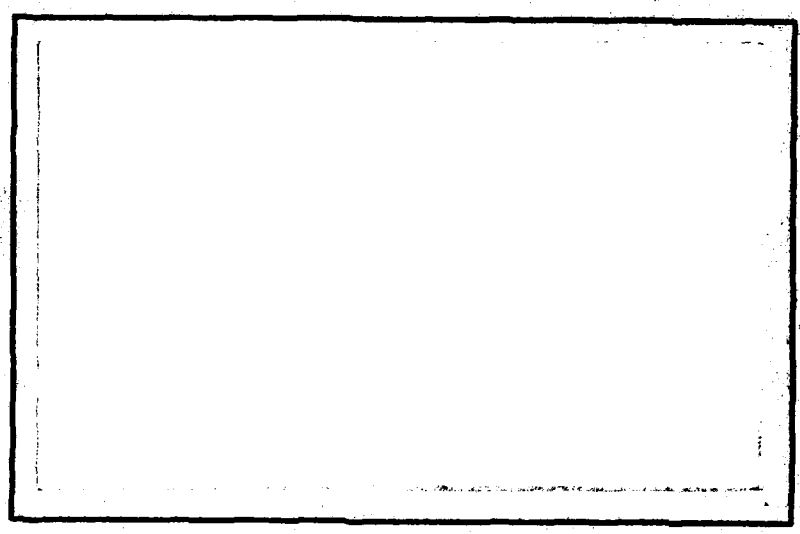

DEPARTMENT OF COMPUTER SCIENCE

Technical Report

A NEW DERIVATION OF SYMMETRIC POSITIVE DEFINITE SECANT UPDATES

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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 Cholsky factorization.

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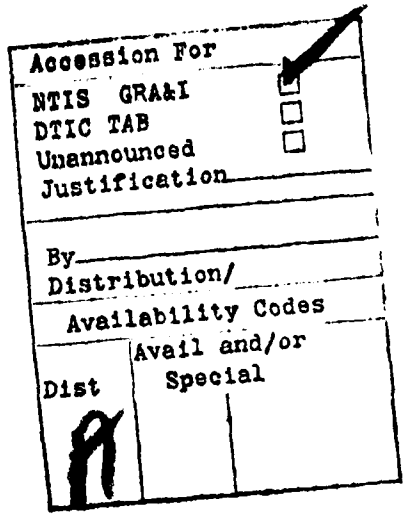

Abstract

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 $J_+ \in R^{n\times n}$ in a quasi-Newton method for solving $F(x) = 0$ whose basic step is

$$x_+ = x_c - J_c^{-1} F(x_c),$$

where $F : R^n \to R^n$, $x_c \in R^n$, and $J_c \in R^{n\times n}$ 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

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

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 $f: R^n \to R$. 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_c. Again it seems as reasonable to minimize the change from $Q(s,y) \cap \{A:A=A^T\}$ to H_c^{-1} as Greenstadt does, as to follow Powell and minimize the change to H_c 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

$$H_+ = H_c + \frac{(y-H_cs)y^T + y(y-H_cs)^T}{y^Ts} - \frac{s^T(y-H_cs)y\ y^T}{(y^Ts)^2} \qquad (1.4)$$

$$\text{or} \quad H_+^{-1} = H_c^{-1} - \frac{H_c^{-1}y\ y^TH_c^{-1}}{y^TH_c^{-1}y} + \frac{s\ s^T}{y^Ts},$$

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

$$H_+^{-1} = H_c^{-1} + \frac{(s-H_c^{-1}y)s^T + s(s-H_c^{-1}y)^T}{s^Ty} - \frac{y^T(s-H_c^{-1}y)s\ s^T}{(s^Ty)^2}$$

$$\text{or} \quad H_+ = H_c - \frac{H_cs\ s^TH_c}{s^TH_cs} + \frac{y\ y^T}{y^Ts}. \qquad (1.5)$$

Since $s^Ty = s^TH\ s$ 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 $y^Ts > 0$. It is well-known that if H_c is symmetric and positive definite, then $y^Ts > 0$ 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 $\| W(H_c-H_+)W\|_F$ 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 $\|W^{-T}(H_c^{-1}-H_+^{-1})W^{-1}\|_F$. 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 $y,s \in R^n$. This lemma is quite easy, and it will form the basis for our subsequent derivations.

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

Proof: If v and J exist then clearly $y = Jv = JJ^Ts$ 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 $v = L^Ts$ 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 $H_c = L_cL_c^T$, 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 $v = J_+^Ts$. 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 $v \in R^n$, find the $J_+ \in R^{n\times n}$ which is nearest L_c in the Frobenius norm and satisfies $J_+v = y$.
2. Solve for v so that $J_+^T s = v$.

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

Theorem 2.2: Let $L_c \in R^{n\times n}$ be nonsingular, $H_c = L_c L_c^T$, $y, s \in R^n$, s nonzero. 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 BFGS update $H_+ = J_+ J_+^T$ is one such, where

$$J_+ = L_c + \frac{(y - \sqrt{\frac{y^T s}{s^T H s}}\, H_c s)(L_c^T s)^T}{\sqrt{\frac{y^T s}{s^T H_c s}}\; s^T H_c s} \qquad (2.1)$$

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 $v \in R^n$, and nonsingular $J_+ \in R^{n\times n}$ such that $J_+v = y$ and $J_+^T s = v$. Therefore

$$v^T v = (J_+^T s)^T (J_+^{-1} y) = s^T y$$

which shows that $s^T y > 0$ 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,

$$J_+ = L_c + \frac{(y - L_c v)v^T}{v^T v} .$$

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

$$v = J_+^T s = L_c^T s + \frac{(y^T s - v^T L_c^T s)}{v^T v} v.$$

This implies that $v = \alpha L_c^T s$ for some scalar α, and so the problem of determining the n components of v is reduced to finding the scalar α. Plugging back in, we see that

$$\alpha = 1 + \frac{(y^T s - \alpha s^T H_c s)}{\alpha^2 s^T H_c s} \cdot \alpha$$

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

$$J_+^T s = v \tag{2.2}$$

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 $y^Ts > 0$. If there is such a matrix, then the DFP update $H_+ = J_+J_+^T$ is one such, where

$$J_+^T = L_c^T + \frac{\left(\sqrt{\frac{y^Ts}{y^TH_c^{-1}y}}\, L_c^{-1}y - L_c^Ts\right)y^T}{y^Ts}$$

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

$$J_+^T = L_c^T + \frac{(v-L_c^Ts)\, v^TL_c^T}{v^TL_c^Ts} \tag{2.3}$$

to satisfy (2.2), then the equation for $y = J_+v$ is

$$y = J_+ v = L_cv + L_cv \left(\frac{v^Tv - s^TL_cv}{v^TL_c^Ts}\right)$$

so $v = \beta L_c^{-1}y$ for some scalar β and plugging back in,

$$\beta = \sqrt{\frac{y^Ts}{y^TH_c^{-1}y}}$$

and

$$v = \sqrt{\frac{y^Ts}{y^TH_c^{-1}y}}\; L_c^{-1}y. \tag{2.4}$$

Again if $y^Ts > 0$, 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 to J_+, and for the DFP, L_c^T to J_+^T. 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 σ^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 σ^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 $R^{n\times n}$, we consider the procedure

1. Assuming we know $v \in R^n$, choose J_+ to solve

$$\min_{J_+ \in Q(y,v)} \| W_L(J_+ - L_c)W_R \|_F \qquad (3.1)$$

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 $M = W_R^{-T}W_R^{-1}$,

$$J_+ = L_c + \frac{(y-L_c v)(Mv)^T}{v^T M v} \tag{3.2}$$

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 $L_c^T s$ 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 $\hat{J}_+ = I$ 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

$$\min_{J^T \in Q(v,s)} \|W_L(J^T - L_c^T) W_R\|_F, \tag{3.3}$$

and then solve for v from

$$y = J_+ v. \tag{3.4}$$

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 $M = (W_R W_R^T)^{-1}$

$$J_+^T = L_c^T + \frac{(v-L_c^T s)(Ms)^T}{s^T Ms} \tag{3.5}$$

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

$$H_+ = J_+ J_+^T = H_c + \frac{(y-H_c s)(Ms)^T+(Ms)(y-H_c s)^T}{s^T Ms} - \frac{s^T(y-H_c s)Mss^T M}{(s^T Ms)^2}, \tag{3.6}$$

where J_+ is given by (3.5) and

$$v = L_c^{-1}(y+\alpha Ms) \tag{3.7}$$

for either root α of

$$\alpha^2 s^T M H_c^{-1} Ms+2\alpha s^T M H_c^{-1} y+y^T H_c^{-1} y-s^T y = 0. \tag{3.8}$$

If

$$(s^T M H_c^{-1} y)^2 \geq (s^T M H_c^{-1} Ms)(y^T H_c^{-1} y-s^T y), \tag{3.9}$$

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),

$$y = J_+ v = L_c v + (Ms)\frac{v^T v-s^T L_c v}{s^T Ms}. \tag{3.10}$$

Thus, for some α, $y + \alpha Ms = L_c v$. Direct substitution into (3.10) shows that (3.4) is satisfied if and only if α is chosen so that

$$y^T s = v^T v = (L_c^{-1}y+\alpha L_c^{-1}Ms)^T(L_c^{-1}y+\alpha L_c^{-1}Ms)$$

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

This is equivalent to α 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 α, 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 $H_c = L_c L_c^T$ be symmetric positive definite matrices and let $s, y \in R^n$ with $s^T y > 0$. If σ is any number for which

$$\sigma^2 > \frac{(s^T M H_c^{-1} Ms)y^T H_c^{-1}y - (s^T M H_c^{-1}y)^2}{(s^T M H_c^{-1} Ms)y^T s} \tag{3.11}$$

then (3.6) applied to $\sigma^2 H_c = (\sigma L_c)(\sigma L_c^T)$ defines a symmetric positive definite H_+, (3.9) is a strict inequality for $\sigma^2 H_c$, v defined by (3.7) for σL_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 $\sigma^2 H_c$,

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

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

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

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

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

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 σ^2 be any positive number. Then the DFP update H_+ of $\sigma^2 H_c$ is positive definite and

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

where

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

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

$$M \in Q\left(\gamma\left[y \pm \sqrt{\frac{y^T s}{s^T H_c s}}\, H_c s\right], s\right)$$

and any scalar γ, (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 σ.

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 $\overline{M} \in Q(y,s)$, the BFGS scaling is

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

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 $(\overline{M} + H_c)/2$.

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 $\{s_1,\ldots,s_m\} \subset R^n$, assume s is linearly independent of the space spanned by the s_i's, and consider the following problem:

Given $H_c = L_cL_c^T$, s, $y \in R^n$ with $y^Ts > 0$ find $H_+ = J_+J_+^T$ such that

$$H_+s = y \text{ and } H_+s_i = H_cs_i,\ i = 1, 1, \ldots, m. \tag{4.1}$$

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

$$(y-H_cs)^Ts_i = 0,\ i = 1, 2, \ldots, m. \tag{4.2}$$

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 $H_c = L_cL_c^T$, and we want $H_+ = J_+J_+^T$.

Projected BFGS Procedure

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

$$\begin{aligned} &\min && \|J_+ - L_c\|_F \\ &J_+ \in Q(y,v) \\ &\text{subject to } && (J_+-L_c)L_c^Ts_i = 0,\ i = 1, \ldots, m \end{aligned} \tag{4.3}$$

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 $L_c, J_+ \in R^{n\times n}$, $s_i \in R^n$. 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

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

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

$$(J_+J_+^T-L_cL_c^T) = J_+(J_+-L_c)^T + (J_+-L_c)L_c^T. \tag{4.9}$$

We see immediately that if (4.7) holds, then (4.6) implies (4.5). Now again from (4.8),

$$s_i^T(J_+J_+^T-L_cL_c^T)s_i = \|(J_+-L_c)^Ts_i\|_2^2 + 2s_i^T(J_+-L_c)L_c^Ts_i$$

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

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

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

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),

$$0 = L_c(J_+-L_c)^Ts_i + (J_+-L_c)J_+^Ts_i.$$

Using this and the fact that $L_c(J_+-L_c)^Ts_i \neq 0$ because (4.6) doesn't hold and L_c is nonsingular, we see that $a \geq 1$. Thus, rank

$(J_+J_+^T - L_CL_C^T) \leq 2k-2.$

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 rank $(J_+ - L_C) = 1$, and $J_+J_+^T \neq L_CL_C^T$, 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 $L_C \in R^{n\times n}$ be nonsingular, $J_+ \in R^{n\times n}$, $s, s_i, y \in R^n$, and let (4.5) hold. Set $H_C = L_CL_C^T$ and $v = J_+^Ts$. If (4.2) holds for s_i, then $(y-L_Cv)^Ts_i = 0$. If $J_+v = y$, rank $(J_+-L_C) = 1$, and $s^Ty \neq y^TH_C^{-1}y$ also hold, then (4.7) holds.

Proof: First we note that

$$\begin{aligned}(y-H_Cs)^Ts_i - (y-L_Cv)^Ts_i &= (L_Cv-H_Cs)^Ts_i \\ &= (L_CJ_+^Ts-L_CL_C^Ts)^Ts_i \\ &= s^T(J_+-L_C)^TL_C^Ts_i,\end{aligned}$$

and so (4.2) and (4.5) imply $(y-L_Cv)^Ts_i = 0$. If we assume that $J_+v = y$, then

$$0 = (y-L_Cv)^Ts_i = v^T(J_+-L_C)^Ts_i, \qquad (4.10)$$

but since rank $(J_+-L_c) = 1$, for some $w_1, w_2 \in R^n$, $(J_+-L_c)^T = w_1 w_2^T$ and (4.10) becomes

$$0 = v^T w_1 w_2^T s_i.$$

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 $y^T s = (J_+v)^T s = v^T J_+^T s = v^T v = y^T H_c^{-1} y$, 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 δ_{ij} denote the Kronecker delta.

Theorem 4.5: Let $L_c \in R^{n\times n}$ be nonsingular, $H_c = L_c L_c^T$, and let $\{s,y,s_1,\ldots,s_m\} \subset R^n$, 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

$$\bar{s} = s - \sum_{i=1}^{m} s_i (s^T H_c s_i)$$

and

$$\bar{y} = y - \sum_{i=1}^{m} H_c s_i (s^T H_c s_i).$$

Set

$$J_+ = L_c + \frac{(\bar{y}-\alpha H_c \bar{s})(\alpha L_c^T \bar{s})}{s^T \bar{y}} \tag{4.11}$$

for $\alpha^2 = \dfrac{s^T\bar{y}}{\bar{s}^T H_c \bar{s}}$ and define $H_+ = J_+ J_+^T$. Then

$$H_+ = H_c + \frac{\bar{y}\bar{y}^T}{s^T\bar{y}} - \frac{H_c\bar{s}\bar{s}^T H_c}{\bar{s}^T H_c \bar{s}}, \tag{4.12}$$

$H_+ s = y$, $(J_+-L_c)L_c^T s_i = 0, i = 1,2,\ldots,m$ and J_+ is real if $s^T\bar{y} > 0$. 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

$$J_+ = L_c + \frac{(y-L_c v)\bar{v}^T}{v^T v}, \tag{4.13}$$

where

$$\bar{v} = v - \sum_{i=1}^{m} L_c^T s_i (v^T L_c^T s_i). \tag{4.14}$$

Thus step 2 of the procedure requires that

$$v = L_c^T s + \bar{v} \frac{(y^T s - v^T L_c^T s)}{\bar{v}^T v} \tag{4.15}$$

which, by (4.14), implies

$$v = \alpha L_c^T s + \sum_{i=1}^{m} \beta_i L_c^T s_i, \tag{4.16}$$

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

$$(L_c^T s)^T L_c^T s_i = v^T L_c^T s_i = \alpha (L_c^T s)^T L_c^T s_i + \beta_i,$$

or

$$\beta_i = (1-\alpha)(L_c^T s)^T L_c s_i.$$

This allows us to rewrite (4.16) as

$$v = \alpha \left[L_c^T s - \sum_{i=1}^{m} L_c^T s_i (L_c^T s)^T L_c^T s_i\right] + \sum_{i=1}^{m} L_c^T s_i (L_c^T s)^T L_c^T s_i \equiv \alpha r + z,$$

where r and z are defined in the obvious way and $r = L_c^T \bar{s}$. Notice that $\bar{v} = v - z$, so $\bar{v} = \alpha r$ and we only need find α to have $\bar{v}$ and hence v. Note also that

$$r^T z = \bar{v}^T z/\alpha = 0,$$

since $\bar{v}^T L_c^T s_i = 0$ for all i.

To find α, direct substitution shows that as in the proof of Proposition 3.1, (4.15) is satisfied if and only if

$$s^T y = v^T v = \alpha^2 r^T r + 2\alpha r^T z + z^T z$$
$$= \alpha^2 r^T r + z^T z.$$

Thus

$$s^T y - z^T z = \alpha^2 \bar{s}^T L_c L_c^T \bar{s},$$

$$s^T y - \sum_{i=1}^{m} [(L_c^T s)^T L_c^T s_i]^2 = \alpha^2 \bar{s}^T H_c \bar{s},$$

$$s^T y - \sum_{i=1}^{m} (s^T H_c s_i)^2 = \alpha^2 \bar{s}^T H_c \bar{s},$$

$$s^T \bar{y} = \alpha^2 \bar{s}^T H_c \bar{s},$$

and $$\alpha^2 = \frac{s^T \bar{y}}{\bar{s}^T H_c \bar{s}}.$$

Next we show that (4.13) reduces to (4.11). Using $\bar{v} = \alpha r$, $r^T z = 0$, $r^T r = \bar{s}^T H_c \bar{s}$, and the value we have just found for α^2,

$$\bar{v}^T v = \alpha r^T v = \alpha r^T (\alpha r + z) = \alpha^2 r^T r = s^T \bar{y}.$$

Also, by the definition of v, $\bar{y}$, and z, and $r = L_c^T \bar{s}$,

$$y - L_c v = y - \alpha L_c r - L_c z$$
$$= y - \alpha H_c \bar{s} - \sum_{i=1}^{m} H_c s_i (s^T H_c s_i)$$
$$= \bar{y} - \alpha H_c \bar{s}$$

and so (4.13) becomes

$$J_+ = L_c + \frac{(\bar{y} - \alpha H_c \bar{s})(\alpha L_c^T \bar{s})^T}{s^T \bar{y}},$$

which is (4.11). Notice that α 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

$$J_+ = L_c + \frac{(y - \sqrt{\frac{y^Ts}{s^TH_cs}}\, H_cs)s^TL_c}{\sqrt{\frac{y^Ts}{s^TH_cs}}\, s^TH_cs} = L_c + wz^T \tag{5.1}$$

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

$$J_+ = L_cQ_c + wz^T$$

or

$$J_+ = L_cD_cV_c + wz^T$$

and find

$$J_+ = L_+Q_+ \tag{5.2}$$

or

$$J_+ = L_+D_+V_+, \tag{5.3}$$

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 $Q_c^T z$ or $V_c^T z$ 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)

$$H_+ = J_+ J_+^T = L_+ Q_+ Q_+^T L_+^T = L_+ L_+^T$$

or

$$H_+ = J_+ J_+^T = L_+ D_+ V_+ V_+^T D_+ L_+^T = L_+ D_+^2 L_+^T,$$

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

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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

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

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

$$J_+ = L_c + \frac{(y - L_c v)(Mv)^T}{v^T M v} \tag{A.1}$$

and step 2 gives

$$v = J_+^T s = L_c^T s + Mv \left(\frac{y^T s - v^T L_c^T s}{v^T M v} \right) \tag{A.2}$$

From (A.2),

$$Mv = \alpha (v - L_c^T s) \tag{A.3}$$

for some scalar α, 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

$$v^T v = y^T s \neq v^T L_c^T s. \tag{A.4}$$

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

$$H_+ = J_+ J_+^T = H_c + \frac{(y - H_c s) w^T + w (y - H_c s)}{w^T s} - \frac{(y - H_c s)^T s \; w w^T}{(w^T s)^2}, \tag{A.5}$$

where

$$w \triangleq y - L_c v \tag{A.6}$$

and v satisfies

$$v = (I-(1/\alpha)M)^{-1} L_c^T s \tag{A.7}$$

for some scalar α such that

$$v^T v = y^T s . \tag{A.8}$$

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

$$M = \beta \left[I + \left(\frac{y^T H_c^{-1} y}{y^T s}\right)^{1/2} L_c^T \bar{H}^{-1} L_c\right]$$

for any positive definite $\bar{H} \in Q(y,s)$ and any positive scalar β, then M is positive definite and the DFP update results from (A.5-8). In fact, if M is any matrix of the form

$$M = \beta_1 I + \beta_2 L_c^T \bar{H}^{-1} L_c,$$

where $\bar{H}$ is defined as above, and β_1, β_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.