ON SOLVING LARGE-SCALE LIMITED-MEMORY QUASI-NEWTON EQUATIONS

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Abstract. We consider the problem of solving linear systems of equations with limited-memory members of the restricted Broyden class and symmetric rank-one matrices. In this paper, we present various methods for solving these linear systems, and propose a new approach based on a practical implementation of the compact representation for the inverse of these limited-memory matrices. Using the proposed approach has an additional benefit: The condition number of the system matrix can be computed efficiently. Numerical results suggest that the proposed method compares favorably in speed and accuracy to other algorithms and is competitive to methods available to only the Broyden-Fletcher-Goldfarb-Shanno update and the symmetric rank-one update.

Limited-memory quasi-Newton methods, compact representation, restricted Broyden class of updates, symmetric rank-one update, Broyden-Fletcher-Goldfarb-Shanno update, Davidon-Fletcher-Powell update, Sherman-Morrison-Woodbury formula

1. Introduction

We consider linear systems of the following form:

$$B_{k+1}r = z, \tag{1}$$

where $r, z \in \Re^n$ and $B_{k+1} \in \Re^{n\times n}$ is a limited-memory quasi-Newton matrix obtained from applying $k+1$ restricted Broyden class updates or symmetric rank-one (SR1) updates to an initial matrix B_0. We assume n is large, and thus, explicitly forming and storing B_{k+1} is impractical or impossible; moreover, in this setting, we assume limited-memory quasi-Newton matrices are used so that $k \ll n$. In this paper, we propose a compact formulation of B_{k+1}^{-1} that can be used to solve (1).

Problems such as (1) arise in quasi-Newton line-search and trust-region methods for large-scale optimization (see, e.g., [**?**, **?**, **?**, **?**]). Assuming $f : \Re^n \to \Re$ is continuously differentiable, traditional quasi-Newton methods for minimization generate a sequence of iterates $\{x_k\}$ such that f is strictly decreasing on this sequence. Moreover, at each iteration, the most-recently computed iterate x_{k+1} is used to update the quasi-Newton matrix by defining a new *quasi-Newton pair* (s_k, y_k) given by

$$s_k \triangleq x_{k+1} - x_k \quad \text{and} \quad y_k \triangleq \nabla f(x_{k+1}) - f(x_k).$$

In the case of the restricted Broyden class and the SR1 updates, B_{k+1} is updated as follows:

$$B_{k+1} = B_k - \frac{1}{s_k^T B_k s_k} B_k s_k s_k^T B_k + \frac{1}{y_k^T s_k} y_k y_k^T + \phi(s_k^T B_k s_k) w_k w_k^T, \tag{2}$$

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with

$$w_k = \frac{y_k}{y_k^T s_k} - \frac{B_k s_k}{s_k^T B_k s_k},$$

where $\phi \in [0,1]$ for the restricted Broyden class of updates and $\phi = y_k^T s_k / (y_k^T s_k - s_k^T B_k s_k$ for the SR1 update (see, e.g., [**?**, **?**, **?**]). The most well-known members of the restricted Broyden class are the Broyden-Fletcher-Goldfarb-Shanno (BFGS) update and Davidon-Fletcher-Powell (DFP) update that are obtained by setting $\phi = 0$ and $\phi = 1$, respectively, in (2). In the case of a quasi-Newton line-search method, at each iteration the quasi-Newton step p_k is computed from solving

$$B_{k+1} p_k = -\nabla f(x_k),$$

which is of the form (1) with $z \triangleq -\nabla f(x_k)$ and $r \triangleq p_k$. Systems of the form (1) also appear in quasi-Newton trust-region methods. At each iteration of these methods an approximate solution to the trust-region subproblem must be computed. The two-norm trust-region subproblem is given by

$$\underset{p \in \Re^n}{\text{minimize}} \;\; \mathcal{Q}(p) \triangleq \nabla f(x_k)^T p + \frac{1}{2} p^T B_{k+1} p \quad \text{subject to} \quad \|p\|_2 \leq \delta_k, \tag{3}$$

where δ_k is the so-called *trust-region radius*. When the solution to the subproblem (3) lies in the strict interior of the trust region, the global solution of the trust-region subproblem is given by p_k^*, where p_k^* satisfies (1) with $z \triangleq -\nabla f(x_k)$ and $r \triangleq p_k^*$. Moreover, when B_{k+1} is a member of the Broyden convex class and $\|B_{k+1}^{-1} \nabla f(x_k)\| \leq \delta_k$ then the global solution of the trust-region subproblem lies in the strict interior, i.e., p_k^* satisfies $B_{k+1}^{-1} p_k^* = -\nabla f(x_k)$. It should be noted systems of the form (1) also arise in preconditioning iterative solvers. For these, we refer the reader to [**?**, **?**].

When n is large, solving systems of the form (1) can be done efficiently in the case of the BFGS update ($\phi = 0$) using the well-known two-loop recursion [**?**]. However, there is no known corresponding recursion method for other updates of the Broyden class; in fact, for this reason many researchers prefer the BFGS update. In this paper we present various methods for solving linear systems of equations with limited-memory quasi-Newton matrices. The main contribution of this paper is a new approach by formulating a compact representation for the inverse of any member of the restricted Broyden class as well as SR1 matrices. In addition, we provide a practical algorithm for computing this formulation in order to solve linear systems such as (1). This compact formulation for the inverse of these matrices is based on ideas found in [**?**], where a compact formulation for the Broyden class of matrices is presented. A benefit of our proposed approach is the ability to calculate the eigenvalues of the limited-memory matrix, and hence, the condition number of the linear system.

This paper is organized in five sections. In Section 2, we review limited-memory quasi-Newton matrices and a variety of methods for solving linear systems with a limited-memory quasi-Newton matrix. In Section 3, we review the compact formulation for matrices obtained using the Broyden class of updates. The compact formulation for the inverse of these matrices is presented in Section 4. Also in this section we provide a practical implementation for solving systems of the form (1). Relationships between compact formulations are also considered. At the end of Section 4, we discuss how to compute the condition number of the linear system

being solved and how to obtain additional computational savings when a new quasi-Newton pair is computed. Finally, in Section 5 numerical experiments demonstrate the competitiveness of this approach.

2. Background

Given an initial matrix B_0, the Broyden class of updates generate a sequence of matrices $\{B_{k+1}\}$ given by

$$B_{k+1} = B_k - \frac{1}{s_k^T B_k s_k} B_k s_k s_k^T B_k + \frac{1}{y_k^T s_k} y_k y_k^T + \phi(s_k^T B_k s_k) w_k w_k^T, \tag{4}$$

with

$$w_k = \frac{y_k}{y_k^T s_k} - \frac{B_k s_k}{s_k^T B_k s_k},$$

where ϕ is a scalar that may depend on y and Bs. The Broyden class of updates is a class of symmetric rank-one or rank-two updates, depending on the choice of ϕ. In practice, B_0 can be any symmetric matrix but is often taken to be a constant multiple of the identity. The *restricted* (or *convex*) Broyden class refers to updates when $\phi \in [0, 1]$. Provided B_0 is a symmetric positive-definite matrix and $y_i^T s_i > 0$ for each i, the restricted Broyden class of updates generates a sequence of symmetric positive-definite matrices.

The most widely-used member of restricted Broyden class is the Broyden-Fletcher-Goldfarb-Shanno (BFGS) update, which is obtained by setting $\phi = 0$. In this case, (4) simplifies to

$$B_{k+1} = B_k - \frac{1}{s_k^T B_k s_k} B_k s_k s_k^T B_k + \frac{1}{y_k^T s_k} y_k y_k^T. \tag{5}$$

The inverse of the BFGS matrix B_{k+1} is given by

$$B_{k+1}^{-1} = \left(I - \frac{s_k y_k^T}{y_k^T s_k}\right) B_k^{-1} \left(I - \frac{y_k s_k^T}{y_k^T s_k}\right) + \frac{s_k s_k^T}{y_k^T s_k},$$

which can be written recursively as

$$\begin{aligned} B_{k+1}^{-1} = (V_k^T \cdots V_0^T) B_0^{-1} (V_0 \cdots V_k) &+ \frac{1}{y_0^T s_0} (V_k^T \cdots V_1^T) s_0 s_0^T (V_1 \cdots V_k) \\ &+ \frac{1}{y_1^T s_1} (V_k^T \cdots V_2^T) s_1 s_1^T (V_2 \cdots V_k) \\ &+ \cdots \\ &+ \frac{1}{y_k^T s_k} s_k s_k^T, \end{aligned} \tag{6}$$

where $V_i = I - \frac{1}{y_i^T s_i} y_i s_i^T$ (see, e.g., [**?**]).

When B_{k+1} is a BFGS matrix, solving linear systems of the form $B_{k+1} r = z$ can be done using the well-known "two-loop recursion" method [**?**]:

Algorithm 1: Two-loop recursion to compute $r = B_k^{-1} z$ when B_k is a BFGS matrix.

$q \leftarrow z$;
for $i = k - 1, \ldots, 0$
  $\alpha_i \leftarrow (s_i^T q)/(y_i^T s_i)$;

$q \leftarrow q - \alpha_i y_i$;
end
$r \leftarrow B_0^{-1} q$;
for $i = 0, \ldots, k-1$
$\beta \leftarrow (y_i^T r)/(y_i^T s_i)$;
$r \leftarrow r + (\alpha_i - \beta) s_i$:
end

Assuming that the inner products $y_i^T s_i$ can be precomputed and B_0 is a scalar multiple of the identity matrix, then the total operation count for Algorithm 1 is $7nk + n$ flops and $2k$ vector inner products.

Other named members of the restricted Broyden class include the the Davidon-Fletcher-Powell (DFP) update, which occurs when $\phi = 1$;

$$B_{k+1} = \left(I - \frac{y_k s_k^T}{y_k^T s_k}\right) B_k \left(I - \frac{s_k y_k^T}{y_k^T s_k}\right) + \frac{y_k y_k^T}{y_k^T s_k}.$$

The DFP update has the same form as the inverse of the BFGS update but with s_k and y_k interchanged; because of this, the BFGS and DFP updates are often referred to as *duals* (or *complements*) of each other [**?**].

The *symmetric rank-one* (SR1) update is obtained by setting $\phi = y_k^T s_k/(y_k^T s_k - s_k^T B_k s_k$; in this case,

$$B_{k+1} = B_k + \frac{1}{s_k^T (y_k - B_k s_k)} (y_k - B_k s_k)(y_k - B_k s_k)^T. \tag{7}$$

The SR1 update is a member of the Broyden class but not the restricted Broyden class. This update exhibits hereditary symmetric but not positive definiteness. In fact, the SR1 update is often used when it is desirable to approximate negative curvature in the underlying function f.

The SR1 update is remarkable in that it is self-dual: initializing with B_0^{-1} instead of B_0, replacing s_k with y_k, and replacing y_k with s_k for all k in (7) results in B_{k+1}^{-1} (see e.g., [**?**]). Thus, $r = B_{k+1}^{-1} z$ can be computed using recursion (see Algorithm 2). The first loop of Algorithm 2 computes $p_i \triangleq s_i - H_i y_i$ for $i = 0, \ldots k$; the final line of Algorithm 2 computes $r = B_{k+1}^{-1} z = B_0^{-1} z + \sum_{i=0}^{k} (p_i^T z)/(p_i^T y_i) p_i$.

Algorithm 2: Computing $r = B_{k+1}^{-1} z$, when B_{k+1} is an SR1 matrix.
for $i = 0, \ldots k$
$p_i = s_i - H_0 y_i$;
for $j = 0 \ldots i-1$
$p_i = p_i - ((p_j^T y_i)/(p_j^T y_j)) p_j$;
end
end
$r \leftarrow H_0 z + \sum_{i=0}^{k} ((p_i^T z)/(p_i^T y_i)) p_i$;

Thus, in the case of SR1 updates, solving linear systems with SR1 matrices can be performed using vector inner products; the cost for solving linear systems with an SR1 matrix is the same as the cost of computing products with an SR1 matrix, which can be done with $(k^2 + 5k + 2)/2$ vector inner products and $(3k^2 +$

$21k + 14)n/2$ floating point operations. It should be noted that unlike members of the restricted Broyden class, SR1 matrices can be indefinite, and in particular, numerically singular. Methods found in [**?**,**?**] can be used to compute the eigenvalues (and thus, the condition number) of SR1 matrices before performing linear solves to help avoid solving ill-conditioned systems.

In large-scale optimization, *limited-memory* versions of these updates are used to control storage requirements. In a limited-memory setting, only the most recent m updates are stored and used to update B_0. In practice, the value of m is small, i.e., less than ten (see e.g., [**?**]). (For more details on limited-memory quasi-Newton matrices and the Broyden convex class of matrices see, e.g., [**?**, **?**, **?**].)

2.1. **Solves with Broyden class.** Solves with members of the Broyden class of matrices when n is large must be done using recursion. Unfortunately, there is no corresponding "two-loop recursion" (Algorithm 1) for any member other than the BFGS update, giving the BFGS update an advantage over other members of this class of quasi-Newton matrices; moreover, no other member exhibits self-duality such as the SR1 update. As a result, linear solves with members of the Broyden class generated by updates other than the BFGS or SR1 update are done at more expense.

2.1.1. *Using the Sherman-Morrison-Woodbury formula.* One approach to perform linear solves with members of the Broyden convex class is to use the Sherman-Morrison-Woodbury (SMW) formula to update the inverse after each rank-one change. In the symmetric case, the SMW formula for a rank-one change is given by

$$(A + \alpha uu^T)^{-1} = A^{-1} - \frac{\alpha}{1 + \alpha u^T A^{-1} u} A^{-1} u u^T A^{-1}. \tag{8}$$

We now show how (8) can be used to compute the inverse of B_{k+1}. First, for $0 \leq j \leq k$, define

$$\begin{array}{rclcrcl} \alpha_{3j} & = & (y_j^T s_j)^{-1}, & & u_{3j} & = & y_j, \\ \alpha_{3j+1} & = & \phi(s_j^T B_j s_j), & & u_{3j+1} & = & \dfrac{y_j}{y_j^T s_j} - \dfrac{B_j s_j}{s_j^T B_j s_j}, \\ \alpha_{3j+2} & = & -(s_j^T B_j s_j)^{-1}, & & u_{3j+2} & = & B_j s_j, \end{array} \tag{9}$$

Letting

$$C_0 = B_0 \quad \text{and} \quad U_i = \alpha_i u_i u_i^T$$

for $0 \leq i \leq 3k$, we define the matrices

$$C_1 = C_0 + U_0, \quad C_2 = C_1 + U_1, \quad \ldots, \quad C_{3(k+1)} = C_{3(k+1)-1} + U_{3(k+1)-1}. \tag{10}$$

By construction, $C_{3(k+1)} = B_{k+1}$. It can be shown that each C_i is positive definite and so $u_i^T C_i^{-1} u_i > 0$ for each i. For the restricted Broyden class, α_{3j} and α_{3j+1}, $j = 0, \ldots, k$ are both strictly positive. Thus, the denominator in (8) is strictly positive for the rank-one changes associated the $3j$ and $3j + 1$, $j = 0, \ldots k$, and thus, the SMW formula is well-defined for these rank-one updates. Since $C_{3j+2} = B_j$ and B_j is positive definite, the rank one update associated with $j + 2$, $j = 0, \ldots k$, results in a positive definite matrix; in other words, (8) is well defined. Thus, solving the system $B_{k+1} r = z$ is equivalent to computing $r = C_{3(k+1)}^{-1} z$. Apply the SMW formula in (8) to obtain the inverse of C_{i+1} from C_i^{-1}, we obtain

$$C_{i+1}^{-1} z = C_i^{-1} z - \frac{\alpha_i}{1 + \alpha_i u_i^T C_i^{-1} u_i} C_i^{-1} u_i u_i^T C_i^{-1} z, \tag{11}$$

for $0 \leq i < 3(k+1)$. Recursively applying (11) to $C_i^{-1}z$, we obtain that

$$C_{i+1}^{-1}z = C_0^{-1}z - \sum_{j=0}^{i} \frac{\alpha_j}{1+\alpha_j u_j^T C_j^{-1} u_j} C_j^{-1} u_j u_j^T C_j^{-1} z, \tag{12}$$

and more importantly,

$$C_{3(k+1)}^{-1}z = C_0^{-1}z - \sum_{j=0}^{3(k+1)-1} \frac{\alpha_j}{1+\alpha_j u_j^T C_j^{-1} u_j} C_j^{-1} u_j u_j^T C_j^{-1} z. \tag{13}$$

Computing (13) can be simplified by defining the following two quantities:

$$\tau_j = \frac{\alpha_j}{1+\alpha_j u_j^T C_j^{-1} u_j} \quad \text{and} \quad p_j = C_j^{-1} u_j. \tag{14}$$

Substituting (14) into (13) yields

$$C_{3(k+1)}^{-1}z = C_0^{-1}z - \sum_{j=0}^{3(k+1)-1} \tau_j (p_j^T z) p_j, \tag{15}$$

where $\tau_j = \alpha_j(1+\alpha_j p_j^T u_j)^{-1}$. The advantage of representation is that computing $C_{3(k+1)}^{-1}z$ requires only vector inner products. Moreover, the vectors p_j can be computed by evaluating (12) at $z = u_j$ for $i = j-1$; that is,

$$p_j = C_j^{-1} u_j = C_0^{-1} u_j - \sum_{i=0}^{j-1} \tau_i (p_i^T u_j) p_i.$$

In Algorithm 3, we present the recursion to solve the linear system $B_{k+1}r = z$ using the SMW formula (see related methods in [**?**, **?**]). We assume B_0 is a an easily-invertible initial matrix. To compute products of the form $B_i s_i$ in Algorithm 3, we refer the reader to Appendix A.

Algorithm 3: Computing $r = B_{k+1}^{-1}z$**.**

$r \leftarrow C_0^{-1}z$;
for $j = 0, \ldots, 3(k+1)-1$
  if $\mod(j,3) = 0$
    $i \leftarrow j/3$;
    $u \leftarrow y_i$;
    $\alpha \leftarrow y_i^T s_i$;
  else if $\mod(j,3) = 1$
    $i \leftarrow (j-1)/3$;
    $u \leftarrow (y_i)/(y_i^T s_i) - (B_i s_i)/(s_i^T B_i s_i)$;
    $\alpha \leftarrow \phi(s_i^T B_i s_i)$;
  else
    $i \leftarrow (j-2)/3$;
    $u \leftarrow B_i s_i$;
    $\alpha \leftarrow -(s_i^T B_i s_i)^{-1}$;
  end
  $p_j \leftarrow C_0^{-1} u$;
  for $l = 0, \ldots, j$

$p_j \leftarrow p_j - \tau_l (p_l^T u) p_l$;
end
$\tau_j \leftarrow \alpha/(1 + \alpha p_j^T u)$;
$r \leftarrow r - \tau_j (p_j^T z) p_j$;
end

2.1.2. *Using a recursion formula.* Alternatively, linear solves with a general member of the Broyden class can be performed using the following recursion formula found in [**?**] for H_{k+1}, the inverse of B_{k+1}:

$$H_{k+1} = H_k + \frac{1}{s_k^T y_k} s_k s_k^T - \frac{1}{y_k^T H_k y_k} H_k y_k y_k^T H_k + \Phi_k (y_k^T H_k y_k) v_k v_k^T, \tag{16}$$

where

$$v_k = \frac{s_k}{y_k^T s_k} - \frac{H_k y_k}{y_k^T H_k y_k} \quad \text{and} \quad \Phi_k = \frac{(1-\phi)(y_k^T s_k)^2}{(1-\phi)(y_k^T s_k)^2 + \phi (y_k^T H_k y_k)(s_k^T B_k s_k)}, \tag{17}$$

and $H_k \triangleq B_k^{-1}$. Thus, the solution to $B_{k+1} r = z$ can be obtained from

$$\begin{aligned} B_{k+1}^{-1} z &= \left(H_0 z + \sum_{i=0}^{k} \frac{1}{s_i^T y_i} s_i s_i^T - \frac{1}{y_i^T H_i y_i} H_i y_i y_i^T H_i + \Phi_i (y_i^T H_i y_i) v_i^T v_i \right) z \\ &= H_0 z + \sum_{i=0}^{k} \frac{s_i^T z}{s_i^T y_i} s_i - \frac{y_k^T H_i z}{y_i^T H_i y_i} H_i y_i + \Phi_i (y_i^T H_i y_i)(v_i^T z) v_i. \end{aligned}$$

In Algorithm 4, we present how to compute the solution r explicitly. Products involving H_i are computed using an algorithm similar to Algorithm **??** and is presented in Appendix B.

Algorithm 4: Computing $r = H_{k+1} z$.
$r \leftarrow H_0 z$;
for $j = 0, \ldots, 3(k+1) - 1$
  if $\mod(j, 3) = 0$
    $i \leftarrow j/3$;
    $u \leftarrow s_i$;
    $\alpha \leftarrow y_i^T s_i$;
  else if $\mod(j, 3) = 1$
    $i \leftarrow (j-1)/3$;
    $u \leftarrow H_i y_i$;
    $\alpha \leftarrow -(y_i^T H_i y_i)^{-1}$;
  else
    $i \leftarrow (j-2)/3$;
    $u \leftarrow (s_i)/(y_i^T s_i) - (H_i y_i)/(y_i^T H_i y_i)$;
    $\Phi \leftarrow (1-\phi)(y_i^T s_i)^2 / \left((1-\phi)(y_i^T s_i)^2 + \phi (y_i^T H_i y_i)(s_i^T B_i s_i) \right)$;
    $\alpha \leftarrow \Phi (y_i^T H_i y_i)$;
  end
  $r \leftarrow r + \alpha (u^T z) u$;
end

3. Compact representation

In this section, we briefly review the compact representation of members of Broyden class of matrices.

Given $k+1$ update pairs of the form $\{(s_i, y_i)\}$, the *compact formulation* of B_{k+1} is given by

$$B_{k+1} = B_0 + \Psi_k M_k \Psi_k^T, \tag{18}$$

where M_k is a square matrix and $B_0 \in \Re^{n\times n}$ is an initial matrix, which is often taken to be a scalar multiple of the identity. (Note that the size of Ψ is not specified.) The compact formulation of members of the Broyden class of updates are defined in terms of

$$\begin{aligned} S_k &= [\ s_0 \ \ s_1 \ \ s_2 \ \ \cdots \ \ s_k\ ] \in \Re^{n\times(k+1)}, \\ Y_k &= [\ y_0 \ \ y_1 \ \ y_2 \ \ \cdots \ \ y_k\ ] \in \Re^{n\times(k+1)}, \end{aligned}$$

and the following decomposition of $S_k^T Y_k \in \Re^{(k+1)\times(k+1)}$:

$$S_k^T Y_k = L_k + D_k + R_k,$$

where L_k is strictly lower triangular, D_k is diagonal, and R_k is strictly upper triangular. Assuming all updates are well defined, Byrd, Nocedal, and Schnabel [**?**] show the compact representation for BFGS matrices ($\phi = 0$) is given by (18) where

$$\Psi_k = \begin{bmatrix} B_0 S_k & Y_k \end{bmatrix} \quad \text{and} \quad M_k = -\begin{bmatrix} S_k^T B_0 S_k & L_k \\ L_k^T & -D_k \end{bmatrix}^{-1}. \tag{19}$$

In the case of DFP updates ($\phi = 1$), the compact formulation is given by (18) with

$$\Psi_k = \begin{bmatrix} B_0 S_k & Y_k \end{bmatrix} \quad \text{and} \quad M_k = -\begin{bmatrix} S_k^T B_0 S_k + D_k & L_k + D_k \\ (L_k + D_k)^T & 0 \end{bmatrix}^{-1}. \tag{20}$$

(Details can be found in [**?**].)

In [**?**], Erway and Marcia generalize these results to all members of the restricted Broyden updates; it is shown that the compact formulation for any member of the restricted Broyden class is given by (18) with

$$\Psi_k = \begin{bmatrix} B_0 S_k & Y_k \end{bmatrix} \quad \text{and} \quad M_k = -\begin{bmatrix} S_k^T B_0 S_k - \phi\Lambda_k & (L_k - \phi\Lambda_k) \\ (L_k - \phi\Lambda_k)^T & -(D_k + \phi\Lambda_k) \end{bmatrix}^{-1}, \tag{21}$$

where

$$\Lambda_k = \underset{0\le i\le k}{\operatorname{diag}}\ (\lambda_i), \quad \text{where } \lambda_i = \frac{1}{-\dfrac{1-\phi}{s_i^T B_i s_i} - \dfrac{\phi}{s_i^T y_i}} \quad \text{for } 0 \le i \le k. \tag{22}$$

Note that this is truly a generalization since when $\phi = 0$ and $\phi = 1$, M_k in (21) simplifies to (19) and (20), respectively. In the case of members of the restricted Broyden class, $\Psi_k \in \Re^{n\times 2(k+1)}$ and $M_k \in \Re^{2(k+1)\times 2(k+1)}$.

Finally, the compact representation of SR1 matrices is given by

$$\Psi_k = Y_k - B_0 S_k \quad \text{and} \quad M_k = (D_k + L_k + L_k^T - S_k^T B_0 S_k)^{-1}, \tag{23}$$

where $\Psi_k \in \Re^{n\times(k+1)}$ and $M_k \in \Re^{(k+1)\times(k+1)}$ (see [**?**]).

In the limited-memory case, $k \ll n$, and thus, M_k is easily inverted.

4. Inverses

In some applications, being able to solve systems with limited-memory matrices is important. In this section, we present the compact formulation for the inverse of any member of the restricted Broyden class of matrices and for SR1 matrices. We then demonstrate how this compact formulation can be used to solve linear systems with these limited-memory matrices. Finally, we discuss computing the condition number of the linear system and potential computational savings when a new quasi-Newton pair is computed.

The main contribution to this paper is a formula for the compact formulation for any member of the restricted Broyden class. It should be noted that the compact formulation for the inverse of a BFGS matrix is already known (see [**?**]). We now derive a general expression for the compact representation of any member of the restricted Broyden class. To do this, we apply the Sherman-Morrison-Woodbury formula (see, e.g., [**?**]) to the compact representation of B_{k+1} found in (18):

$$B_{k+1}^{-1} = B_0^{-1} + B_0\Psi_k \left(-M_k^{-1} - \Psi_k^T B_0 \Psi_k\right)^{-1} \Psi_k^T B_0.$$

For quasi-Newton matrices it is conventional to let H_i denote the inverse of B_i for each i; using this notation, the inverse of B_{k+1}^{-1} is given by

$$H_{k+1} = H_0 + H_0\Psi_k \left(-M_k^{-1} - \Psi_k^T H_0 \Psi_k\right)^{-1} \Psi_k^T H_0. \tag{24}$$

Since $H_0\Psi_k = H_0[B_0S_k \;\; Y_k] = [S_k \;\; H_0Y_k]$, (24) can be written as

$$H_{k+1} = H_0 + [\; S_k \quad H_0Y_k \;](-M_k^{-1} - \Psi_k^T H_0 \Psi_k)^{-1} \begin{bmatrix} S_k^T \\ Y_k^T H_0 \end{bmatrix}. \tag{25}$$

Finally, (25) can be simplified using

$$\Psi_k^T H_0 \Psi_k = \begin{bmatrix} S_k^T B_0 S_k & S_k^T Y_k \\ Y_k^T S_k & Y_k^T H_0 Y_k \end{bmatrix}$$

to obtain

$$\begin{aligned}
(-M_k^{-1} - \Psi_k^T H_0 \Psi_k)^{-1} &= \left(\begin{bmatrix} S_k^T B_0 S_k - \phi\Lambda_k & (L_k - \phi\Lambda_k) \\ (L_k - \phi\Lambda_k)^T & -(D_k + \phi\Lambda_k) \end{bmatrix} - \begin{bmatrix} S_k^T B_0 S_k & S_k^T Y_k \\ Y_k^T S_k & Y_k^T H_0 Y_k \end{bmatrix} \right)^{-1} \\
&= \begin{bmatrix} -\phi\Lambda_k & L_k - \phi\Lambda_k - S_k^T Y_k \\ L_k^T - \phi\Lambda_k - Y_k^T S_k & -D_k - \phi\Lambda_k - Y_k^T H_0 Y_k \end{bmatrix}^{-1} \\
&= \begin{bmatrix} -\phi\Lambda_k & -R_k - D_k - \phi\Lambda_k \\ -R_k^T - D_k - \phi\Lambda_k & -D_k - \phi\Lambda_k - Y_k^T H_0 Y_k \end{bmatrix}^{-1}.
\end{aligned}$$

In other words, the compact formulation for the inverse of a member of the restricted Broyden class is given by

$$H_{k+1} = H_0 + \tilde{\Psi}_k \tilde{M}_k \tilde{\Psi}_k^T \quad \text{where} \quad \tilde{\Psi}_k \triangleq [S_k \;\; H_0Y_k], \tag{26}$$

and

$$\tilde{M}_k \triangleq \begin{bmatrix} -\phi\Lambda_k & -R_k - D_k - \phi\Lambda_k \\ -R_k^T - D_k - \phi\Lambda_k & -D_k - \phi\Lambda_k - Y_k^T H_0 Y_k \end{bmatrix}^{-1}. \tag{27}$$

In the case of the BFGS update ($\phi = 0$), equation (26) simplifies to

$$\begin{aligned}\tilde{M}_k &= (-M_k^{-1} - \Psi_k^T H_0 \Psi_k)^{-1} \\ &= \begin{bmatrix} 0 & -R_k - D_k \\ -R_k^T - D_k & -D_k - Y_k^T H_0 Y_k \end{bmatrix}^{-1} \\ &= \begin{bmatrix} \bar{R}_k^{-T}(D_k + Y_k^T H_0 Y_k)\bar{R}_k^{-1} & -\bar{R}_k^{-T} \\ -\bar{R}_k^{-1} & 0 \end{bmatrix},\end{aligned}$$

where $\bar{R}_k = R_k + D_k$. Thus, the compact representation for the inverse of a BFGS matrix is given by

$$H_{k+1} = H_0 + \begin{bmatrix} S_k & H_0 Y_k \end{bmatrix} \begin{bmatrix} \bar{R}_k^{-T}(D_k + Y_k^T H_0 Y_k)\bar{R}_k^{-1} & -\bar{R}_k^{-T} \\ -\bar{R}_k^{-1} & 0 \end{bmatrix} \begin{bmatrix} S_k^T \\ Y_k^T H_0 \end{bmatrix}, \tag{28}$$

which is equivalent to that found in [**?**, Equation (2.6)].

The compact formulation for the inverse of an SR1 matrix can be derived using the same strategy as for the restricted Broyden class. The SMW formula applied to the compact formulation of an SR1 with Ψ_k and M_k defined as in (23) yields

$$H_{k+1} = H_0 + H_0(Y_k - B_0 S_k)\left(-M_k - \Psi_k^T H_0 \Psi_k\right)^{-1}(Y_k - B_0 S_k)^T H_0.$$

Substituting in for M_k using (23) together with the identity

$$\Psi_k^T H_0 \Psi_k = Y_k^T H_0 Y_k - S_k^T Y_k - Y_k^T S_k + S_k^T B_0 S_k,$$

yields

$$\begin{aligned}H_{k+1} &= H_0 + (H_0 Y_k - S_k)\big(- (D_k + L_k + L_k^T - S_k^T B_0 S_k) \\ &\qquad -(Y_k^T H_0 Y_k - S_k^T Y_k - Y_k^T S_k + S_k^T B_0 S_k)\big)^{-1}(H_0 Y_k - S_k)^T \\ &= H_0 + (S_k - H_0 Y_k)^T (D_k + R_k + R_k^T - Y_k^T H_0 Y_k)^{-1}(S_k - H_0 Y_k)^T.\end{aligned}$$

In other words, the compact formulation for the inverse of an SR1 matrix is given by

$$H_{k+1} = H_0 + \tilde{\Psi}_k \tilde{M}_k \tilde{\Psi}_k^T \quad \text{where} \quad \tilde{\Psi}_k \triangleq [S_k - H_0 Y_k], \tag{29}$$

and $\tilde{M}_k \triangleq (D_k + R_k + R_k^T - Y_k^T H_0 Y_k)^{-1}$. Algorithm 5 details how to solve a linear system defined by an L-SR1 matrix via the compact representation for its inverse.

Algorithm 5: Computing $r = B_{k+1}^{-1} z$ using (29) when B_{k+1} is an SR1 matrix.

Define H_0, S_k and Y_k;
Form $S_k^T Y_k = L_k + D_k + R_k$;
Form $\tilde{\Psi}_k = S_k - H_0 Y_k$;
$\tilde{M}_k \leftarrow (D_k + R_k + R_k^T - Y_k^T H_0 Y_k)^{-1}$;
$r = H_0 z + \tilde{\Psi}_k \tilde{M}_k \tilde{\Psi}_k z$;

4.1. **Relationships between updates.** Well-known relationships between different updates of the restricted class are preserved with the compact formulation for the inverse. In particular, we show that the BFGS and the DFP are duals of each (see Section 2.1) and we argue that the SR1 matrix is self-dual (see Section 2.1).

Consider the compact formulation for the inverse of a BFGS matrix (i.e., $\phi = 0$) in (28). This is equivalent to

$$\begin{aligned} H_{k+1} &= H_0 + \begin{bmatrix} H_0 Y_k & S_k \end{bmatrix} \begin{bmatrix} 0 & -\bar{R}_k^{-1} \\ -\bar{R}_k^{-T} & \bar{R}_k^{-T}(D_k + Y_k^T H_0 Y_k)\bar{R}_k^{-1} \end{bmatrix} \begin{bmatrix} Y_k^T H_0 \\ S_k^T \end{bmatrix} \\ &= H_0 - \begin{bmatrix} H_0 Y_k & S_k \end{bmatrix} \begin{bmatrix} Y_k^T H_0 Y_k + D_k & \bar{R}_k^T \\ \bar{R}_k & 0 \end{bmatrix}^{-1} \begin{bmatrix} Y_k^T H_0 \\ S_k^T \end{bmatrix}. \end{aligned}$$

Now we consider interchanging B_0 with H_0 and Y_k with S_k. Notice that if S_k and Y_k are interchanged then the upper triangular part of $S_k^T Y_k$ corresponds to the lower triangular part of $Y_k^T S_k$, implying that L_k and R_k must also be interchanged. Putting this all together yields:

$$B_{k+1} = B_0 - \begin{bmatrix} B_0 S_k & Y_k \end{bmatrix} \begin{bmatrix} S_k^T B_0 S_k + D_k & (L_k + D_k)^T \\ L_k + D_k & 0 \end{bmatrix}^{-1} \begin{bmatrix} S_k^T B_0 \\ Y_k^T \end{bmatrix},$$

which is the compact formulation for a DFP matrix. In other words, the BFGS and DFP are complementary updates of each other. (In a similar manner one can show that the compact formulation a BFGS matrix can be obtained by replacing B_0 for H_0 as well as y_k with s_k in the compact formulation for the inverse of a DFP matrix.)

Finally, it is worth noting that the inverse of compact formulation for an SR1 matrix is self-dual in the sense of Section 2.1. That is, replacing H_0 with B_0 and S_k with Y_k (and, thus, R_k with L_k) in (29) yields the compact formulation for the SR1 matrix given by (23).

4.2. **Recursive formulation.** In this section, we present a practical method to compute $\tilde{M}_k$ in (26) given by (27). We begin by providing an alternative expression for $\tilde{M}_0$ that will allow us to define a recursion method to compute $\tilde{M}_k$.

Lemma 1. *Suppose $H_1 = H_0 + \tilde{\Psi}_0 \tilde{M}_0 \tilde{\Psi}_0^T$, is the inverse of a member of the restricted Broyden class of updates after performing one update. Then,*

$$\tilde{M}_0 = \begin{bmatrix} \tilde{\alpha}_0 & \tilde{\beta}_0 \\ \tilde{\beta}_0 & \tilde{\delta}_0 \end{bmatrix}, \tag{30}$$

where

$$\tilde{\alpha}_0 = \frac{1}{s_0^T y_0} + \Phi_0 \frac{y_0^T H_0 y_0}{(s_0^T y_0)^2}, \quad \tilde{\beta}_0 = -\frac{\Phi_0}{y_0^T s_0}, \quad \tilde{\delta}_0 = -\frac{1-\Phi_0}{y_0^T H_0 y_0}, \tag{31}$$

and Φ_0 is as in (17).

Proof. Expanding (16), yields

$$\begin{aligned} H_1 = H_0 &+ \left(\frac{1}{s_0^T y_0} + \Phi_0 \frac{y_0^T H_0 y_0}{(s_0^T y_0)^2} \right) s_0 s_0^T - \frac{\Phi_0}{y_0^T s_0} H_0 y_0 s_0^T \\ &- \frac{\Phi_0}{y_0^T s_0} s_0 y_0^T H_0 - \frac{1-\Phi_0}{y_0^T H_0 y_0} H_0 y_0 y_0^T H_0, \end{aligned}$$

which simplifies to

$$H_1 = H_0 + \begin{bmatrix} s_0 & H_0 y_0 \end{bmatrix} \begin{bmatrix} \tilde{\alpha}_0 & \tilde{\beta}_0 \\ \tilde{\beta}_0 & \tilde{\delta}_0 \end{bmatrix} \begin{bmatrix} s_0^T \\ y_0^T H_0 \end{bmatrix}, \tag{32}$$

where $\tilde{\alpha}_0$, $\tilde{\beta}_0$, and $\tilde{\delta}_0$ are defined as in (31) and Φ_0 is given by (17). Note the (32) is of the form $H_1 = H_0 + \tilde{\Psi}_0 \tilde{M}_0 \tilde{\Psi}_0^T$.

We now show that $\tilde{M}_0$ defined by (30) and (31) is equivalent to (27) with $k = 0$. To see this, we simplify the entries of (30). First, define

$$\Delta_0 \triangleq (1-\phi)(y_0^T s_0)^2 + \phi(y_0^T H_0 y_0)(s_0^T B_0 s_0).$$

Then,

$$\Phi_0 = \frac{(1-\phi)(s_0^T y_0)^2}{\Delta_0},$$

and thus,

$$\tilde{\alpha}_0 = \frac{1}{s_0^T y_0} + \frac{(1-\phi) y_0^T H_0 y_0}{\Delta_0}, \quad \tilde{\beta}_0 = -\frac{(1-\phi)(s_0^T y_0)}{\Delta_0}, \quad \text{and} \quad \tilde{\delta}_0 = -\frac{\phi(s_0^T B_0 s_0)}{\Delta_0}.$$

Consider the inverse of (30), which is given by

$$\begin{bmatrix} \tilde{\alpha}_0 & \tilde{\beta}_0 \\ \tilde{\beta}_0 & \tilde{\delta}_0 \end{bmatrix}^{-1} = \frac{1}{\tilde{\alpha}_0 \tilde{\delta}_0 - \tilde{\beta}_0^2} \begin{bmatrix} \tilde{\delta}_0 & -\tilde{\beta}_0 \\ -\tilde{\beta}_0 & \tilde{\alpha}_0 \end{bmatrix}. \tag{33}$$

We now simplify the entries on the right side of (33) The determinant of (30) is given by

$$\begin{aligned} \tilde{\alpha}_0 \tilde{\delta}_0 - \tilde{\beta}_0^2 &= -\frac{1-\Phi_0}{(s_0^T y_0)(y_0^T H_0 y_0)} - \frac{\Phi_0(1-\Phi_0)}{(s_0^T y_0)^2} - \frac{\Phi_0^2}{(s_0^T y_0)^2} \\ &= -\frac{\phi s_0^T B_0 s_0}{\Delta_0 s_0^T y_0} - \frac{1-\phi}{\Delta_0} \\ &= \frac{1}{\Delta_0}\left(\frac{s_0^T B_0 s_0}{\lambda_0}\right), \end{aligned}$$

where λ_0 is defined in (22). Thus, the first entry of (33) is given by

$$\frac{\tilde{\delta}_0}{\tilde{\alpha}_0 \tilde{\delta}_0 - \tilde{\beta}_0^2} = -\frac{\phi(s_0^T B_0 s_0)}{\Delta_0} \frac{\Delta_0 \lambda_0}{s_0^T B_0 s_0} = -\phi \lambda_0. \tag{34}$$

The off-diagonal elements of the right-hand side of (33) simplify as follows:

$$\begin{aligned} \frac{\tilde{\beta}_0}{\tilde{\alpha}_0 \tilde{\delta}_0 - \tilde{\beta}_0^2} &= -\left(\frac{(1-\phi)(s_0^T y_0)}{\Delta_0}\right)\left(\Delta_0 \left(\frac{\lambda_0}{s_0^T B_0 s_0}\right)\right) \\ &= -\frac{(1-\phi) s_0^T y_0}{-(1-\phi) - \phi \dfrac{s_0^T B_0 s_0}{s_0^T y_0}} \\ &= -\frac{(1-\phi)(s_0^T y_0)^2 + \phi s_0^T B_0 s_0 (s_0^T y_0) - \phi s_0^T B_0 s_0 (s_0^T y_0)}{-(1-\phi) s_0^T y_0 - \phi s_0^T B_0 s_0} \\ &= s_0^T y_0 + \phi \frac{s_0^T B_0 s_0 (s_0^T y_0)}{-(1-\phi) s_0^T y_0 - \phi s_0^T B_0 s_0} \\ &= s_0^T y_0 + \phi \lambda_0. \end{aligned} \tag{35}$$

Finally, the last entry of (33) can be simplified as follows:

(36)
$$\begin{aligned}
\frac{\tilde{\alpha}_0}{\tilde{\alpha}_0\tilde{\delta}_0 - \tilde{\beta}_0^2} &= \frac{1}{s_0^T y_0}\frac{\Delta_0\lambda_0}{s_0^T B_0 s_0} + (1-\phi)y_0^T H_0 y_0 \frac{\lambda_0}{s_0^T B_0 s_0} \\
&= \frac{\lambda_0}{(s_0^T y_0)(s_0^T B_0 s_0)}\Big(\Delta_0 + (1-\phi)(y_0^T H_0 y_0)(s_0^T y_0)\Big) \\
&= \frac{1}{-(1-\phi)s_0^T y_0 - \phi s_0^T B_0 s_0}\Big(\Delta_0 + (1-\phi)(y_0^T H_0 y_0)(s_0^T y_0)\Big) \\
&= \frac{(1-\phi)(s_0^T y_0)^2 + \phi(y_0^T H_0 y_0)(s_0^T B_0 s_0) + (1-\phi)(y_0^T H_0 y_0)(s_0^T y_0)}{-(1-\phi)s_0^T y_0 - \phi(s_0^T B_0 s_0)} \\
&= \frac{(1-\phi)(s_0^T y_0)^2 + \phi(s_0^T B_0 s_0)(s_0^T y_0)}{-(1-\phi)s_0^T y_0 - \phi(s_0^T B_0 s_0)} - \frac{\phi(s_0^T B_0 s_0)(s_0^T y_0)}{-(1-\phi)s_0^T y_0 - \phi(s_0^T B_0 s_0)} \\
&\quad + \frac{\phi(y_0^T H_0 y_0)(s_0^T B_0 s_0) + (1-\phi)(y_0^T H_0 y_0)s_0^T y_0}{-(1-\phi)s_0^T y_0 - \phi(s_0^T B_0 s_0)} \\
&= -s_0^T y_0 - \phi\lambda_0 - y_0^T H_0 y_0.
\end{aligned}$$

Thus, (33) together with (34) (36) and (37) gives

$$\begin{bmatrix} \tilde{\alpha}_0 & \tilde{\beta}_0 \\ \tilde{\beta}_0 & \tilde{\delta}_0 \end{bmatrix}^{-1} = \begin{bmatrix} -\phi\lambda_0 & -s_0^T y_0 - \phi\lambda_0 \\ -s_0^T y_0 - \phi\lambda_0 & -s_0^T y_0 - \phi\lambda_0 - y_0^T H_0 y_0 \end{bmatrix},$$

showing that $\tilde{M}_0$ defined by (30) and (31) is equivalent to (27) with $k = 0$. □

Together with Lemma 1, the following theorem shows how $\tilde{M}_k$ is related to $\tilde{M}_{k-1}$; from this, we present an algorithm to compute $\tilde{M}_k$ using recursion.

Theorem 1. *Suppose $H_{j+1} = H_0 + \tilde{\Psi}_j \tilde{M}_j \tilde{\Psi}_j^T$ as in (26) for all $j \in \{0, \ldots, k\}$, is the inverse of a member of the Broyden class of updates for a fixed $\phi \in [0, 1]$. If $\tilde{M}_0$ is defined by (30), then for all $j \in \{1, \ldots k\}$, $\tilde{M}_j$ satisfies the recursion relation*

$$\tilde{M}_j = \Pi_j^T \begin{bmatrix} \tilde{M}_{j-1} + \tilde{\delta}_j \tilde{u}_j \tilde{u}_j^T & \tilde{\beta}_j \tilde{u}_j & \tilde{\delta}_j \tilde{u}_j \\ \tilde{\beta}_j \tilde{u}_j^T & \tilde{\alpha}_j & \tilde{\beta}_j \\ \tilde{\delta}_j \tilde{u}_j^T & \tilde{\beta}_j & \tilde{\delta}_j \end{bmatrix} \Pi_j, \tag{37}$$

where

$$\Pi_j = \begin{bmatrix} I_j & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & I_j & 0 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix}, \tag{38}$$

is such that

$$\begin{bmatrix} \tilde{\Psi}_{j-1} & s_j & H_0 y_j \end{bmatrix} \Pi_j = \tilde{\Psi}_j,$$

and

$$\tilde{\alpha}_j = \frac{1}{s_j^T y_j} + \Phi_j \frac{y_j^T H_j y_j}{(s_j^T y_j)^2}, \quad \tilde{\beta}_j = -\frac{\Phi_j}{y_j^T s_j}, \quad \tilde{\delta}_j = -\frac{1 - \Phi_j}{y_j^T H_j y_j},$$

and $\tilde{u}_j = \tilde{M}_{j-1} \tilde{\Psi}_{j-1}^T y_j$.

Proof. This proof is by induction on j. For the base case, we show that equation (37) holds for $j = 1$. Setting $k = 1$ in (16) yields

$$H_2 = H_1 + \begin{bmatrix} s_1 & H_1 y_1 \end{bmatrix} \begin{bmatrix} \tilde{\alpha}_1 & \tilde{\beta}_1 \\ \tilde{\beta}_1 & \tilde{\delta}_1 \end{bmatrix} \begin{bmatrix} s_1^T \\ y_1^T H_1 \end{bmatrix}, \tag{39}$$

where

$$\tilde{\alpha}_1 = \frac{1}{s_1^T y_1} + \Phi_1 \frac{y_1^T H_1 y_1}{(s_1^T y_1)^2}, \quad \tilde{\beta}_1 = -\frac{\Phi_1}{y_1^T s_1}, \quad \text{and} \quad \tilde{\delta}_1 = -\frac{1 - \Phi_1}{y_1^T H_1 y_1}.$$

By Lemma 1, (39) can be written as

$$H_2 = H_0 + \tilde{\Psi}_0 \tilde{M}_0 \tilde{\Psi}_0^T + \begin{bmatrix} s_1 & H_1 y_1 \end{bmatrix} \begin{bmatrix} \tilde{\alpha}_1 & \tilde{\beta}_1 \\ \tilde{\beta}_1 & \tilde{\delta}_1 \end{bmatrix} \begin{bmatrix} s_1^T \\ y_1^T H_1 \end{bmatrix}, \tag{40}$$

where $\tilde{\Psi}_0 = [S_0 \;\; H_0 Y_0]$ and $\tilde{M}_0$ is given by (30). Letting $\tilde{u}_1 = \tilde{M}_0 \tilde{\Psi}_0^T y_1$, we have that

$$H_1 y_1 = \left(H_0 + \tilde{\Psi}_0 \tilde{M}_0 \tilde{\Psi}_0^T \right) y_1 = H_0 y_1 + \tilde{\Psi}_0 \tilde{u}_1. \tag{41}$$

Substituting (41) into the last quantity on the right side of (40) yields

$$\begin{aligned} \begin{bmatrix} s_1 & H_1 y_1 \end{bmatrix} \begin{bmatrix} \tilde{\alpha}_1 & \tilde{\beta}_1 \\ \tilde{\beta}_1 & \tilde{\delta}_1 \end{bmatrix} \begin{bmatrix} s_1^T \\ y_1^T H_1 \end{bmatrix} &= \begin{bmatrix} s_1 & H_0 y_1 + \tilde{\Psi}_0 \tilde{u}_1 \end{bmatrix} \begin{bmatrix} \tilde{\alpha}_1 & \tilde{\beta}_1 \\ \tilde{\beta}_1 & \tilde{\delta}_1 \end{bmatrix} \begin{bmatrix} s_1^T \\ y_1^T H_0 + \tilde{u}_1^T \tilde{\Psi}_0^T \end{bmatrix} \\ &= \begin{bmatrix} \tilde{\Psi}_0 & s_1 & H_0 y_1 \end{bmatrix} \begin{bmatrix} \tilde{\delta}_1 \tilde{u}_1 \tilde{u}_1^T & \tilde{\beta}_1 \tilde{u}_1 & \tilde{\delta}_1 \tilde{u}_1 \\ \tilde{\beta}_1 \tilde{u}_1^T & \tilde{\alpha}_1 & \tilde{\beta}_1 \\ \tilde{\delta}_1 \tilde{u}_1^T & \tilde{\beta}_1 & \tilde{\delta}_1 \end{bmatrix} \begin{bmatrix} \tilde{\Psi}_0^T \\ s_1^T \\ y_1^T H_0 \end{bmatrix}. \end{aligned}$$

Letting Π_1 be defined as in (38) with $j = 1$, gives that $\begin{bmatrix} \tilde{\Psi}_0 & s_1 & H_0 y_1 \end{bmatrix} \Pi_1 = \tilde{\Psi}_1$, and thus,

$$H_2 = H_0 + \tilde{\Psi}_1 \Pi_1^T \bar{M}_1 \Pi_1 \tilde{\Psi}_1^T,$$

where

$$\bar{M}_1 \triangleq \begin{bmatrix} \tilde{M}_0 + \tilde{\delta}_1 \tilde{u}_1 \tilde{u}_1^T & \tilde{\beta}_1 \tilde{u}_1 & \tilde{\delta}_1 \tilde{u}_1 \\ \tilde{\beta}_1 \tilde{u}_1^T & \tilde{\alpha}_1 & \tilde{\beta}_1 \\ \tilde{\delta}_1 \tilde{u}_1^T & \tilde{\beta}_1 & \tilde{\delta}_1 \end{bmatrix}.$$

It remains to show that $\tilde{M}_1 = \Pi_1^T \bar{M}_1 \Pi_1$; however, for simplicity, we instead show $\tilde{M}_1^{-1} = \Pi_1^T \bar{M}_1^{-1} \Pi$.

Notice that $\bar{M}_1$ can be written as the product of three matrices:

$$\bar{M}_1 = \begin{bmatrix} I_2 & 0 & \tilde{u}_1 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} \tilde{M}_0 & 0 & 0 \\ 0 & \tilde{\alpha}_1 & \tilde{\beta}_1 \\ 0 & \tilde{\beta}_1 & \tilde{\delta}_1 \end{bmatrix} \begin{bmatrix} I_2 & 0 & 0 \\ 0 & 1 & 0 \\ \tilde{u}_1^T & 0 & 1 \end{bmatrix}.$$

Define

$$\tilde{N}_0 = \begin{bmatrix} \tilde{\alpha}_1 & \tilde{\beta}_1 \\ \tilde{\beta}_1 & \tilde{\delta}_1 \end{bmatrix}.$$

Then, $\bar{M}_1^{-1}$ is given by

$$\bar{M}_1^{-1} = \begin{bmatrix} I & 0 & 0 \\ 0 & 1 & 0 \\ -\tilde{u}_1^T & 0 & 1 \end{bmatrix} \begin{bmatrix} \tilde{M}_0^{-1} & 0 \\ 0 & \tilde{N}_0^{-1} \end{bmatrix} \begin{bmatrix} I & 0 & -\tilde{u}_1 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix}, \tag{42}$$

where it can be shown, using similar computations as in the proof of Lemma 1, that

$$\begin{aligned}\tilde{N}_0^{-1} &= \frac{1}{\tilde{\alpha}_1\tilde{\delta}_1 - \tilde{\beta}_1^2}\begin{bmatrix}\tilde{\delta}_1 & -\tilde{\beta}_1\\ -\tilde{\beta}_1 & \tilde{\alpha}_1\end{bmatrix}\\ &= \begin{bmatrix}-\phi\lambda_1 & -s_1^Ty_1 - \phi\lambda_1\\ -s_1^Ty_1 - \phi\lambda_1 & -s_1^Ty_1 - \phi\lambda_1 - y_1^TH_1y_1\end{bmatrix}.\end{aligned}$$

Substituting $\tilde{N}_0^{-1}$ into (42) and simplifying yields

$$\bar{M}_1^{-1} = \begin{bmatrix}\tilde{M}_0^{-1} & 0 & -\tilde{\Psi}_0^Ty_1\\ 0 & -\phi\lambda_1 & -s_1^Ty_1 - \phi\lambda_1\\ -y_1^T\tilde{\Psi}_0 & -s_1^Ty_1 - \phi\lambda_1 & \tilde{u}_1^TM_0^{-1}\tilde{u}_1 - s_1^Ty_1 - \phi\lambda_1 - y_1^TH_1y_1\end{bmatrix}. \tag{43}$$

Terms in the (3,3)-entry in the right side of (43) can be simplified using that $\tilde{M}_0^{-1}\tilde{u}_1 = \tilde{\Psi}_0^Ty_1$ and that $y_1^TH_1y_1 = y_1^TH_0y_1 + y_1^T\tilde{\Psi}_0\tilde{M}_0\tilde{\Psi}_0^Ty_1$ as follows:

$$\begin{aligned}\tilde{u}_1^T\tilde{M}_0^{-1}\tilde{u}_1 - y_1^TH_1y_1 &= y_1^T\tilde{\Psi}_0\tilde{M}_0\tilde{\Psi}_0^Ty_1 - y_1^TH_1y_1\\ &= -y_1^TH_0y_1 + y_1^TH_1y_1 - y_1^TH_1y_1\\ &= -y_1^TH_0y_1.\end{aligned}$$

Thus,

$$\bar{M}_1^{-1} = \begin{bmatrix}\tilde{M}_0^{-1} & 0 & -\tilde{\Psi}_0^Ty_1\\ 0 & -\phi\lambda_1 & -s_1^Ty_1 - \phi\lambda_1\\ -y_1^T\tilde{\Psi}_0 & -s_1^Ty_1 - \phi\lambda_1 & -s_1^Ty_1 - \phi\lambda_1 - y_1^TH_0y_1\end{bmatrix}. \tag{44}$$

By Lemma 1,

$$\tilde{M}_0^{-1} = \begin{bmatrix}\tilde{\alpha}_0 & \tilde{\beta}_0\\ \tilde{\beta}_0 & \tilde{\delta}_0\end{bmatrix}^{-1} = \begin{bmatrix}-\phi\lambda_0 & -s_0^Ty_0 - \phi\lambda_0\\ -s_0^Ty_0 - \phi\lambda_0 & -s_0^Ty_0 - \phi\lambda_0 - y_0^TH_0y_0\end{bmatrix}.$$

This, together with the substitution $\tilde{\Psi}_0^Ty_1 = \begin{pmatrix}S_0^Ty_1\\ Y_0^TH_0y_1\end{pmatrix}$, gives that

$$\begin{aligned}\Pi_1^T\bar{M}_1^{-1}\Pi_1 &= \Pi_j^T\begin{bmatrix}\tilde{M}_0^{-1} & 0 & -\tilde{\Psi}_0^Ty_1\\ 0 & -\phi\lambda_1 & -s_1^Ty_1 - \phi\lambda_1\\ -y_1^T\tilde{\Psi}_0 & -s_1^Ty_1 - \phi\lambda_1 & -s_1^Ty_1 - \phi\lambda_1 - y_1^TH_0y_1\end{bmatrix}\Pi_j\\
&= \left[\begin{array}{cc|cc}-\phi\lambda_0 & 0 & -s_0^Ty_0 - \phi\lambda_0 & -S_0^Ty_1\\ 0 & -\phi\lambda_1 & 0 & -s_1^Ty_1 - \phi\lambda_1\\ \hline -s_0^Ty_0 - \phi\lambda_0 & 0 & -s_0^Ty_0 - \phi\lambda_0 - y_0^TH_0y_0 & -Y_0^TH_0y_1\\ -y_1^TS_0 & -s_1^Ty_1 - \phi\lambda_1 & -y_1^TH_0Y_0 & -s_1^Ty_1 - \phi\lambda_1 - y_1^TH_0y_1\end{array}\right]\\
&= \left[\begin{array}{cc|cc}-\phi\Lambda_0 & 0 & -R_0 - D_0 - \phi\Lambda_0 & -S_0^Ty_1\\ 0 & -\phi\lambda_1 & 0 & -s_1^Ty_1 - \phi\lambda_1\\ \hline -R_0^T - D_0 - \phi\Lambda_0 & 0 & -D_0 - \phi\Lambda_1 - Y_0^TH_0Y_0 & -Y_0^TH_0y_1\\ -y_1^TS_0 & -s_1^Ty_1 - \phi\lambda_1 & -y_1^TH_0Y_0 & -s_1^Ty_1 - \phi\lambda_1 - y_1^TH_0y_1\end{array}\right]\\
&= \begin{bmatrix}-\phi\Lambda_1 & -R_1 - D_1 - \phi\Lambda_1\\ -R_1^T - D_1 - \phi\Lambda_1 & -D_1 - \phi\Lambda_1 - Y_1^TH_0Y_1\end{bmatrix}\\
&= \tilde{M}_1^{-1},\end{aligned}$$

proving the base case.

The inductive step is similar to the base case. For the inductive step, we assume the theorem holds for $k = 1, \dots j-1$ and now show it holds for $k = j$. We begin, as before, setting $k = j$ in (16) to obtain

$$H_{j+1} = H_j + \begin{bmatrix} s_j & H_j y_j \end{bmatrix} \begin{bmatrix} \tilde{\alpha}_j & \tilde{\beta}_j \\ \tilde{\beta}_j & \tilde{\delta}_j \end{bmatrix} \begin{bmatrix} s_j^T \\ y_j^T H_j \end{bmatrix}, \tag{45}$$

where

$$\tilde{\alpha}_j = \frac{1}{s_j^T y_j} + \Phi_j \frac{y_j^T H_j y_j}{(s_j^T y_j)^2}, \quad \tilde{\beta}_j = -\frac{\Phi_j}{y_j^T s_j}, \quad \text{and} \quad \tilde{\delta}_j = -\frac{1-\Phi_j}{y_j^T H_j y_j},$$

Using the induction hypothesis, (45) becomes

$$H_{j+1} = H_0 + \tilde{\Psi}_{j-1} \tilde{M}_{j-1} \tilde{\Psi}_{j-1} + \begin{bmatrix} s_j & H_j y_j \end{bmatrix} \begin{bmatrix} \tilde{\alpha}_j & \tilde{\beta}_j \\ \tilde{\beta}_j & \tilde{\delta}_j \end{bmatrix} \begin{bmatrix} s_j^T \\ y_j^T H_j \end{bmatrix}.$$

Similar to the base case,

$$\begin{aligned} \begin{bmatrix} s_j & H_j y_j \end{bmatrix} \begin{bmatrix} \tilde{\alpha}_j & \tilde{\beta}_j \\ \tilde{\beta}_j & \tilde{\delta}_j \end{bmatrix} \begin{bmatrix} s_j^T \\ y_j^T H_j \end{bmatrix} &= \begin{bmatrix} s_j & H_0 y_j + \tilde{\Psi}_{j-1} \tilde{u}_j \end{bmatrix} \begin{bmatrix} \tilde{\alpha}_j & \tilde{\beta}_j \\ \tilde{\beta}_j & \tilde{\delta}_j \end{bmatrix} \begin{bmatrix} s_j^T \\ y_j^T H_0 + \tilde{u}_j^T \tilde{\Psi}_{j-1}^T \end{bmatrix} \\ &= \begin{bmatrix} \tilde{\Psi}_{j-1} & s_j & H_0 y_j \end{bmatrix} \begin{bmatrix} \tilde{\delta}_j \tilde{u}_j \tilde{u}_j^T & \tilde{\beta}_j \tilde{u}_j & \tilde{\delta}_j \tilde{u}_j \\ \tilde{\beta}_j \tilde{u}_j^T & \tilde{\alpha}_j & \tilde{\beta}_j \\ \tilde{\delta}_j \tilde{u}_j^T & \tilde{\beta}_j & \tilde{\delta}_j \end{bmatrix} \begin{bmatrix} \tilde{\Psi}_{j-1}^T \\ s_j^T \\ y_j^T H_0 \end{bmatrix}, \end{aligned}$$

where $\tilde{u}_j = \tilde{M}_{j-1} \tilde{\Phi}_{j-1}^T y_j$. With Π_j defined as in (38), then $\begin{bmatrix} \tilde{\Psi}_{j-1} & s_j & H_0 y_j \end{bmatrix} \Pi_j = \tilde{\Psi}_j$, and so

$$H_j = H_0 + \tilde{\Psi}_j \Pi_j^T \bar{M}_j \Pi_j \tilde{\Psi}_j^T,$$

where

$$\bar{M}_j \triangleq \begin{bmatrix} \tilde{M}_{j-1} + \tilde{\delta}_j \tilde{u}_j \tilde{u}_j^T & \tilde{\beta}_j \tilde{u}_j & \tilde{\delta}_j \tilde{u}_j \\ \tilde{\beta}_j \tilde{u}_j^T & \tilde{\alpha}_j & \tilde{\beta}_j \\ \tilde{\delta}_j \tilde{u}_j^T & \tilde{\beta}_j & \tilde{\delta}_j \end{bmatrix}. \tag{46}$$

It remains to show that $\tilde{M}_j = \Pi_j^T \bar{M}_j \Pi_j$; however, for simplicity, we instead show $\tilde{M}_j^{-1} = \Pi_j^T \bar{M}_j^{-1} \Pi_j$ using a similar argument as in the base case. In particular, similar to (43), it can be shown that

$$\bar{M}_j^{-1} = \begin{bmatrix} \tilde{M}_{j-1}^{-1} & 0 & -\tilde{\Psi}_{j-1}^T y_j \\ 0 & -\phi \lambda_j & -s_j^T y_j - \phi \lambda_j \\ -y_j^T \tilde{\Psi}_{j-1} & -s_j^T y_j - \phi \lambda_j & -s_j^T y_j - \phi \lambda_j - y_j^T H_0 y_j \end{bmatrix}.$$

By the inductive hypothesis that (27) holds for $k = j-1$,

$$\tilde{M}_{j-1}^{-1} = \begin{bmatrix} -\phi \Lambda_{j-1} & -R_{j-1} - D_{j-1} - \phi \Lambda_{j-1} \\ -R_{j-1}^T - D_{j-1} - \phi \Lambda_{j-1} & -D_{j-1} - \phi \Lambda_k - Y_{j-1}^T H_0 Y_{j-1} \end{bmatrix}$$

and so,

$$\begin{aligned}
\Pi_j^T \bar{M}_j^{-1} \Pi_j &= \Pi_j^T \begin{bmatrix} \tilde{M}_{j-1}^{-1} & 0 & -\tilde{\Psi}_{j-1}^T y_j \\ 0 & -\phi\lambda_j & -s_j^T y_j - \phi\lambda_j \\ -y_j^T \tilde{\Psi}_{j-1} & -s_j^T y_j - \phi\lambda_j & -s_j^T y_j - \phi\lambda_j - y_j^T H_0 y_j \end{bmatrix} \Pi_j \\
&= \left[\begin{array}{cc|cc} -\phi\Lambda_{j-1} & 0 & -R_{j-1} - D_{j-1} - \phi\Lambda_{j-1} & -S_{j-1}^T y_j \\ 0 & -\phi\lambda_j & 0 & -s_j^T y_j - \phi\lambda_j \\ \hline -R_{j-1}^T - D_{j-1} - \phi\Lambda_{j-1} & 0 & -D_{j-1} - \phi\Lambda_k - Y_{j-1}^T H_0 Y_{j-1} & -Y_{j-1}^T H_0 y_j \\ -y_j^T S_{j-1} & -s_j^T y_j - \phi\lambda_j & -y_j^T H_0 Y_{j-1} & -s_j^T y_j - \phi\lambda_j - y_j^T H_0 y_j \end{array}\right] \\
&= \begin{bmatrix} -\phi\Lambda_j & -R_j - D_j - \phi\Lambda_j \\ -R_j^T - D_j - \phi\Lambda_j & -D_j - \phi\Lambda_k - Y_j^T H_0 Y_j \end{bmatrix} \\
&= \tilde{M}_j^{-1},
\end{aligned}$$

proving the induction step. □

Using Theorem 1, Algorithm 6 computes $\tilde{M}_k$ and then uses the compact formulation for the inverse to solve linear systems of the form (1). There are two parts to `for` loop in Algorithm 4: The first half of the loop is used to build products of the form $s_j^T B_j s_j$; the second half of the loop computes $\tilde{M}_k$, making use of $s_j^T B_j s_j$ to compute Ψ_j. Thus, when $\phi = 0$ or $\phi = 1$, Ψ_j can be quickly computed as $\Phi = 1$ and $\Phi = 0$, respectively; in other words, the first six lines of the `for` loop can be skipped when $\phi = 0$ or $\phi = 1$.

Algorithm 6: Computing $r = B_{k+1}^{-1} z$ using (26).
Define ϕ, B_0, and H_0;
Form M_0 using (21) and $\tilde{M}_0$ using (30);
Let $\Psi_0 = (B_0 s_0 \; y_0)$ and $\tilde{\Psi}_0 = (s_0 \; H_0 y_0)$;
for $j = 1 : k$

% Part 1: Compute $s_j^T B_j s_j$
$u_j \leftarrow M_{j-1}(\Psi_{j-1}^T s_j)$;
$s_j^T B_j s_j \leftarrow s_j^T B_0 s_j + (s_j^T \Psi_{j-1}) u_j$;
$\alpha_j \leftarrow -(1-\phi)/(s_j^T B_j s_j)$;
$\beta_j \leftarrow -\phi/(y_j^T s_j)$;
$\delta_j \leftarrow (1 + \phi(s_j^T B_j s_j)/(y_j^T s_j))/(y_j^T s_j)$;
$M_j \leftarrow \Pi_j \begin{pmatrix} M_{j-1} + \alpha_j u_j u_j^T & \alpha_j u_j & \beta_j u_j \\ \alpha_j u_j^T & \alpha_j & \beta_j \\ \beta_j u_j^T & \beta_j & \delta_j \end{pmatrix} \Pi_j^T$, where Π_j is as in (38);

%Part 2: Compute $\tilde{M}_j$
$\tilde{u}_j \leftarrow \tilde{M}_{j-1}(\tilde{\Psi}_{j-1}^T y_j)$;
$y_j^T H_j y_j \leftarrow y_j^T H_0 y_j + (y_j^T \tilde{\Psi}_{j-1}) \tilde{u}_j$;
$\Phi_j = (1-\phi)(y_j^T s_j)^2 / ((1-\phi)(y_j^T s_j)^2 + \phi(y_j^T H_j y_j)(s_j^T B_j s_j))$;
$\tilde{\alpha}_j \leftarrow (1 + \Phi_j(y_j^T H_j y_j)/(y_j^T s_j))/(y_j^T s_j)$;

$\tilde{\beta}_j \leftarrow -\Phi_j/(y_j^T s_j)$;
$\tilde{\delta}_j \leftarrow -(1-\Phi_j)/(y_j^T H_j y_j)$;
$\tilde{M}_j \leftarrow \Pi_j^T \begin{pmatrix} \tilde{M}_{j-1} + \delta_j \tilde{u}_j \tilde{u}_j^T & \tilde{\beta}_j \tilde{u}_j & \tilde{\delta}_j \tilde{u}_j \\ \tilde{\beta}_j \tilde{u}_j^T & \tilde{\alpha}_j & \tilde{\beta}_j \\ \tilde{\delta}_j \tilde{u}_j^T & \tilde{\beta}_j & \tilde{\delta}_j \end{pmatrix} \Pi_j$, where Π_j is as in (38);

end
$r = H_0 z + \tilde{\Psi}_k \tilde{M}_k \tilde{\Psi}_k^T z$;

For Algorithm 6, the quantities $S_k^T B_0 S_k$, $Y_k^T H_0 Y_k$, and $S_k^T Y_k$ can be precomputed. Assuming B_0 is a scalar multiple of the identity matrix and $H_0 = B_0^{-1}$, then forming $S_k^T B_0 S_k$ and $Y_k^T H_0 Y_k$ requires $(k+1)(k+2)n$ flops each; forming $S_k^T Y_k$ requires $(k+1)^2(2n-1)$ flops. Also, the computations for u_j and $\tilde{u}_j$ in Algorithm 6 can be simplified by noting that

$$\Psi_{j-1}^T s_j = \begin{bmatrix} S_{j-1}^T B_0 s_j \\ Y_{j-1}^T s_j \end{bmatrix} \quad \text{and} \quad \tilde{\Psi}_{j-1}^T y_j = \begin{bmatrix} S_{j-1}^T y_j \\ Y_{j-1}^T H_0 y_j \end{bmatrix}. \tag{47}$$

In other words, $\Psi_{j-1}^T s_j$ is a $2j$ vector whose first j entries are the first j entries in the $(j+1)$th column of $S_k^T B_0 S_k$ and whose last j entries are the first j entries in the $(j+1)$th row of $S_k^T Y_k$; similarly, $\tilde{\Psi}_{j-1}^T y_j$ is a vector whose first j entries are the first j entries in the $(j+1)$th column of $S_k^T Y_k$ and whose last j entries are the first jth entries in the $(j+1)$th column of $Y_k^T H_0 Y_k$. Thus, computing u_j and $\tilde{u}_j$ only requires $2j(4j-1)$ flops each.

Computing the scalar $s_j^T B_j s_j$ in the second line of the `for` loop requires performing one inner product between $\Psi_{j-1}^T s_j$ and u_j and then summing this with $s_j^T B_0 s_j$, resulting in an operation cost of $4j$. This is the same cost is associated with forming $y_j^T H_j y_j$ in the second line of Part 2 of the `for` loop. The scalar Φ_j requires 10 flops to compute. The other scalars ($\alpha_j, \beta_j, \delta_j, \tilde{\alpha}_j, \tilde{\beta}_j$, and $\tilde{\delta}_j$) requires a total of 14 flops, not including multiplying by -1 in the definitions of β_j and $\tilde{\beta}_j$. Finally, forming the matrices M_j and $\tilde{M}_j$ requires $24j^2 + 16j$ flops each. Thus, excluding the cost of forming $S_k^T B_0 S_k$, $S_k^T Y_k$, and $Y_k^T H_0 Y_k$, the operation count for computing $\tilde{M}_k$ in Algorithm 6 is given by

$$\sum_{j=1}^{k} 4j(4j-1) + 8j + 24 + 24j^2 + 16j = \frac{1}{3}\left(40k^3 + 90k^2 + 122k\right).$$

4.3. **Efficient solves after updates.** To compute the factors in (24), it is necessary to form the matrices L_k, D_k and R_k. After a new quasi-Newton pair has been computed, updating (24) can be done efficiently by storing $S_k^T S_k$, $Y_k^T Y_k$ and $S_k^T Y_k$. In this case, to update H_{k+1} we add a column to (and possibly delete a column from) S_k and Y_k; the corresponding changes can then be made in $S_k^T S_k$, $Y_k^T Y_k$ and $S_k^T Y_k$ (see [**?**] for more details).

In the practical implementation given in Algorithm 6, it is necessary to compute $\Psi_{j-1}^T s_j$ and $\tilde{\Psi}_{j-1}^T y_j$ given by (47), which can be formed using the stored quantities $S_k^T S_k$, $Y_k^T Y_k$, and $S_k^T Y_k$. To compute these quantities when a new quasi-Newton pair of updates is obtained we apply the same strategy as described above by adding (and possibly deleting) columns in S_k and Y_k, enabling $\Psi_{j-1}^T s_j$ and $\tilde{\Psi}_{j-1}^T y_j$

to be updated efficiently. With these updates, the work required for Algorithm 6 is significantly reduced.

4.4. **Computing condition numbers.** Provided the initial approximate Hessian B_0 is taken to be a scalar multiple of the identity, (i.e., $B_0 = \gamma I$), it is possible to compute the condition number of B_{k+1} in (1). To do this, we consider the condition number of $H_{k+1} = B_{k+1}^{-1}$. The eigenvalues of H_{k+1} can be obtained from the compact representation of H_{k+1} together with the techniques from [**?**, **?**]. For completeness, we review this approach below.

Suppose B_{k+1} is a member of the restricted Broyden class. The eigenvalues of H_{k+1} can be computed using the compact formulation for H_{k+1} given in (26):

$$H_{k+1} = H_0 + \tilde{\Psi}_k \tilde{M}_k \tilde{\Psi}_k^T.$$

Letting $\tilde{\Psi}_k = QR$ be the QR decomposition of $\tilde{\Psi}_k$ where $Q \in \Re^{n\times n}$ is an orthogonal matrix and $R \in \Re^{n\times 2(k+1)}$ is an upper triangular matrix. Then,

$$\begin{aligned} H_{k+1} &= H_0 + \tilde{\Psi}_k \tilde{M}_k \tilde{\Psi}_k^T \\ &= H_0 + QR\tilde{M}_k R^T Q^T. \end{aligned} \tag{48}$$

The matrix $R\tilde{M}_k R^T$ is a real symmetric $n \times n$ matrix. However, since $\tilde{\Psi}_k \in \Re^{n\times 2(k+1)}$ has at most rank $2(k+1)$, then R can be written in the form

$$R = \begin{pmatrix} R_1 \\ 0 \end{pmatrix},$$

where $R_1 \in 2(k+1) \times 2(k+1)$. Thus,

$$R\tilde{M}_k R^T = \begin{pmatrix} R_1 \\ 0 \end{pmatrix} \tilde{M}_k \begin{pmatrix} R_1^T & 0 \end{pmatrix} = \begin{pmatrix} R_1\tilde{M}_k R_1^T & 0 \\ 0 & 0 \end{pmatrix}.$$

Since $R_1\tilde{M}_k R_1^T \in \Re^{2(k+1)\times 2(k+1)}$, its spectral decomposition can be computed explicitly. Letting $V_1 D_1 V_1^T$ is the spectral decomposition of $R_1\tilde{M}_k R_1^T$ and substituting into (49) yields:

$$H_{k+1} = H_0 + QVDV^TQ^T$$

where

$$V \triangleq \begin{pmatrix} V_1 & 0 \\ 0 & 0 \end{pmatrix} \in \Re^{n\times n} \quad \text{and} \quad D \triangleq \begin{pmatrix} D_1 & 0 \\ 0 & 0 \end{pmatrix} \in \Re^{n\times n}.$$

Thus,

$$H_{k+1} = H_0 + QVDV^TQ^T = QV(\gamma^{-1}I + D)V^TQ^T,$$

giving the spectral decomposition of H_{k+1}. In particular, the matrix H_{k+1} has an eigenvalue of γ^{-1} with multiplicity $n - 2(k+1)$ and $2(k+1)$ eigenvalues given by $\gamma^{-1} + d_i$ for $1 \le i \le 2(k+1)$ where d_i denotes the ith diagonal element of D_1. Thus, the condition number of H_{k+1} can be computed as the ratio of the largest eigenvalue to the smallest eigenvalue (in magnitude). The condition number of B_{k+1} is the reciprocal of this value.

When B_{k+1} a quasi-Newton matrix generated by SR1 updates, the procedure is similar except $\tilde{\Psi}_k$ has half as many columns resulting in $(k+1)$ eigenvalues given by $\gamma^{-1} + d_i$ for $1 \le i \le (k+1)$ and $n - (k+1)$ eigenvalues of γ^{-1}. After a new quasi-Newton pair is computed it is possible to update the QR factorization (for details, see [**?**]).

5. Numerical experiments

In this section, we demonstrate the accuracy of the proposed method for solving quasi-Newton equations. We solve the following linear system:

$$B_{k+1}p_k = -g_k \tag{49}$$

where B_{k+1} is an SR1 matrix or a member of the restricted Broyden class of updates. For SR1 matrices, we compare the following methods:

(1) The self-duality method (Algorithm 2)
(2) Compact inverses formulation (Algorithm 5)

For members of the restricted Broyden class of updates, we considered three values of ϕ: $0.00, 0.50$, and 0.99 and compare the following methods:

(1) Recursive SMW approach (Algorithm 3)
(2) Recursion to compute products with H_{k+1} (Algorithm 4)
(3) Compact inverses formulation (Algorithm 6)

Additionally, when $\phi = 0.00$, we also test the "two-loop recursion" (Algorithm 1).

We consider problem sizes (n) ranging from $10,000$ to $1,000,000$. We present the norms of the relative residuals:

$$\frac{\|B_{k+1}p_k - (-g_k)\|_2}{\|g_k\|_2},$$

and the time (in seconds) needed to compute each solution. The number of limited memory updates was set to five.

We simulate the first five iterations of an unconstrained line-search method. We generate the initial point x_0 and the gradients $g_j = \nabla f(x_j)$, for $0 \le j \le 5$, randomly and compute the subsequent iterations

$$x_{j+1} = x_j - \alpha_j H_j g_j, \qquad \text{for } 0 \le j \le 5,$$

where $H_j = B_j^{-1}$ is the inverse of the quasi-Newton matrix.

Results.

The results are presented in Tables 1–7. All algorithms were able to solve the linear systems to high accuracy. The update-specific two-loop recursion (Algorithm 1) for L-BFGS matrices performed the best in terms of computational time. However, for the (general) restricted Broyden class matrices the compact inverse formulation outperformed the other methods. For the SR1 case, the compact inverse formulation outperformed the algorithm based on self-duality (Algorithm 2).

Table 1. Relative error and computational time (in seconds) for SR1 matrices.

n	Self-Duality (Alg. 2)		Compact Inverses (Alg. 5)	
	Rel. Error	Time	Rel. Error	Time
10,000	1.98e-15	4.47e-03	6.10e-15	1.04e-03
50,000	2.24e-14	7.25e-03	7.57e-14	1.89e-03
100,000	5.07e-14	1.66e-02	6.44e-14	4.61e-03
1,000,000	8.67e-13	2.93e-01	2.26e-12	4.66e-02

TABLE 2. Relative error for Broyden class matrices with $\phi = 0.00$ (BFGS).

n	Two-Loop Recursion (Alg. 1)	Recursive SMW (Alg. 3)	Recursive H_{k+1} (Alg. 4)	Compact Inverses (Alg. 6)
10,000	4.88e-16	4.63e-16	5.37e-16	3.59e-16
50,000	2.93e-16	4.44e-16	3.61e-16	4.20e-16
100,000	6.64e-16	3.74e-16	6.16e-16	3.81e-16
1,000,000	1.47e-15	1.46e-15	1.45e-15	1.51e-15

TABLE 3. Computational time (in seconds) for Broyden class matrices with $\phi = 0.00$ (BFGS).

n	Two-Loop Recursion (Alg. 1)	Recursive SMW (Alg. 3)	Recursive H_{k+1} (Alg. 4)	Compact Inverses (Alg. 6)
10,000	8.40e-04	6.71e-03	4.83e-03	4.65e-03
50,000	4.03e-03	3.75e-02	2.34e-02	6.95e-03
100,000	6.17e-03	8.09e-02	5.44e-02	1.29e-02
1,000,000	1.38e-01	1.42e+00	8.90e-01	1.16e-01

TABLE 4. Relative error for Broyden class matrices with $\phi = 0.50$.

n	Recursive SMW (Alg. 3)	Recursive H_{k+1} (Alg. 4)	Compact Inverses (Alg. 6)
10,000	9.90e-16	8.37e-16	8.15e-16
50,000	4.25e-16	6.80e-16	5.82e-15
100,000	7.00e-16	6.31e-16	9.14e-16
1,000,000	2.77e-16	2.40e-16	3.56e-16

TABLE 5. Computational time (in seconds) for Broyden class matrices with $\phi = 0.50$.

n	Recursive SMW (Alg. 3)	Recursive H_{k+1} (Alg. 4)	Compact Inverses (Alg. 6)
10,000	8.62e-03	7.10e-03	6.08e-03
50,000	4.23e-02	2.39e-02	6.21e-03
100,000	8.31e-02	5.60e-02	1.22e-02
1,000,000	1.49e+00	8.96e-01	1.20e-01

6. CONCLUDING REMARKS

We derived the compact formulation for members of the restricted Broyden class and the SR1 update. With this compact formulation, we showed how to solve linear systems defined by limited-memory quasi-Newton matrices. Numerical results suggest that this proposed approach is efficient and accurate. This approach has

TABLE 6. Relative error for Broyden class matrices with $\phi = 0.99$.

n	Recursive SMW (Alg. 3)	Recursive H_{k+1} (Alg. 4)	Compact Inverses (Alg. 6)
10,000	8.33e-16	1.59e-15	1.63e-15
50,000	8.45e-15	1.21e-14	3.88e-15
100,000	7.28e-14	6.67e-14	2.67e-14
1,000,000	2.59e-15	1.80e-15	3.29e-15

TABLE 7. Computational time (in seconds) for Broyden class matrices with $\phi = 0.99$.

n	Recursive SMW (Alg. 3)	Recursive H_{k+1} (Alg. 4)	Compact Inverses (Alg. 6)
10,000	8.87e-03	9.65e-03	4.89e-03
50,000	3.84e-02	2.56e-02	6.24e-03
100,000	8.29e-02	5.21e-02	1.21e-02
1,000,000	1.51e+00	8.44e-01	1.20e-01

two distinct advantages over existing procedures for solving limited-memory quasi-Newton systems. First, there is a natural way to use the compact formulation for the inverse to obtain the condition number of the linear system. Second, when a new quasi-Newton pair is computed, computational savings can be achieved by simple updates to the matrix factors in the compact formulation.

Future work includes integrating this linear solver inside line-search and trust-region methods for large-scale optimization.

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Appendix A. At each iteration, Algorithm 3 computes α and u, which are defined in (9) and require matrix-vector products involving the matrices B_i for $0 \leq i \leq k$. The main difficulty in computing α and u is the computation of matrix-vector products with the matrices B_i for each i. Note that if we are able to form $u_{3j+2} = B_j s_j$, then we are able to compute all other terms that use $B_j s_j$ in (9). In what follows, we show how to compute u_{3j+2} without storing B_i for $0 \leq i \leq k$. This idea is based on Procedure 7.6 in [**?**].

We begin by writing $C_{3(k+1)}$ in (10) as follows:

$$C_{3(k+1)} \quad = \quad B_0 + \sum_{j=0}^{k} \alpha_{3j} u_{3j} u_{3j}^T + \alpha_{3j+1} u_{3j+1} u_{3j+1}^T + \alpha_{3j+2} u_{3j+2} u_{3j+2}^T,$$

where α_i and u_i are defined by (9). Since $B_j = C_{3j}$, then

$$\begin{aligned} u_{3j+2} &= B_j s_j \\ &= \left(B_0 + \sum_{i=0}^{j-1} \alpha_{3i} u_{3i} u_{3i}^T + \alpha_{3i+1} u_{3i+1} u_{3i+1}^T + \alpha_{3i+2} u_{3i+2} u_{3i+2}^T \right) s_j \\ &= B_0 s_j + \sum_{i=0}^{j-1} \alpha_{3i} (u_{3i}^T s_j) u_{3i} + \alpha_{3i+1} (u_{3i+1}^T s_j) u_{3i+1} + \alpha_{3i+2} (u_{3i+2}^T s_j) u_{3i+2}. \end{aligned}$$

All the terms in the above summation only involve vectors that have been previously computed. Having computed u_{3j+2}, it is then possible to compute $\alpha_{3j+1}, \alpha_{3j+2}$, and u_{3j+1}. (The other terms α_{3j} and u_{3j} do not depend on $B_j s_j$.) The following algorithm computes the terms α and u that are used in Algorithm 3.

Algorithm A.1: Unrolling the limited-memory Broyden convex class formula.

for $j = 0, \ldots, k$

$u_{3j} \leftarrow y_j$;

$\alpha_{3j} \leftarrow 1/(s_j^T y_j)$;

$u_{3j+2} \leftarrow B_0 s_j + \sum_{i=0}^{j-1} \left[\alpha_{3i} (u_{3i}^T s_j) u_{3i} + \alpha_{3i+1} (u_{3i+1}^T s_j) u_{3i+1} + \alpha_{3i+2} (u_{3i+2}^T s_j) u_{3i+2} \right]$;

$\alpha_{3j+2} \leftarrow -1/(s_j^T u_{3j+2})$;

$u_{3j+1} \leftarrow \alpha_{3j} y_j + \alpha_{3j+2} u_{3j+2}$;

$\alpha_{3j+1} = -\phi/\alpha_{3j+2}$;

end

Appendix B. The following algorithm computes products involving the matrices H_i for $0 \leq i \leq k$ for use in Algorithm 4. The algorithm avoids storing any matrices, and matrix-vector products are computed recursively. The derivation of this algorithm is similar to that for Algorithm A.1.

Algorithm B.2: Unrolling the limited-memory Broyden convex class formula.

for $j = 0, \ldots, k$

$\hat{u}_{3j} \leftarrow s_j$;

$\hat{\alpha}_{3j} \leftarrow 1/(s_j^T y_j)$;

$\hat{u}_{3j+1} \leftarrow H_0 y_j + \sum_{i=0}^{j-1} \left[\hat{\alpha}_{3i} (\hat{u}_{3i}^T y_j) \hat{u}_{3i} + \hat{\alpha}_{3i+1} (\hat{u}_{3i+1}^T y_j) \hat{u}_{3i+1} + \hat{\alpha}_{3i+2} (\hat{u}_{3i+2}^T y_j) \hat{u}_{3i+2} \right]$;

$\hat{\alpha}_{3j+1} \leftarrow -1/(y_j^T \hat{u}_{3j+2})$;

$\hat{u}_{3j+2} \leftarrow \hat{\alpha}_{3j} s_j + \hat{\alpha}_{3j+2} \hat{u}_{3j+2}$;

Compute α_{3j+2} using Algorithm A.1;

$\Phi_j \leftarrow (1-\phi)/(1 - \phi + \phi \hat{\alpha}_{3j}^2 / (\hat{\alpha}_{3j+1} \alpha_{3j+2}))$;

$\hat{\alpha}_{3j+2} = -\Phi_j / \hat{\alpha}_{3j+2}$;

end

References

[1] O. Burdakov, L. Gong, Y.-X. Yuan, and S. Zikrin, *On efficiently combining limited memory and trust-region techniques*, Tech. Report 2013:13, Linkping University, The Institute of Technology, 2013.

[2] R. H. Byrd, J. Nocedal, and R. B. Schnabel, *Representations of quasi-Newton matrices and their use in limited-memory methods*, Math. Program., 63 (1994), pp. 129–156.

[3] A. R. Conn, N. I. M. Gould, and P. L. Toint, *Trust-Region Methods*, Society for Industrial and Applied Mathematics (SIAM), Philadelphia, PA, 2000.

[4] J. E. Dennis, Jr and J. J. Moré, *Quasi-newton methods, motivation and theory*, SIAM Review, 19 (1977), pp. 46–89.

[5] J. B. Erway, V. Jain, and R. F. Marcia, *Shifted limited-memory DFP systems*, in 2013 Asilomar Conference on Signals, Systems and Computers, Nov 2013, pp. 1033–1037.

[6] J. B. Erway and R. F. Marcia, *Limited-memory BFGS systems with diagonal updates*, Linear Algebra and its Applications, 437 (2012), pp. 333–344.

[7] J. B. Erway and R. F. Marcia, *On efficiently computing the eigenvalues of limited-memory quasi-newton matrices*, SIAM Journal on Matrix Analysis and Applications, 36 (2015), pp. 1338–1359.

[8] G. H. Golub and C. F. Van Loan, *Matrix Computations*, The Johns Hopkins University Press, Baltimore, Maryland, third ed., 1996.

[9] I. Griva, S. G. Nash, and A. Sofer, *Linear and nonlinear programming*, Society for Industrial and Applied Mathematics, Philadelphia, 2009.

[10] D. G. Luenberger and Y. Ye, *Linear and nonlinear programming*, vol. 116, Springer, 2008.

[11] K. S. Miller, *On the Inverse of the Sum of Matrices*, Mathematics Magazine, 54 (1981), pp. 67–72.

[12] J. L. Morales and J. Nocedal, *Automatic preconditioning by limited memory quasi-newton updating*, SIAM Journal on Optimization, 10 (2000), pp. 1079–1096.

[13] J. Nocedal, *Updating quasi-Newton matrices with limited storage*, Mathematics of Computation, 35 (1980), pp. 773–782.

[14] J. Nocedal and S. J. Wright, *Numerical Optimization*, Springer-Verlag, New York, second ed., 2006.

[15] D. P. O'Leary and A Yeremin, *The linear algebra of block quasi-newton algorithms*, Linear Algebra and Its Applications, 212 (1994), pp. 153–168.

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