

Toward Direct Sparse Updates
of Cholesky Factors

by

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Abstract

A very important problem in numerical optimization is to find a way to update a sparse Hessian approximation so that it will be positive definite under reasonable circumstances. This problem has motivated research, which is yet to show much progress, toward a "sparse BFGS method." In this paper, we suggest a different approach to the problem based on using a sparse Broyden, or Schubert, update directly on the Cholesky factor of the current Hessian approximation to define the next Hessian approximation implicitly in terms of its Cholesky factorization. This approach has the added advantage of being able to cheaply find the Newton step, since no factorization step is required. The difficulty with our approach is in finding a satisfactory secant or quasi-Newton condition to use in the update.

Key words

quasi-Newton methods, continuous minimization, sparse Hessians.

1. Introduction

Let $f: \mathbf{R}^n \rightarrow \mathbf{R}$, and consider the problem of finding a local minimizer of f . Often, a solution to this problem can be obtained using a quasi-Newton method which is basically an iterative procedure of the form

$$x_{k+1} = x_k - B_k^{-1} \nabla f(x_k) \quad k = 0, 1, 2, \dots$$

where $\nabla f(x_k)$ is the gradient of f at x_k and B_k is some approximation to the Hessian of f at x_k . The sequence of matrices $\{B_k\}$ is often generated by the least-change secant update (l.c.s.u.) approach, i.e. in going from B_k to B_{k+1} , we want to change B_k as little as possible in some sense while preserving its structure, e.g. symmetry, sparsity, positive definiteness, and forcing B_{k+1} to satisfy the secant equation

$$B_{k+1} s_k = y_k$$

with $s_k = x_{k+1} - x_k$, $y_k = \nabla f_{k+1} - \nabla f_k$. For further details on the l.c.s.u. idea the reader is referred to Dennis and Schnabel (1979).

For small dense problems the BFGS update developed independently by Broyden (1970), Fletcher (1970), Goldfarb (1970), and Shanno (1970),

$$B_{k+1} = B_k + \frac{y_k y_k^T}{y_k^T s_k} - \frac{B_k s_k s_k^T B_k}{s_k^T B_k s_k}$$

has been found to be the best among the class of l.c.s.u. that preserve symmetry and positive definiteness. However, for larger problems with sparse Hessians, the situation is less clear. Recently, a considerable amount of work has gone into extending the known dense updates to

preserve sparsity using the least-change secant update framework (Marwil 1978; Toint 1977,1978,1979,1981; Shanno 1981; Dennis and Schnabel 1979). The resulting updates preserve symmetry, sparsity, and satisfy the secant equation. However, they do not necessarily maintain positive definiteness, and they exhibit rather unsatisfactory performance in practice. An interesting different approach is developed in Griewank and Toint (1982a,b,c, 1983). Thus, a major problem in this area is how to generate sparse symmetric positive-definite secant updates that perform well in practice.

In this report, we will point out an approach to derive a family of sparse symmetric positive-definite secant updates. The motivation for this work is based on the following derivation of the BFGS update by Dennis and Schnabel (1981):

Assuming $B_c = L_c L_c^T$ is the current symmetric positive-definite approximation to the Hessian of f , obtain $B_+ = J_+ J_+^T$ as follows:

(1) For arbitrary $v \in \mathbf{R}^n$, solve for

$$J_+ = \operatorname{argmin} \|J - L_c\|_F \quad \text{s.t.} \quad Jv = y.$$

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

The solution J_+ is the Broyden update (Broyden 1965) of L_c sending $v = \frac{\sqrt{y^T s}}{|L_c^T s|} L_c^T s$ to y . Dennis and Schnabel (1981) prove that $J_+ J_+^T$ is exactly the BFGS update of $B_c = L_c L_c^T$. From $B_+ = J_+ J_+^T$, we can get the Cholesky factors of B_+ in $O(n^2)$ operations by forming the LQ factorization of J_+ without ever forming B_+ (Goldfarb 1976), since

$$B_+ = J_+ J_+^T = L_+ Q_+ Q_+^T L_+^T = L_+ L_+^T.$$

Note that what we really want all along is the Cholesky factorization of B_+ , not B_+ itself. Thus it seems reasonable to update L_c by a sparse Broyden or Schubert formula (Broyden 1971, Dennis and Schnabel 1979, Marwil 1979, Schubert 1970) to get L_+ directly using the l.c.s.u. idea as in Dennis and Marwil (1982). This way we can ensure that the resulting $B_+ = L_+ L_+^T$ is positive definite and symmetric, and we can also preserve the sparsity structure of L_c , if there is any. In Section 2, we will consider some instances of this updating scheme. Section 3 outlines our test algorithm for the minimization problem together with the new update. In Section 4, we will discuss some of the computational results. Finally, Section 5 is a brief look at some possible future work.

2. The Update Method

Let $Q(z_1, z_2)$ denote $\{M \in \mathbb{R}^{n \times n} : Mz_2 = z_1 \text{ for } z_1, z_2 \in \mathbb{R}^n\}$. Let \mathbf{L} denote the space of lower triangular matrices with some fixed sparsity pattern chosen from the sparsity of the Hessian as in George and Liu (1981).

An interesting approach to the problem of finding a sparse symmetric positive-definite update would be to solve the following problem:

Problem 1. Given $y, s \in \mathbb{R}^n$ such that $y^T s > 0$, find

$$L_+ = \operatorname{argmin} \|L - L_c\|_F \text{ s.t. } L \in \mathbf{L} \text{ and } LL^T \in Q(y, s).$$

At the moment, a computationally viable solution to the problem is not obvious (see Greenstadt (1983)). Hence we seek a related but "easier" problem by sparsifying the BFGS derivation of Section 1. The following notation will be very useful:

$P_X(\cdot)$ represents the orthogonal projection of (\cdot) onto X in the Frobenius norm;

z_j denotes the vector z with the sparsity of the j^{th} row of L_c ;

$(z_j)_i$ is the i^{th} component of z_j ;

z^j is the vector z with the sparsity of the j^{th} column of L_c ;

$(z^T z^j)^+$ is the pseudo-inverse of $z^T z^j$;

and

e_j is the j^{th} unit vector.

If we try to modify the BFGS derivation in the most straightforward way, then we run into apparent difficulty as follows:

(1) For arbitrary $v \in \mathbb{R}^n$,

$$L_+ = \operatorname{argmin} \|L - L_c\|_F \text{ s.t. } L \in \mathcal{L} \cap Q(y, v)$$

is solved by the appropriate sparse Broyden update

$$L_+ = L_c + \sum_{i=1}^n (v_i^T v_i)^+ e_i^T (y - L_c v) e_i v_i^T,$$

(if (1) has a solution -- more on this later.)

(2) Solve for v such that $v = L_+^T s$. But this yields the rather formidable system

$$v = L_c^T s + \sum_{i=1}^n (v_i^T v_i)^+ e_i^T (y - L_c v) s_i v_i$$

to solve for v .

Instead of trying to solve for v , we will turn the problem around and try to incorporate $v = L_+^T s$ into the variational problem whose

solution defines L_+ . This leads to the following problem:

Problem 2. Given $v \neq 0$, $y, s \in \mathbb{R}^n$ such that $v^T v = y^T s$, find

$$L_+ = \operatorname{argmin} \|L - L_c\|_F \text{ s.t. } L \in Q(y, v) \cap \mathbf{L} \cap Q(v, s)^T,$$

where $Q(v, s)^T$ is the set of transposes of matrices in $Q(v, s)$.

The remainder of this section is devoted to the presentation of results on the solution to Problem 2. In particular, $v^T v = y^T s$ is shown to be necessary for feasibility, although it is quite unlikely to be sufficient. In the event that Problem 2 is not feasible, i.e. $Q(y, v) \cap \mathbf{L} \cap Q(v, s)^T = \emptyset$, we provide a generalized inverse type solution.

Theorem 2.1. If $\nabla^2 f(x)$ is symmetric, positive definite and has the same sparsity pattern for every $x \in [x_c, x_+]$; and if every symmetric positive-definite matrix with that same sparsity pattern has a Cholesky factor in \mathbf{L} , then there exists some $v \in \mathbb{R}^n$ such that Problem 2 has a solution. If $v \in \mathbb{R}^n$ and $Q(y, v) \cap Q(v, s)^T \neq \emptyset$, then $y^T s = v^T v \geq 0$, with equality only for $y=0$.

Proof: The proof is accomplished by drawing slightly different conclusions from standard arguments. We write

$$y = \left[\int_0^1 \nabla^2 f(x_c + ts) dt \right] s \equiv Bs,$$

where B is a symmetric positive-definite matrix with the sparsity of the Hessian. Thus by hypothesis, for some $L \in \mathbf{L}$, $B = LL^T$. Set $v = L^T s$, and note that $L \in Q(y, v)$ with $v=0$ only if $y=0$ and

$$y^T s = (LL^T s)^T s = (L^T s)^T (L^T s) = v^T v \geq 0.$$

Thus L is a feasible point for the Problem 2 corresponding to this v , and by standard arguments, feasibility is enough to ensure a solution.

If the reader is unfamiliar with such existence results, then we give the explicit solution in the next theorem.

Now to see the necessity of the condition that $v^T v = y^T s \geq 0$ for feasibility, let $J \in Q(y, v) \cap Q(v, s)^T$. Then,

$$0 \leq v^T v = (J^{-1} y)^T (J^T s) = y^T s.$$

If $v^T v = 0$, then $v = 0$, so $y = Jv = 0 = J^{-T} v = s$.

Short of the impractical construction of the proof, we don't know how to find a v for which Problem 2 is feasible. Our next theorem, a corollary of results in Dennis and Schnabel (1979), gives a formula for $L_+ \in L$ which solves Problem 2 whenever it has a solution and when it doesn't have a real solution, the formula gives a generalized solution.

Theorem 2.2. Let $P \in \mathbb{R}^{n \times n}$ be the matrix whose j th column is given by

$$P e_j = \left[\frac{v^T v_j}{v^T v} \right] e_j - \sum_{i=1}^j (s^T s^i)^+ \left[\frac{(v_j)_i v_i s_j}{v^T v} \right] s^i, \quad (2.1)$$

and let w be any solution to the least squares problem

$$\min_{w \in \mathbb{R}^n} \| Pw - (y - P_{\mathbf{A}}(L_c)v) \|_2^2,$$

where

$$P_{\mathbf{A}}(L_c) = L_c + \sum_{i=1}^n (s^T s^i)^+ e_i^T (v - L_c^T s) s^i e_i^T.$$

Then in the Frobenius norm,

$$L_+ = L_c + \sum_{i=1}^n \left\{ \frac{v_i}{v^T v} w^i + (s^T s^i)^+ \left[e_i^T (v - L_c^T s) - \frac{v_i}{v^T v} s^T w^i \right] s^i \right\} e_i^T, \quad (2.2)$$

is an element of L closest to $Q(v,s)^T$. Among these closest points, it is also a closest point to $Q(y,v)$. Among all such points, it is the unique closest point to L_c . Thus, if Problem 2 is feasible, then L_+ is its unique solution.

Proof: It will be convenient to establish some further notation. We will always use closest or nearest to mean in the Frobenius norm. Let

$$A = M(L^T, Q(v,s))^T = \{L \in L : L^T \text{ is a nearest point to } Q(v,s)\}.$$

It is shown in Dennis and Schnabel (1979) that for A_1, A_2 affine, $M(A_1, A_2)$ is affine and it is $A_1 \cap A_2$, if the intersection is nonempty. Thus, A is affine and its parallel subspace is $S = [L^T \cap Q(0,s)]^T$.

From Theorem 4.5 in Dennis and Schnabel (1979),

$$P_S \left(\frac{wv^T}{v^T v} \right) = \left[P_{L^T} \left(\frac{vw^T}{v^T v} \right) + \sum_{i=1}^n (s^T s^i)^+ e_i^T (-P_{L^T} \left(\frac{vw^T}{v^T v} \right) s) e_i (s^i)^T \right]^T,$$

where $P_{L^T} \left(\frac{vw^T}{v^T v} \right) = \sum_{i=1}^n \frac{v_i}{v^T v} e_i (w^i)^T$. Hence,

$$\begin{aligned} P_S \left(\frac{wv^T}{v^T v} \right) &= \sum_{i=1}^n \frac{v_i}{v^T v} w^i e_i^T - \sum_{i=1}^n (s^T s^i)^+ e_i^T \left[\sum_{k=1}^n \frac{v_k}{v^T v} e_k (s^T w^k) \right] s^i e_i^T \\ &= \sum_{i=1}^n \frac{v_i}{v^T v} w^i e_i^T - \sum_{i=1}^n (s^T s^i)^+ \frac{v_i}{v^T v} (s^T w^i) s^i e_i^T. \end{aligned}$$

Thus,

$$P_A(L_c) = L_c + \sum_{i=1}^n (s^T s^i)^+ e_i^T (v - L_c^T s) s^i e_i^T.$$

Also from Theorem 3.2 in Dennis and Schnabel (1979), we know that

$$L_+ = P_A(L_c) + P_S \left(\frac{wv^T}{v^T v} \right), \quad (2.3)$$

where w is any solution to the least squares problem

$$\min_{w \in \mathbb{R}^n} \|Pw - (y - P_{\mathbf{A}}(L_c)v)\|_2^2,$$

with the j^{th} column of \mathbf{P} given by

$$Pe_j = P_{\mathbf{S}} \left(\frac{e_j v^T}{v^T v} \right) \quad \text{for } j = 1, 2, \dots, n. \quad (2.4)$$

It is straightforward to show this to be (2.1), but we will give the proof since some facts about projectors are used. First note that once we have done so, the proof of the theorem is complete because (2.2) can be obtained by substituting the expressions for the projections into (2.3).

$$\text{Now } P_{\mathbf{L}} \left(\frac{ve^T}{v^T v} \right) = \left[\frac{v e^T}{v^T v} \right].$$

Hence,

$$\begin{aligned} P_{\mathbf{S}} \left(\frac{e_j v^T}{v^T v} \right) &= \left[P_{\mathbf{S}}^T \left(P_{\mathbf{L}} \left(\frac{ve^T}{v^T v} \right) \right) \right]^T \\ &= \left[P_{\mathbf{L}} \left(\frac{ve^T}{v^T v} \right) + \sum_{i=1}^n (s^T s^i)^+ e_i^T \left(-P_{\mathbf{L}} \left(\frac{ve^T}{v^T v} \right) s \right) e_i (s^i)^T \right]^T \\ &= \left[\frac{v e^T}{v^T v} - \sum_{i=1}^n (s^T s^i)^+ \left[\frac{e_i^T v e^T s}{v^T v} \right] e_i (s^i)^T \right]^T. \end{aligned}$$

Consequently by (2.4), the j^{th} column of \mathbf{P} is

$$\begin{aligned} Pe_j &= \left[\frac{v^T v e_j}{v^T v} \right] e_j - \sum_{i=1}^n (s^T s^i)^+ \left[\frac{(v \cdot)_i v \cdot s \cdot j}{v^T v} \right] s^i \\ &= \left[\frac{v^T v e_j}{v^T v} \right] e_j - \sum_{i=1}^j (s^T s^i)^+ \left[\frac{(v \cdot)_i v \cdot s \cdot j}{v^T v} \right] s^i, \end{aligned}$$

because v_j is zero in every coordinate past the j^{th} . This completes the proof.

If Problem 2 is not feasible, then Theorem 2.2 gave a solution to the generalized problem

$$L_+ = \operatorname{argmin} \|L - L_c\|_F \text{ s.t. } L \in \mathbf{M}(\mathbf{M}(L, Q(v, s)^T), Q(y, v)).$$

We could have chosen to solve another generalization of Problem 2:

$$L_+ = \operatorname{argmin} \|L - L_c\|_F \text{ s.t. } L \in \mathbf{M}(\mathbf{M}(L, Q(y, v)), Q(v, s)^T).$$

The solution to this problem can be obtained using the same principles as in the proof of Theorem 2.2.

Hence, if we have some reasonable choice rule for v , $L_+ L_+^T$ with L_+ given by (2.2) would give a sparse symmetric positive-definite update of $B_c = L_c L_c^T$.

3. Algorithm

In this section, we will outline our test algorithm for the minimization problem using our updating procedure.

Given x_0, L_0 . For $k = 0, 1, 2, \dots$

- (1) Compute $f(x_k), \nabla f(x_k)$ and test for convergence.
- (2) Calculate p_k so that $L_k L_k^T p_k = -\nabla f(x_k)$.
- (3) Calculate λ_k satisfying

$$f(x_k + \lambda_k p_k) \leq f(x_k) + 10^{-4} \lambda_k \nabla f_k^T p_k$$

- (4) Set $x_{k+1} = x_k + \lambda_k p_k$, $s = x_{k+1} - x_k$, $y = \nabla f_{k+1} - \nabla f_k$.
- (5) Use some choice rule to pick a v . (More on this later.)
- (6) Form the right-hand side of the least squares problem:

$$y - P_{\mathbf{A}}(L_k)v = y - L_k v - \sum_{i=1}^n (s^T s^i)^+ e_i^T (v - L_k^T s) v_i s^i.$$

(7) Accumulate \mathbf{P} column by column using (2.1).

(8) Solve the least squares problem for w :

$$Pw = y - P_{\mathbf{A}}(L_k)v$$

(9) Update L_k to get L_{k+1} using (2.2).

Some remarks should be made about steps (5) and (8).

Remark 1. For a given choice of v the update L_+ only solves Problem 2 provided that $\mathbf{A} \cap Q(y, v)$ is nonempty, i.e., Problem 2 is feasible. Moreover, since we trust the l.c.s.u. idea, we certainly hope that the vector v that we pick will give us an L_+ which is not too far from L_c . For example, if we ignore sparsity in the lower triangular factors, then we might want L_+ to satisfy

$$\|L_+ - L_c\|_F \leq \|L_{\text{BFGS}} - L_c\|_F, \quad (3.1)$$

where L_{BFGS} is the lower triangular matrix obtained from the BFGS Cholesky update procedure. There is no obvious way to choose v which satisfies both these conditions. Since $v = \frac{\sqrt{y^T s}}{|L_c^T s|} L_c^T s$ gives the BFGS update when used with the BFGS procedure, it would seem reasonable to test our updating procedure using this v . However, we do take sparsity into account, at least to require L_+ to be lower triangular, so this choice for v cannot guarantee that $\mathbf{A} \cap Q(y, v)$ be nonempty, and in fact, it may not give an L_+ that satisfies (3.1).

If \mathbf{L} is the subspace of lower triangular matrices without any additional sparsity, then the other choice of v for which both

$\mathbf{A} \cap \mathbf{Q}(y, v) \neq \emptyset$ and (3.1) are satisfied is $v = L_{\text{BFGS}}^T s$. The truth of this statement is obvious since L_{BFGS} itself belongs to $\mathbf{A} \cap \mathbf{Q}(y, v)$. We want to point out that this choice for v is not a practical one since it requires that we know L_{BFGS} . However, since we are trying to test the usefulness of applying l.c.s.u. to the factor, this v is interesting for our purposes.

Remark 2. The solution of the least squares problem in step 8 is important in our procedure. In the testing, we used the SVD to solve this problem and found that the matrix \mathbf{P} is always ill-conditioned with condition number ranging between 10^9 and 10^{18} . In all cases tested, \mathbf{P} usually had $n-1$ "nice" singular values and one relatively bad one. We used the following criteria to determine the numerical rank of \mathbf{P} . Let σ_i denote the i^{th} singular value of \mathbf{P} , then

$$\sigma_i = 0 \quad \text{if} \quad \sigma_i < \sqrt{\text{macheps}} \|\mathbf{P}\|_{\infty}$$

where $\text{macheps} \approx 10^{-18}$ is the machine epsilon of the arithmetic used. Though this seems reasonable, we have observed that in some cases our minimization algorithm performs better without it. This probably indicates that the size of the residual is more important than the well-posedness of the least-squares problem. When some σ_i is set to 0, (3.1) is sometimes not satisfied even though we know that theoretically for $v = L_{\text{BFGS}}^T s$ this could never happen.

4. Discussion of Computational Results

The following updates were tested in the algorithm of Section 3:

- (A) L_+ given by the BFGS Cholesky update,
- (B) L_+ given by (2.2) with $v = L_{\text{BFGS}}^T s$

$$(C) \quad L_+ \text{ given by (2.2) with } v = \frac{\sqrt{y^T s}}{|L_c^T s|} L_c^T s$$

In general, (C) gave very poor performance for the reasons that we have already discussed; so we will shift our attention to (A) and (B). The test problems used were the 18 problems documented in More' et al (1981). Moreover, to test for robustness of the algorithms, we followed the idea of More' et al in starting at $x_0 = x_s$, $10x_s$, and $100x_s$ respectively, where x_s is the standard start for the test problem. This gave us a total of 54 test cases.

All the runs were made in 18-digit arithmetic without any rescaling of the problems and with a default maximum stepsize allowed in the line search $STEPMX = \max\{10^3, 10^3 \|x_0\|_2\}$. Also, convergence was assumed when either

$$\max_i \left\{ \frac{|x_i^k - x_i^{k-1}|}{\max\{|x_i^k|, 1\}} \right\} \leq STPTOL = 10^{-5},$$

or

$$\max_i \left\{ \frac{|\nabla f(x^k)_i| \max\{|x_i^k|, 1\}}{\max\{|f(x^k)|, 1\}} \right\} \leq GRDTOL = 10^{-5}.$$

In a lot of cases, (B) is certainly competitive with (A). However the following observations were made in the cases where (B) performs poorly:

- (1) Drastic changes in the Newton step occur frequently.
- (2) (B) is not robust in the sense that it performs very poorly far away from the solution, e.g. when $x_0 = 100x_s$.

- (3) The steps generated by (B) usually do not lead to a decrease in function value as large as does the BFGS update. Even if we add a β -condition to our line search, i.e., $\nabla f_{k+1}^T p_k \geq \beta \nabla f_k^T p_k$, the same behavior persists no matter how accurate the line search is chosen to be, e.g. for $\beta=0.01$.
- (4) If we switch from (B) to (A) using whatever information the algorithm has accumulated up to that point, then the BFGS update always seems to be able to converge to the solution quite rapidly from what is supposed to be "bad" information.
- (5) Let $\text{DIFF} = \|L_{\text{BFGS}} - L_c\|_F^2 - \|L_+ - L_c\|_F^2$. We observe that in the case where (B) is doing poorly, DIFF is always relatively large; when (B) performs better or as well as the BFGS update, DIFF is always relatively small. Hence (B) is only good when L_+ is near L_{BFGS} . Does this say that doing a least change secant update of L_c is not sensible? We don't really know since it only tells us that our procedure does not give a reasonable update for the choice of $v = L_{\text{BFGS}}^T s$. The following is a possible explanation of this behavior. Since we are at L_c , we need to compute L_{BFGS} to get $v = L_{\text{BFGS}}^T s$. Hence in the case where L_{BFGS} is far away from L_c , the information that we use to obtain L_+ will not reflect the current information contained in L_c . It would seem more reasonable to have a choice rule that used information at the current step to determine a v that satisfies both (3.1) and $A \cap Q(y, v) \neq \emptyset$.

Although this discussion is based on extensive computational results, we feel that there is little point to including actual numbers of function and gradient evaluations here. Our experiments are

continuing and it is our plan to publish all test results together, if at all.

5. Conclusions

We would really like to be able to solve Problem 1, but we considered the apparently more tractable Problem 2, and we have developed what should be a reasonable way to update a sparse Cholesky factorization by updating L_c to get L_+ directly. Unfortunately, the whole procedure is based on the choice of the vector v . It is reasonable to conjecture that if our idea has merit, then the obstacle is the determination of v as mentioned at the end of the last section. This is somewhat similar to the problem of making a useful partially separable decomposition in the Griewank-Toint approach (Griewank and Toint 1983). We also would need to find a cheap way to solve the least squares problem in Step 8 of the algorithm to make our algorithm useful. There are other ways to simplify Problem 1 that may turn out to be more useful; for example, we might linearize the constraint $L_+L_+^T s = y$ in L_+ . (See Greenstadt, 1983.)

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