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Properties of the block BFGS update and its application to the limited-memory block BNS method for unconstrained minimization[1]

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Abstract:

A block version of the BFGS variable metric update formula and its modifications are investigated. In spite of the fact that this formula satisfies the quasi-Newton conditions with all used difference vectors and that the improvement of convergence is the best one in some sense for quadratic objective functions, for general functions it does not guarantee that the corresponding direction vectors are descent. To overcome this difficulty, but at the same time utilize the advantageous properties of the block BFGS update, a block version of the limited-memory variable metric BNS method for large scale unconstrained optimization is proposed. The global convergence of the algorithm is established for convex sufficiently smooth functions. Numerical experiments demonstrate the efficiency of the new method.

Keywords:
Unconstrained minimization, block variable metric methods, limited-memory methods, the BFGS update, global convergence, numerical results

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1 Introduction

In this paper we propose a block version of the widely used BNS method, see [1], for large scale unconstrained optimization

$$\min f(x): \ x \in \mathcal{R}^N,$$

where it is assumed that the problem function $f : \mathcal{R}^N \to \mathcal{R}$ is differentiable.

The BNS method belongs to the variable metric (VM) or quasi-Newton (QN) line search iterative methods, see [6], [12]. They start with an initial point $x_0 \in \mathcal{R}^N$ and generate iterations x_{k+1} by the process $x_{k+1} = x_k + s_k$, $s_k = t_k d_k$, $k \ge 0$, where d_k is the direction vector and the stepsize $t_k > 0$ is chosen in such a way that

$$f_{k+1} - f_k \le \varepsilon_1 t_k g_k^T d_k, \qquad g_{k+1}^T d_k \ge \varepsilon_2 g_k^T d_k \tag{1.1}$$

(the Wolfe line search conditions, see e.g. [15]), $0 < \varepsilon_1 < 1/2$, $\varepsilon_1 < \varepsilon_2 < 1$, $f_k = f(x_k)$ and $g_k = \nabla f(x_k)$. Usually $d_k = -H_k g_k$ with a symmetric positive definite matrix H_k; typically H_0 is a multiple of I and H_{k+1} is obtained from H_k by a VM update to satisfy the QN condition (secant equation)

$$H_{k+1} y_k = s_k \tag{1.2}$$

(see [6], [12]), where $y_k = g_{k+1} - g_k$. For $k \ge 0$ we denote

$$B_k = H_k^{-1}, \qquad b_k = s_k^T y_k,$$

(note that $b_k > 0$ for $g_k \ne 0$ by (1.1)). To simplify the notation we frequently omit index k and replace index $k+1$ by symbol $+$ and index $k-1$ by symbol $-$.

Among VM methods, the BFGS method, see [6], [12], [15], belongs to the most efficient; the update formula preserves positive definite VM matrices and can be written in the following quasi-product form

$$H_+ = \frac{1}{b} s s^T + \Big(I - \frac{1}{b} s y^T\Big) H \Big(I - \frac{1}{b} y s^T\Big). \tag{1.3}$$

The BFGS method can be easily modified for the large-scale optimization; the BNS and L-BFGS (see [8], [14], [9] - subroutine PLIS) methods represent its well-known limited-memory adaptations. In every iteration we recurrently update matrix $\zeta_k I$, $\zeta_k > 0$, (without forming an approximation of the inverse Hessian matrix explicitly) by the BFGS method, using m couples of vectors $(s_{k-\tilde{m}}, y_{k-\tilde{m}}), \dots, (s_k, y_k)$ successively, where

$$\tilde{m} = \min(k, \hat{m}-1), \quad m = \tilde{m} + 1 \tag{1.4}$$

and $\hat{m} > 1$ is a given parameter. In case of the BNS method, matrix H_+ can be expressed either in the form, see [1],

$$H_+ = \zeta I + \Big[S, \zeta Y\Big] \begin{bmatrix} U^{-T}(D + \zeta Y^T Y)U^{-1} & -U^{-T} \\ -U^{-1} & 0 \end{bmatrix} \begin{bmatrix} S^T \\ \zeta Y^T \end{bmatrix},$$

where $S_k = [s_{k-\tilde{m}}, \dots, s_k]$, $Y_k = [y_{k-\tilde{m}}, \dots, y_k]$, $D_k = \mathrm{diag}[b_{k-\tilde{m}}, \dots, b_k]$, $(U_k)_{i,j} = (S_k^T Y_k)_{i,j}$ for $i \le j$, $(U_k)_{i,j} = 0$ otherwise (an upper triangular matrix), or in the form, also given in [1]

$$H_+ = S U^{-T} D U^{-1} S^T + \zeta \Big(I - S U^{-T} Y^T\Big)\Big(I - Y U^{-1} S^T\Big). \tag{1.5}$$

This indicate that direction vectors can be calculated efficiently without computing of H_+ explicitly, see [1].

For S^TY nonsingular and any $\bar{H} \in \mathcal{R}^{N\times N}$, the BFGS update formula (1.3) can be easily generalized to the following block version

$$H_+ = S(S^TY)^{-1}S^T + P^T\bar{H}P\,, \quad P = I - Y(S^TY)^{-1}S^T, \tag{1.6}$$

which satisfies the QN conditions $H_+Y = S$, i.e. for the whole block of stored difference vectors. This generalization of the BFGS update of $\bar{H}$ was derived by Schnabel [16] for S^TY and $\bar{H}$ symmetric positive definite, using a variational approach, and by Hu and Storey [7] for quadratic functions, using corrections for the exact line search. Both in [16] and in [7], some modifications of matrices Y (and also S in [7]) are proposed with intent to replace S^TY by a symmetric positive definite matrix. Note that these modifications disturb the QN conditions from previous iterations.

Formula (1.6) is not directly applicable to general functions, since it does not guarantee that the corresponding direction vectors are descent if the matrix S^TY is not positive definite (i.e. $S^TY + Y^TS$ symmetric positive definite). To overcome this difficulty and at the same time utilize the advantageous properties of the block BFGS update in the limited-memory context, in each iteration we determine $n \geq 1$ and split matrices S and Y in such a way that $S = [S_{[1]}, \ldots, S_{[n]}]$, $Y = [Y_{[1]}, \ldots, Y_{[n]}]$, where all blocks $S_{[i]}^TY_{[i]}$ are positive definite. Afterwards we replace the BNS formula (1.5) by n successive updates of an initial VM matrix H_I (ζI for the BNS method (1.5)) using a modification of the block BFGS update (1.6) with matrices $S_{[i]}$, $Y_{[i]}$ instead of S, Y (the block BNS method, see Section 4). Obviously, for $n = m$ we obtain the BNS method. The question how to form suitable blocks $S_{[i]}, Y_{[i]}$ will be discussed in Section 5. Numerical results indicate that this approach can improve results significantly compared to the BNS and L-BFGS method.

In spite of the fact that matrix H_+ is unsymmetric generally, we use the conventional direction vector $d_+ = -H_+g_+$, such that $z^* = x_+ + d_+$ solves the problem $g(z^*) = 0$, $g(z) = g_+ + H_+^{-1}(z - x_+)$ (a linear model for gradients which respects the QN conditions: $g(x_+) = g_+$, $g(x) = g$ for $H_+y = s$, $g(x_-) = g_-$ for $H_+y = s$ and $H_+y_- = s_-, \ldots$). In this way, for ill-conditioned problems we usually obtained better results than e.g. with the vector $\bar{d}_+ = -(1/2)(H_+ + H_+^T)g_+$, which minimizes the quadratic function $\bar{Q}(\bar{d}) = \bar{d}^T(H_+ + H_+^T)^{-1}\bar{d} + g_+^T\bar{d}$.

In Section 2 we derive the block BFGS update for general functions, present its properties and modifications and show some connections with the corrected BFGS update, see [18] and [17]. In Section 3 we focus on quadratic functions and show optimality of the block BFGS method and a role of unit stepsizes. In Section 4 we investigate the block BNS method and derive a convenient formula similar to (1.5) to represent the resulting VM matrix and a related formula for efficient calculation of the direction vector. The corresponding algorithm is described in Section 5. The global convergence of the algorithm is established in Section 6 and numerical results are reported in Section 7.

We will denote by $\|\cdot\|_F$ the Frobenius matrix norm, by $\|\cdot\|$ the spectral matrix norm, by $|\cdot|$ the size of both scalars and vectors (the Euclidean vector norm) and by $[A]_{n_1}^{n_2}$ the principal submatrix of A with both row and column indices of entries from n_1 to n_2.

2 The block BFGS update

Using a variational approach, we will derive the block BFGS update (1.6) for general functions, investigate its generalized form and show some connections with methods based on vector corrections from previous iterations for conjugacy.

2.1 Derivation and basic properties

To derive the basic variant of the block BFGS update, given by Theorem 2.2, we utilize Theorem 2.1, which is a block version (with S, Y instead of s, y) of Corollary 2.3 in [3].

Lemma 2.1. *Suppose that a matrix $J \in \mathcal{R}^{N\times m}$ has a full rank, $u \in \mathcal{R}^m$ and $x^* = J(J^TJ)^{-1}u$. Then x^* is the unique solution to $\min_{x\in\mathcal{R}^N} |x|$ s.t. $J^Tx = u$.*

Proof. Obviously $J^Tx^* = u$. Let $x' = x^* + v$ and $J^Tx' = u$ for some $v \in \mathcal{R}^N$. Then $J^Tv = 0$, thus $|x'|^2 = u^T(J^TJ)^{-1}u + |v|^2$, which yields the desired conclusion. □

Theorem 2.1. *Let $S, Y \in \mathcal{R}^{N\times m}$, $A, W_L, W_R \in \mathcal{R}^{N\times N}$, W_L, W_R nonsingular, $V = W_R^T W_R Y$ and let the matrix Y have a full rank. Then V^TY is nonsingular and the unique solution to*

$$\min_{A_N\in\mathcal{R}^{N\times N}} ||W_L^{-1}(A_N - A)W_R^{-1}||_F \quad s.t. \quad A_NY = S \tag{2.1}$$

is

$$A_N = AP_V + S(V^TY)^{-1}V^T, \quad P_V = I - Y(V^TY)^{-1}V^T. \tag{2.2}$$

Proof. We denote $\Omega = W_L^{-1}(A_N - A)W_R^{-1} \triangleq [\omega_1, \dots, \omega_N]^T$ and $J = W_RY$. Since $J^T\Omega^T = (\Omega W_RY)^T = (A_NY - AY)^TW_L^{-T}$, problem (2.1) can be rewritten as

$$\min_{\omega_i\in\mathcal{R}^N} \sum_{i=1}^N |\omega_i|^2 \quad s.t. \quad J^T\Omega^T = (S - AY)^TW_L^{-T}.$$

Denoting $[u_1, \dots, u_N] = (S - AY)^TW_L^{-T}$, this can be broken up into N disjoint problems

$$\min_{\omega_i\in\mathcal{R}^N} |\omega_i|^2 \quad s.t. \quad J^T\omega_i = u_i, \quad i = 1, \dots, N.$$

Using Lemma 2.1 (J has obviously full rank), we get $\Omega^T= J(J^TJ)^{-1}(S-AY)^TW_L^{-T}$, i.e.

$$\begin{aligned} W_L^{-1}(A_N - A)W_R^{-1} &= \Omega = W_L^{-1}(S - AY)(J^TJ)^{-1}J^T, \\ A_N - A &= (S - AY)(J^TJ)^{-1}J^TW_R, \end{aligned}$$

which gives (2.2) and nonsingularity of V^TY by $J^TW_R = V^T$ and $J^TJ = V^TY$. □

Since the matrix A_N is meant as an approximation of the inverse Hessian matrix, thus near to a symmetric matrix, and since the nearest symmetric matrix to any matrix M in the Frobenius norm is $\frac{1}{2}(M+M^T)$ by Lemma 4.1 in [3], we will construct a matrix A^* satisfying $A^*Y = S$ nearest to the subspace of symmetric matrices in $\mathcal{R}^{N\times N}$. Following the approach used in [3], we will find $\lim_{i\to\infty} A_i$, where in view of Theorem 2.1

$$A_0 = AP_V+S(V^TY)^{-1}V^T, \quad A_{i+1}= (1/2)(A_i+A_i^T)P_V + S(V^TY)^{-1}V^T, \quad i = 0, 1, \dots \tag{2.3}$$

Theorem 2.2. *Let the assumptions of Theorem 2.1 be satisfied and sequence* $\{A_i\}_{i=0}^{\infty}$ *be defined by (2.3). Then*

$$\lim_{i\to\infty} A_i = (1/2)P_V^T(A+A^T)P_V + V(V^TY)^{-T}S^TP_V + S(V^TY)^{-1}V^T \triangleq A^*. \qquad (2.4)$$

Moreover, if $T\in\mathcal{R}^{m\times m}$ *is nonsingular and* $V=ST$, *we obtain the block BFGS update (1.6) with* $H_+ = A^*$, $\bar{H} = (1/2)(A+A^T)$.

Proof. First we prove (the matrix V^TY is nonsingular by Theorem 2.1)

$$A_i = (1/2^i)Z + A^*, \qquad Z = V(V^TY)^{-T}(A^TY-S)^TP_V, \qquad (2.5)$$

$i=1,2,\dots,$ by induction. For $i=1$ it is true, since from (2.3) we get

$$\begin{aligned} A_1 - S(V^TY)^{-1}V^T &= \tfrac{1}{2}\left(A_0+A_0^T\right)P_V = \tfrac{1}{2}\left(AP_V+P_V^TA^T+V(V^TY)^{-T}S^T\right)P_V \\ &= \tfrac{1}{2}\left(I-P_V^T\right)AP_V + \tfrac{1}{2}P_V^T(A+A^T)P_V + \tfrac{1}{2}V(V^TY)^{-T}S^TP_V \\ &= \tfrac{1}{2}V(V^TY)^{-T}(A^TY-S)^TP_V + V(V^TY)^{-T}S^TP_V + \tfrac{1}{2}P_V^T(A+A^T)P_V \end{aligned}$$

by $V^TP_V = 0$, $P_V^2 = P_V$ and $I-P_V^T = V(V^TY)^{-T}Y^T$.

Suppose that (2.5) is true for some $i\ge 1$. By $V^TP_V = 0$ and $P_V^2 = P_V$ we obtain

$$(A^*)^TP_V = \frac{1}{2}P_V^T(A+A^T)P_V + V(V^TY)^{-T}S^TP_V = A^* - S(V^TY)^{-1}V^T = A^*P_V$$

and $ZP_V = Z$, $Z^TP_V = 0$, which by (2.3) and (2.5) yields

$$A_{i+1} = \frac{1}{2}(A_i+A_i^T)P_V + S(V^TY)^{-1}V^T = \frac{1}{2^{i+1}}Z + (A^* - S(V^TY)^{-1}V^T) + S(V^TY)^{-1}V^T,$$

i.e. (2.5) is true for $i+1$, which completes the induction. Consequently, this implies (2.4).

Finally, let $V = ST$. Then $P_V = I - Y(T^TS^TY)^{-1}T^TS^T = I - Y(S^TY)^{-1}S^T = P$ (see (1.6)), $S^TP_V = 0$ and

$$A^* = \frac{1}{2}P^T(A+A^T)P + S(S^TY)^{-1}S^T, \qquad (2.6)$$

which is (1.6) with $H_+ = A^*$, $\bar{H} = (1/2)(A+A^T)$. □

In the sequel, we give some properties of the block BFGS update, similar to the well-known properties of the standard BFGS update. To be able to prove some assertions (e.g. Corollary 2.1) easily, we will investigate the generalized form of (1.6)

$$H_+ = S(S^TY\,C)^{-1}S^T + \left(I - S(S^TY)^{-T}Y^T\right)\bar{H}\left(I - Y(S^TY)^{-1}S^T\right) \qquad (2.7)$$

(i.e. (1.6) with Y replaced by YC), where we consider any nonsingular matrices $\bar{H}\in\mathcal{R}^{N\times N}$ and $S^TY, C\in\mathcal{R}^{m\times m}$. First we prove the following lemmas.

Lemma 2.2. *Let* $W_i\in\mathcal{R}^{\mu\times\nu}$, $\mu>0, \nu>0$, $i=1,\dots,4$, *and* $W_4^TW_3 = I$. *Then*

$$\det\left(I + W_1W_2^T - W_3W_4^T\right) = \det\left(W_2^TW_3\right).\det\left(W_4^TW_1\right). \qquad (2.8)$$

Proof. Denoting $\alpha = \det\left(I + W_1W_2^T - W_3W_4^T\right)$, we can write

$$\begin{vmatrix} I & W_2^T & 0 \\ -W_1 & I & W_3 \\ 0 & W_4^T & I \end{vmatrix} = \begin{vmatrix} I & W_2^T & 0 \\ 0 & I+W_1W_2^T & W_3 \\ 0 & W_4^T & I \end{vmatrix} = \begin{vmatrix} I & W_2^T & 0 \\ 0 & I+W_1W_2^T-W_3W_4^T & W_3 \\ 0 & 0 & I \end{vmatrix} = \alpha.$$

The initial determinant on the left can be rewritten in another way as follows:

$$\alpha = \begin{vmatrix} I & W_2^T & 0 \\ -W_1 & I & W_3 \\ W_4^T W_1 & 0 & I - W_4^T W_3 \end{vmatrix} = \begin{vmatrix} I & W_2^T & 0 \\ -W_1 & I & W_3 \\ W_4^T W_1 & 0 & 0 \end{vmatrix} = \begin{vmatrix} I & W_2^T & -W_2^T W_3 \\ -W_1 & I & 0 \\ W_4^T W_1 & 0 & 0 \end{vmatrix}$$

by $W_4^T W_3 = I$. To obtain the desired result, we multiply the third block column of the last determinant by -1 and interchange it with the first block column. □

Lemma 2.3. *Let $A \in \mathcal{R}^{N\times N}$ be a positive definite (not necessarily symmetric) matrix. Then A is nonsingular and matrix A^{-1} is also positive definite.*

Proof. Obviously, A is nonsingular. Let $q \in \mathcal{R}^N$, $q \neq 0$, $p = A^{-1}q$. Then $q^T A^{-1} q = p^T A^T p = p^T A p > 0$. □

Theorem 2.3. *Let matrices $S^T Y$ and C be nonsingular and let the matrix H_+ be given by (2.7). Then $H_+ Y = SC^{-1}$ and*

(a) if we replace the matrices S, Y in (2.7) by ST_S, YT_Y with $T_S, T_Y \in \mathcal{R}^{m\times m}$ nonsingular, then the corresponding matrix H_+ can be also written in the form (2.7) with C replaced by $T_Y\, C\, T_S^{-1}$,

(b) for $\bar H, H_+$ and $S^T \bar B S$ nonsingular and $\bar B = \bar H^{-1}$, the matrix $B_+ = H_+^{-1}$ is given by

$$B_+ = \bar B - \bar B S(S^T \bar B S)^{-1} S^T \bar B + YC(S^T Y)^{-T} Y^T, \tag{2.9}$$

(c) for $\bar H, H_+$ and $S^T \bar B S$ nonsingular, the determinant of B_+ is

$$\det B_+ = \det \bar B \,.\, \det(S^T Y\, C) / \det(S^T \bar B S). \tag{2.10}$$

(d) for $\bar H$ and $S^T Y\, C$ positive definite, also H_+ is positive definite.

Proof. (a) We simply replace S, Y by ST_S, YT_Y in (2.7) and rewrite the relation.

(b) Denoting $B'_+ = \bar B - \bar B S(S^T \bar B S)^{-1} S^T \bar B + YC(S^T Y)^{-T} Y^T$, we have $B'_+ S = YC$, thus we get from (2.7)

$$\begin{aligned} B'_+ H_+ &= YC(S^T Y\, C)^{-1} S^T + \left(B'_+ - YC(S^T Y)^{-T} Y^T\right) \bar H \left(I - Y(S^T Y)^{-1} S^T\right) \\ &= Y(S^T Y)^{-1} S^T + \left(I - \bar B S(S^T \bar B S)^{-1} S^T\right)\left(I - Y(S^T Y)^{-1} S^T\right) \\ &= I - \bar B S(S^T \bar B S)^{-1} S^T + \bar B S(S^T \bar B S)^{-1} S^T Y(S^T Y)^{-1} S^T = I. \end{aligned}$$

(c) Using (2.9) and Lemma 2.2 with $W_1 = \bar H Y C$, $W_2^T = (S^T Y)^{-T} Y^T$, $W_3 = S(S^T \bar B S)^{-1}$, $W_4^T = S^T \bar B$, we get

$$\begin{aligned} \det B_+ &= \det \bar B \,.\, \det\left(I - S(S^T \bar B S)^{-1} S^T \bar B + \bar H Y C(S^T Y)^{-T} Y^T\right) \\ &= \det \bar B \,.\, \det\left(I - W_3 W_4^T + W_1 W_2^T\right) = \det \bar B \,.\, \det\left((S^T \bar B S)^{-1}\right) . \det(S^T Y\, C)\,. \end{aligned}$$

(d) Let $q \in \mathcal{R}^N$, $q \neq 0$. If $S^T q \neq 0$, then $q^T H_+ q \geq q^T S(S^T Y\, C)^{-1} S^T q > 0$ by Lemma 2.3, otherwise $q^T H_+ q = q^T \bar H q > 0$. □

Corollary 2.1. *Let the matrices $S^T Y$ and $\bar H$ be nonsingular, $\bar H$ symmetric, $\bar B = \bar H^{-1}$, and let the matrices $S^T \bar B S$ and H_+ given by (2.7) with $C = I$ (i.e. by (1.6)) be nonsingular. Then*

$$\Big(\frac{1}{2}\Big(H_+ + H_+^T\Big)\Big)^{-1} = \bar{B} - \bar{B}S\Big(S^T\bar{B}S\Big)^{-1}S^T\bar{B} + Y\Big(\frac{1}{2}\Big(S^TY + Y^TS\Big)\Big)^{-1}Y^T, \quad (2.11)$$
$$\frac{1}{2}\Big(B_+ + B_+^T\Big) = \bar{B} - \bar{B}S\Big(S^T\bar{B}S\Big)^{-1}S^T\bar{B} + \frac{1}{2}Y\Big((S^TY)^{-1} + (Y^TS)^{-1}\Big)Y^T, \quad (2.12)$$
$$\det\Big(\frac{1}{2}\Big(H_+ + H_+^T\Big)\Big)^{-1} = \det\bar{B}\,.\det\Big(\frac{1}{2}\Big((S^TY)^{-1} + (Y^TS)^{-1}\Big)\Big)^{-1}\Big/\det(S^T\bar{B}S)\,, \quad (2.13)$$
$$\det\frac{1}{2}\Big(B_+ + B_+^T\Big) = \det\bar{B}\,.\det\frac{1}{2}\Big(S^TY + Y^TS\Big)/\det(S^T\bar{B}S)\,. \quad (2.14)$$

Proof. From (1.6) we obtain $\frac{1}{2}(H_+ + H_+^T) = \frac{1}{2}S((S^TY)^{-1} + (Y^TS)^{-1})S^T + P^T\bar{H}P$, which can be written in the form (2.7) with $C = (\frac{1}{2}(I + (Y^TS)^{-1}S^TY))^{-1}$ and H_+ replaced by $\frac{1}{2}(H_+ + H_+^T)$. Using Theorem 2.3 (b) – (c), we get (2.11) – (2.13). Since (2.12) can be written in the form (2.9) with $C = \frac{1}{2}(I + (S^TY)^{-1}Y^TS)$ and B_+ replaced by $\frac{1}{2}(B_+ + B_+^T)$, Theorem 2.3 (c) yields (2.14). $\square$

2.2 Connections with methods based on vector corrections

The following lemma shows that if we correct vectors s, y suitably, the BFGS update of the block BFGS update with submatrices S_P, Y_P of S, Y with columns from previous iterations (i.e. without s, y) can be expressed as the block BFGS update (2.7).

Lemma 2.4. *Let $S \triangleq [S_P, s]$, $Y \triangleq [Y_P, y]$, the matrices $S_P^TY_P$, T_S^P, $T_Y^P \in \mathcal{R}^{\tilde{m}\times\tilde{m}}$ be nonsingular, $C_P = T_Y^P(T_S^P)^{-1}$, $P_P = I - Y_P(S_P^TY_P)^{-1}S_P^T$, $\tilde{s} = P_P^Ts$, $\tilde{y} = P_Py$, $\tilde{b} = \tilde{s}^T\tilde{y} \neq 0$ and*

$$H_P = S_P(S_P^TY_P\,C_P)^{-1}S_P^T + P_P^T\bar{H}P_P \quad (2.15)$$

(i.e. (2.7) with S, Y, C replaced by S_P, Y_P, C_P), where $\bar{H}$ is a nonsingular matrix. Then also the corrected BFGS update

$$H_+ = \frac{1}{\tilde{b}}\,\tilde{s}\tilde{s}^T + \Big(I - \frac{1}{\tilde{b}}\,\tilde{s}\tilde{y}^T\Big)H_P\Big(I - \frac{1}{\tilde{b}}\,\tilde{y}\tilde{s}^T\Big) \quad (2.16)$$

of H_P can be equivalently written in the form (2.7) with $C = T_YT_S^{-1}$, where

$$T_S = \begin{bmatrix} T_S^P & -(S_P^TY_P)^{-T}Y_P^Ts \\ & 1 \end{bmatrix}, \quad T_Y = \begin{bmatrix} T_Y^P & -(S_P^TY_P)^{-1}S_P^Ty \\ & 1 \end{bmatrix} \quad (2.17)$$

(the upper block triangular matrices). Moreover, $S_P^TB_+\tilde{s} = \tilde{s}^TH_P^{-1}S_P = 0$ holds and if $\bar{H}$ and $S_P^TY_P\,C_P$ are symmetric matrices, then also H_P, H_+ and $S^TY\,C$ are symmetric.

Proof. Setting $\bar{S} = S\,T_S, \bar{Y} = Y\,T_Y$, we obtain $\bar{S} = [S_PT_S^P, s - S_P(S_P^TY_P)^{-T}Y_P^Ts\,] = [S_PT_S^P, P_P^Ts\,] = [S_PT_S^P, \tilde{s}\,]$ and similarly $\bar{Y} = [Y_PT_Y^P, P_Py\,] = [Y_PT_Y^P, \tilde{y}\,]$, which yields

$$\bar{S}^T\bar{Y} = \begin{bmatrix} (T_S^P)^TS_P^TY_PT_Y^P & (T_S^P)^TS_P^TP_Py \\ s^TP_PY_PT_Y^P & \tilde{b} \end{bmatrix} = \begin{bmatrix} (T_S^P)^TS_P^TY_PT_Y^P & 0 \\ 0 & \tilde{b} \end{bmatrix} \quad (2.18)$$

by $P_P^TS_P = P_PY_P = 0$. Using (2.18), we get

$$\bar{S}(\bar{S}^T\bar{Y})^{-1}\bar{S}^T = S_P(S_P^TY_PC_P)^{-1}S_P^T + \frac{1}{\tilde{b}}\tilde{s}\tilde{s}^T, \quad \bar{Y}(\bar{S}^T\bar{Y})^{-1}\bar{S}^T = Y_P(S_P^TY_P)^{-1}S_P^T + \frac{1}{\tilde{b}}\tilde{y}\tilde{s}^T. \quad (2.19)$$

Setting $\tilde{P} = I - (1/\tilde{b})\,\tilde{y}\tilde{s}^T$, from (2.16) we obtain successively

$$
\begin{aligned}
H_+ &= \frac{1}{\tilde b}\tilde s\tilde s^T + \tilde P^T H_P \tilde P \;=\; \frac{1}{\tilde b}\tilde s\tilde s^T + \tilde P^T S_P (S_P^T Y_P\, C_P)^{-1} S_P^T \tilde P + \tilde P^T P_P^T \bar H P_P \tilde P \\
&= \frac{1}{\tilde b}\tilde s\tilde s^T + S_P (S_P^T Y_P\, C_P)^{-1} S_P^T + \left(I - \frac{1}{\tilde b}\tilde s\tilde y^T\right) P_P^T \bar H P_P \left(I - \frac{1}{\tilde b}\tilde y\tilde s^T\right) \\
&= \frac{1}{\tilde b}\tilde s\tilde s^T + S_P (S_P^T Y_P\, C_P)^{-1} S_P^T + \left(P_P^T - \frac{1}{\tilde b}\tilde s\tilde y^T P_P^T\right) \bar H \left(P_P - \frac{1}{\tilde b} P_P \tilde y\tilde s^T\right) \\
&= \frac{1}{\tilde b}\tilde s\tilde s^T + S_P (S_P^T Y_P\, C_P)^{-1} S_P^T \\
&\quad + \left(I - S_P (S_P^T Y_P)^{-T} Y_P^T - \frac{1}{\tilde b}\tilde s\tilde y^T\right) \bar H \left(I - Y_P (S_P^T Y_P)^{-1} S_P^T - \frac{1}{\tilde b}\tilde y\tilde s^T\right)
\end{aligned}
$$

by $P_P^2 = P_P$ and $P_P^T S_P = 0$, which yields $\tilde P^T S_P = S_P - (1/\tilde b)\tilde s\tilde y^T P_P^T S_P = S_P$. Using (2.19), from this we have

$$
H_+ = \bar S(\bar S^T \bar Y)^{-1}\bar S^T + \left(I - \bar S(\bar S^T \bar Y)^{-T}\bar Y^T\right)\bar H\left(I - \bar Y(\bar S^T \bar Y)^{-1}\bar S^T\right), \tag{2.20}
$$

which can be written in the form (2.7) by Theorem 2.3*(a)*.

Since $H_+\tilde y = \tilde s$ and $H_P Y_P = S_P\, C_P^{-1}$, i.e. $H_P^{-1} S_P = Y_P C_P$ by (2.16) and (2.15), we have $S_P^T B_+ \tilde s = S_P^T \tilde y = S_P^T P_P y = 0$ and $\tilde s^T H_P^{-1} S_P = \tilde s^T Y_P C_P = s^T P_P Y_P C_P = 0$ by $P_P^T S_P = P_P Y_P = 0$.

If $\bar H$ and $S_P^T Y_P\, C_P$ are symmetric matrices, then also H_P and $(T_S^P)^T S_P^T Y_P T_Y^P$ are symmetric by (2.15) and $(T_S^P)^T S_P^T Y_P T_Y^P = (T_S^P)^T (S_P^T Y_P\, C_P) T_S^P$, which yields the symmetry of the matrices H_+, $\bar S^T \bar Y$ and $S^T Y\, C$ by (2.16), (2.18) and by the equality $S^T Y\, C = T_S^{-T}(\bar S^T \bar Y)\, T_S^{-1}$. □

In view of the relations $S_P^T B_+ \tilde s = \tilde s^T H_P^{-1} S_P = 0$, we can regard the transformations $s \to \tilde s = P_P^T s = s - S_P (S_P^T Y_P)^{-T} Y_P^T s$, $y \to \tilde y = P_P y = y - Y_P (S_P^T Y_P)^{-1} S_P^T y$ (or the transformations $S \to \bar S$, $Y \to \bar Y$) in Lemma 2.4 as corrections from previous iterations for conjugacy, which shows some connections with methods [18] and [17], where similar corrections are used.

Although variational characterizations of such corrections are significant mainly for quadratic functions, see Section 3, the following theorem indicates that we can expect good properties of the block BFGS update also for functions similar to quadratic (e.g. near to a local minimum).

Theorem 2.4. *Let* $S \triangleq [S_P, s]$, $Y \triangleq [Y_P, y]$, $\ddot s = s + S_P\sigma$, $\ddot y = y + Y_P\sigma$, $\sigma \in \mathcal{R}^{\tilde m}$, $\tilde m \geq 1$, $\tilde s = P_P^T s$, $\tilde y = P_P\, y$, $P_P = I - Y_P (S_P^T Y_P)^{-1} S_P^T$, $\ddot b = \ddot s^T \ddot y$, $\tilde b = \tilde s^T \tilde y$ *and* $S^T Y$ *be symmetric positive definite. Then* $\ddot b \geq \tilde b$ *and* $\tilde b = s^T \tilde y > 0$ *for any* $\sigma \in \mathcal{R}^{\tilde m}$. *Moreover, let* H_P *be given by (2.15) with* $C_P = I$, H_+ *by (1.6) and* $\ddot a = \ddot y^T H_P \ddot y$, $\tilde a = \tilde y^T H_P \tilde y$. *If we define* $\ddot H_+$ *by*

$$
\ddot H_+ = \frac{1}{\ddot b}\,\ddot s\ddot s^T + \left(I - \frac{1}{\ddot b}\,\ddot s\ddot y^T\right) H_P \left(I - \frac{1}{\ddot b}\,\ddot y\ddot s^T\right) \tag{2.21}
$$

(the corrected BFGS update) and if a symmetric positive definite matrix $\bar G$ *satisfying* $\bar G S = Y$ *is given, then within* $\sigma \in \mathcal{R}^{\tilde m}$ *we have* $\bar G\ddot s = \ddot y$, $\ddot a \geq \tilde a$ *and*

$$
\|\bar G^{1/2}\ddot H_+ \bar G^{1/2} - I\|_F^2 = (1 - \ddot a/\ddot b)^2 - 2\,|\,\bar G^{1/2}(\ddot s - H_P \ddot y)\,|^2/\ddot b + \|\bar G^{1/2} H_P \bar G^{1/2} - I\|_F^2\,; \tag{2.22}
$$

this value is minimized by the choice $\ddot s = \tilde s$, $\ddot y = \tilde y$, *when* $\ddot H_+ = H_+$.

Proof. From $\tilde{s} = P_P^T s$ and $\tilde{y} = P_P\, y$ we obtain $\tilde{b} = s^T \tilde{y}$ by $P_P^2 = P_P$, which gives

$$\tilde{b} = b - s^T Y_P (S_P^T Y_P)^{-1} S_P^T y\,. \tag{2.23}$$

From $\ddot{s} = s + S_P \sigma$ and $\ddot{y} = y + Y_P \sigma$ we get $\ddot{b} = b + 2y^T S_P \sigma + \sigma^T S_P^T Y_P \sigma$, which can be written as

$$\ddot{b} = b - y^T S_P (S_P^T Y_P)^{-1} S_P^T y + \Big(\sigma + (S_P^T Y_P)^{-1} S_P^T y\Big)^T S_P^T Y_P \Big(\sigma + (S_P^T Y_P)^{-1} S_P^T y\Big)\,. \tag{2.24}$$

Since the matrices $S^T Y, S_P^T Y_P$ are symmetric positive definite by assumption, we have $\tilde{b} > 0$ by (2.23), Theorem 2.22 in [5] and $S_P^T y = Y_P^T s$. Comparing (2.24) and (2.23), we can see that always $\ddot{b} \ge \tilde{b}$ holds.

Let $\bar{G} S = Y$ with $\bar{G}$ symmetric positive definite. Obviously $\bar{G}\ddot{s} = \ddot{y}$ and $\bar{G}\tilde{s} = y - Y_P (S_P^T Y_P)^{-T} Y_P^T s = \tilde{y}$. Denoting $w = \bar{G}^{1/2}\ddot{s}$, $\tilde{w} = \bar{G}^{1/2}\tilde{s}$, $W = \bar{G}^{1/2} H_P \bar{G}^{1/2}$, $\ddot{W} = \bar{G}^{1/2} \ddot{H}_+ \bar{G}^{1/2}$ and $M = I - W$, we have $|w|^2 = \ddot{b} \ge \tilde{b} = |\tilde{w}|^2 > 0$ and (2.21) can be written in the form

$$\ddot{W} = (1/|w|^2) w w^T + \ddot{P} W \ddot{P} = I - \ddot{P} M \ddot{P}, \qquad \ddot{P} = I - (1/|w|^2) w w^T, \tag{2.25}$$

by $\bar{G}\ddot{s} = \ddot{y}$ and $\ddot{P}^2 = \ddot{P}$. In view of the fact that the trace of a product of two square matrices is independent of the order of the multiplication, from (2.25) we obtain

$$\begin{aligned} \|I - \ddot{W}\|_F^2 &= \|\ddot{P} M \ddot{P}\|_F^2 = \mathrm{Tr}(\ddot{P} M \ddot{P} M) = \mathrm{Tr}\Big(\Big[M - (1/|w|^2) w w^T M\Big]^2\Big) \\ &= \|M\|_F^2 - \mathrm{Tr}\Big(w w^T M^2 + M w w^T M - \Big[w^T M w / |w|^2\Big]\, w w^T M\Big)/|w|^2 \\ &= \|M\|_F^2 - 2|Mw|^2/|w|^2 + (w^T M w)^2/|w|^4, \end{aligned} \tag{2.26}$$

i.e. (2.22) by $Mw = \bar{G}^{1/2}(\ddot{s} - H_P \ddot{y})$ and $w^T M w = \ddot{b} - \ddot{a}$. In view of $H_P Y_P = S_P$ by (2.15) and in view of $s^T Y_P = y^T S_P$ by symmetry of $S^T Y$, values $|Mw|$ and $w^T M w$ are independent of σ, as we can see from

$$\begin{aligned} \ddot{s} - H_P \ddot{y} &= s + S_P \sigma - H_P y - H_P Y_P \sigma = s - H_P y\,, \\ \ddot{b} - \ddot{a} &= (\ddot{s} - H_P \ddot{y})^T \ddot{y} = (s - H_P y)^T (y + Y_P \sigma) = s^T y - y^T H_P y + (s^T Y_P - y^T S_P)\sigma. \end{aligned}$$

In view of (2.26) we can write $\|I - \ddot{W}\|_F^2 = \varphi(|\tilde{w}|^2/|w|^2)$, where function

$$\varphi(\xi) = \xi^2 (\tilde{w}^T M \tilde{w})^2/|\tilde{w}|^4 - 2\,\xi |M\tilde{w}|^2/|\tilde{w}|^2 + \|M\|_F^2 \tag{2.27}$$

is nonincreasing on $[0,1]$, since $\varphi'(\xi)/2 = \xi(\tilde{w}^T M \tilde{w})^2/|\tilde{w}|^4 - |M\tilde{w}|^2/|\tilde{w}|^2 \le 0$ for $\xi \in [0,1]$ by the Schwarz inequality. Therefore value $\|I - \ddot{W}\|_F^2$ is minimized by the choice $\ddot{s} = \tilde{s}$, $\ddot{y} = \tilde{y}$, which gives $|w| = |\tilde{w}|$, i.e. maximizes $|\tilde{w}|/|w|$. For this choice, matrices $\ddot{H}_+$ and H_+ are identical by Lemma 2.4, where for $C_P = I$ (i.e. $T_S^P = T_Y^P$) and $S^T Y$ symmetric we have $T_S = T_Y$, thus $C = I$.

The rest follows immediately from $\ddot{a} = (\ddot{a} - \ddot{b}) + \ddot{b} = (\tilde{a} - \tilde{b}) + \ddot{b} \ge (\tilde{a} - \tilde{b}) + \tilde{b}$. □

Seemingly, in accordance with Theorem 2.4, the block BFGS update should be advantageous in case that the matrix $S^T Y$ is positive definite and near to symmetric (e.g. near to a local minimum). Paradoxically, the standard BFGS update often gives better results if $S^T Y$ is almost symmetric and the Hessian matrix is ill-conditioned. Therefore we will use, in addition to the block BFGS update, i.e. update (2.21) of H_P with

$$\ddot{s} = \tilde{s}, \qquad \ddot{y} = \tilde{y} \tag{2.28}$$

by Lemma 2.4, also the standard BFGS update of H_P, i.e. (2.21) with

$$\ddot{s} = s, \qquad \ddot{y} = y, \tag{2.29}$$

or a special update of H_P given by (2.21) with

$$\ddot{s} = s - (s^T y_-/b_-)s_-, \qquad \ddot{y} = y - (y^T s_-/b_-)y_-, \tag{2.30}$$

which can be more robust than the block BFGS update. In Section 4 we show how it can be used within the block BNS method. The question how to choose a suitable update will be discussed in Section 5. For functions similar to quadratic, the choice (2.30) can also be characterized variationally:

Theorem 2.5. *Let $\hat{S} = [s_-, s]$, $\hat{Y} = [y_-, y]$, $\hat{s} = s-(s^T y_-/b_-)s_-$, $\hat{y} = y-(y^T s_-/b_-)y_-$, $\ddot{s} = s-\alpha s_-$, $\ddot{y} = y-\alpha y_-$, $\alpha \in \mathcal{R}$, $\hat{b} = \hat{s}^T\hat{y}$, $\ddot{b} = \ddot{s}^T\ddot{y}$. Then $\hat{b} = s^T\hat{y}$; if the matrix $\hat{S}^T\hat{Y}$ is symmetric positive definite, then $\ddot{b} \geq \hat{b} > 0$ for any $\alpha \in \mathcal{R}$. Moreover, let H_P be given by (2.15) with $C_P = I$ and $\ddot{a} = \ddot{y}^T H_P \ddot{y}$. If we define $\ddot{H}_+$ by (2.21) and a symmetric positive definite matrix $\bar{G}$ satisfying $\bar{G}\hat{S} = \hat{Y}$ is given, then within $\alpha \in \mathcal{R}$ the relations $\bar{G}\ddot{s} = \ddot{y}$ and (2.22) hold. Besides, the values $\ddot{a}$ and (2.22) are minimized by the choice $\ddot{s} = \hat{s}$, $\ddot{y} = \hat{y}$.*

Proof. We have $\hat{s}^T\hat{y} = s^T\hat{y} - (s^T y_-/b_-)s_-^T[y-(s_-^T y/b_-)y_-] = s^T\hat{y}$. If the matrix $\hat{S}^T\hat{Y}$ is symmetric positive definite, then $s^T y_- = y^T s_-$, the value $\ddot{b} = b - 2\alpha s^T y_- + \alpha^2 b_-$ is minimized by $\alpha = s^T y_-/b_-$, i.e. by $\ddot{s} = \hat{s}$, $\ddot{y} = \hat{y}$ and the minimum value is $\hat{b} = s^T\hat{y} = b - s^T y_-\, s_-^T y/b_-$ with $\hat{b} > 0$ by Theorem 2.22 in [5].

Let $\bar{G}\hat{S} = \hat{Y}$ with $\bar{G}$ symmetric positive definite. Setting $\sigma = (0, \dots, 0, -\alpha)^T$ and replacing $\tilde{s}$ by $\hat{s}$, $\tilde{y}$ by $\hat{y}$, $\tilde{b}$ by $\hat{b}$ and $\tilde{a}$ by $\hat{y}^T H_P \hat{y}$, we can proceed in the same way as in the proof of Theorem 2.4. □

3 Results for quadratic functions

In this section we suppose that f is a quadratic function with a symmetric positive definite Hessian G (thus $GS = Y$ and $S^T Y = S^T G S$ is a symmetric matrix) and show optimality of the block BFGS method and a role of unit stepsizes, which are very frequent, not only for quadratic functions. Here we consider only the G-conjugacy of vectors.

The following theorem shows that the block BFGS update gives the best improvement of convergence in some sense for linearly independent direction vectors.

Theorem 3.1. *Let f be a quadratic function $f(x) = \frac{1}{2}(x-\bar{x})^T G(x-\bar{x})$, $\bar{x} \in \mathcal{R}^N$, with a symmetric positive definite matrix G, $k > 0$, the vectors $s_{k-\tilde{m}}, \dots, s_k$ be linearly independent and let $\tilde{S}_i = [s_{k-\tilde{m}}, \dots, s_i]$, $\tilde{Y}_i = [y_{k-\tilde{m}}, \dots, y_i]$, $\tilde{P}_i = I - \tilde{Y}_i(\tilde{S}_i^T\tilde{Y}_i)^{-1}\tilde{S}_i^T$, $i = k-\tilde{m}, \dots, k$, $\ddot{s}_i = s_i + \tilde{S}_{i-1}\sigma_{i-1}$, $\ddot{y}_i = y_i + \tilde{Y}_{i-1}\sigma_{i-1}$, $\sigma_{i-1} \in \mathcal{R}^{i-1}$, $\tilde{s}_i = \tilde{P}_{i-1}^T s_i$, $\tilde{y}_i = \tilde{P}_{i-1} y_i$, $i = k-\tilde{m}+1, \dots, k$, $\ddot{s}_{k-\tilde{m}} = \tilde{s}_{k-\tilde{m}} = s_{k-\tilde{m}}$, $\ddot{y}_{k-\tilde{m}} = \tilde{y}_{k-\tilde{m}} = y_{k-\tilde{m}}$. Then $\tilde{S}_i^T\tilde{Y}_i$ are symmetric positive definite and $\ddot{s}_i^T\ddot{y}_i \geq \tilde{s}_i^T\tilde{y}_i > 0$, $i = k-\tilde{m}, \dots, k$. Moreover, if $\bar{H}$ is a symmetric positive definite matrix and if we define H_{k+1} by (1.6) and $\ddot{H}_{k+1}$ by $\ddot{H}_{k-\tilde{m}} = \bar{H}$ and*

$$\ddot{H}_{i+1} = (1/\ddot{s}_i^T\ddot{y}_i)\, \ddot{s}_i\ddot{s}_i^T + \Big(I - (1/\ddot{s}_i^T\ddot{y}_i)\, \ddot{s}_i\ddot{y}_i^T\Big)\ddot{H}_i\Big(I - (1/\ddot{s}_i^T\ddot{y}_i)\, \ddot{y}_i\ddot{s}_i^T\Big), \tag{3.1}$$

$i = k-\tilde{m}, \dots, k$, then value $\|G^{1/2}\ddot{H}_{k+1}G^{1/2} - I\|_F$ is minimized and the matrices $\ddot{H}_{k+1}$ and H_{k+1} are identical and symmetric positive definite for $\ddot{s}_i = \tilde{s}_i$, $\ddot{y}_i = \tilde{y}_i$, $i = k-\tilde{m}+1, \dots, k$.

Proof. Since the columns of $S=\tilde{S}_k$ are linearly independent, the matrices $\tilde{S}_i^T\tilde{Y}_i = \tilde{S}_i^T G\tilde{S}_i$, $i=k-\tilde{m},\ldots,k$, are symmetric positive definite and we can set $\tilde{H}_{i+1}=\tilde{S}_i(\tilde{S}_i^T\tilde{Y}_i)^{-1}\tilde{S}_i^T + \tilde{P}_i^T\bar{H}\tilde{P}_i$, $i=k-\tilde{m},\ldots,k$. Using successively Theorem 2.4 with $\bar{G}=G$ and $S=\tilde{S}_i$, $Y=\tilde{Y}_i$, $H_P=\tilde{H}_i$, $H_+=\tilde{H}_{i+1}$, $i=k-\tilde{m}+1,\ldots,k$, we get that values $\|G^{1/2}\ddot{H}_{i+1}G^{1/2}-I\|_F$ are minimized and the matrices $\ddot{H}_{i+1}$ and $\tilde{H}_{i+1}$ are identical and symmetric positive definite for the choice $\ddot{s}_i=\tilde{s}_i$, $\ddot{y}_i=\tilde{y}_i$, $i=k-\tilde{m}+1,\ldots,k$, when $\ddot{H}_{k+1}=\tilde{H}_{k+1}=H_{k+1}$. □

In Section 2 we mentioned the similarity to the methods based on the corrections from previous iterations for conjugacy. The following theorem, which can be proved similarly as Theorem 3.3 in [18], shows that in two successive iterations with VM matrices H, H_+ obtained by the block BFGS updates, the only unit stepsize is sufficient to have all stored direction vectors from previous iterations conjugate with vector s_+.

Note that the vectors $S_P^T y_+$, $Y_P^T s_+$ from the preceding iteration are used for functions near to quadratic in the process of the suitable update formula selection, see Section 5.

Theorem 3.2. *Let f be a quadratic function $f(x)=\frac{1}{2}(x-\bar{x})^T G(x-\bar{x})$, $\bar{x}\in\mathcal{R}^N$, let G,H,H_+ be symmetric positive definite matrices satisfying $HY_P=S_P$ and $H_+Y=S$, where $S\triangleq[S_P,s]$, $Y\triangleq[Y_P,y]$, let $d=-Hg$, $d_+=-H_+g_+$ and $t=1$, i.e. $s=d$. Then $S_P^T y_+ = Y_P^T s_+ = 0$, i.e. all columns of S_P are conjugate with vector s_+.*

4 The block BNS method

In this section we will derive some representations of matrix H_+ which generalize the BNS formula (1.5). For this purpose, we split matrices S, Y in such a way that $S=[S_{[1]},\ldots,S_{[n]}]$, $Y=[Y_{[1]},\ldots,Y_{[n]}]$ and use the theory in Section 2 for the matrices $S_{[i]},Y_{[i]}$ instead of S,Y, where $n\in[1,m]$ is calculated in such a way that all blocks $S_{[i]}^T Y_{[i]}$ are positive definite (i.e. $S_{[i]}^T Y_{[i]} + Y_{[i]}^T S_{[i]}$ are symmetric positive definite), which is satisfied e.g. for $n=m$, when we get the BNS method.

To construct the matrix H_+, in view of (2.6) we set $H_{[1]}=H_I$, $H_+=H_{[n+1]}$, where

$$H_{[i+1]}=S_{[i]}(S_{[i]}^T Y_{[i]} C_{[i]})^{-1} S_{[i]}^T + \frac{1}{2} P_{[i]}^T\Big(H_{[i]}+H_{[i]}^T\Big)P_{[i]},\quad P_{[i]}=I-Y_{[i]}(S_{[i]}^T Y_{[i]})^{-1}S_{[i]}^T, \tag{4.1}$$

for $S_{[i]}^T Y_{[i]} C_{[i]}$ nonsingular, $i=1,\ldots,n$. We consider arbitrary nonsingular matrices $H_I, C_{[i]}$, although only the choice $H_I=\zeta I$, $\zeta>0$, $C_{[i]}=I$ is used in Sections 5−7. Obviously, all matrices $H_{[i]}$ are positive definite for this choice by Theorem 2.3 (d) and have only a theoretical significance (are not formed explicitly). Note that notation here is partly different than in the previous sections.

In the process of splitting matrices S,Y, we start with the matrices $S_{[n]},Y_{[n]}$ to have maximum of the latest QN conditions satisfied (for $C_{[n]}=I$). Thus to test positive definiteness of the blocks $S_{[i]}^T Y_{[i]}$, $i=n,\ldots,1$, we use the RL factorization arranged in reverse order compared to the usual LU factorization. The following lemma converts the problem of the RL factorization to the same problem of a smaller dimension, see Section 5 for details.

Lemma 4.1. *Suppose that $A,R,L\in\mathcal{R}^{\mu\times\mu}$, $\mu>0$, $u,v\in\mathcal{R}^{\mu}$, $\alpha\in\mathcal{R}$, $\alpha\neq 0$,*

$$\bar{A}=\begin{bmatrix} A & u \\ v^T & \alpha \end{bmatrix},\quad \bar{R}=\begin{bmatrix} R & u \\ & \alpha \end{bmatrix},\quad \bar{L}=\begin{bmatrix} L & \\ (1/\alpha)\,v^T & 1 \end{bmatrix} \tag{4.2}$$

($\bar{R}$ is an upper block triangular matrix, $\bar{L}$ lower block triangular). Then to get $\bar{A}=\bar{R}\bar{L}$, it suffices to find R, L satisfying $A-(1/\alpha)uv^T=RL$. Moreover,

(a) if $u=v$ then the matrix $\bar{A}$ is symmetric positive definite if and only if both $\alpha>0$ and the matrix $A-(1/\alpha)uv^T$ is symmetric positive definite,

(b) if the matrix $\bar{A}$ is positive definite, then $\alpha>0$ and $A-(1/\alpha)uv^T$ is positive definite.

Further, if principal minors $\det[\bar{A}]_i^{\mu+1}$ (see the end of Section 1) are nonzero, $i=1,\ldots,\mu+1$, then we can continue in this way repeatedly, i.e. the whole factorization process is well defined, and the result factorization is unique.

Proof. Let $A-(1/\alpha)uv^T=RL$. Using relations for $\bar{R},\bar{L}$ in (4.2), we obtain

$$\bar{R}\bar{L}=\begin{bmatrix} RL+(1/\alpha)uv^T & u \\ v^T & \alpha \end{bmatrix}=\bar{A}\,.$$

Using Theorem 2.22 in [5], we get (a). Let $\bar{A}$ be positive definite. Then also $\bar{A}^{-1}$ is positive definite by Lemma 2.3, obviously together with all its principal submatrices. Similarly we deduce that $\alpha>0$ (a principal submatrix of $\bar{A}$). Since the matrix $A-(1/\alpha)uv^T$ (the Schur complement of entry α in $\bar{A}$) is the inverse of a principal submatrix of $\bar{A}^{-1}$ by Theorem 1.23 in [5], it is positive definite by Lemma 2.3. Finally, the existence and uniqueness of the factorization under the conditions above follows from Theorem 1.24 in [5], considering the rows and columns of $\bar{A},\bar{R},\bar{L}$ arranged in reverse order. □

The following lemma generalizes the approach used in the proof of Theorem 2.2 in [1].

Lemma 4.2. *Let $\mu,\nu>0$, $S_L,Y_L\in\mathcal{R}^{N\times\mu}$, $S_R,Y_R\in\mathcal{R}^{N\times\nu}$, $S_C=[S_L,S_R]$, $Y_C=[Y_L,Y_R]$, $U_L,E_L\in\mathcal{R}^{\mu\times\mu}$, $C_R\in\mathcal{R}^{\nu\times\nu}$, $\bar{H}_I\in\mathcal{R}^{N\times N}$, U_L, $S_R^TY_R$ and C_R nonsingular,*

$$H_L = S_LU_L^{-T}E_LU_L^{-1}S_L^T+(I-S_LU_L^{-T}Y_L^T)\bar{H}_I(I-Y_LU_L^{-1}S_L^T)\,, \tag{4.3}$$

$$H_C = S_R(S_R^TY_R\,C_R)^{-1}S_R^T+P_R^TH_LP_R,\quad P_R=I-Y_R(S_R^TY_R)^{-1}S_R^T\,. \tag{4.4}$$

Then matrix H_C can be written in the form

$$H_C=S_CU_C^{-T}E_CU_C^{-1}S_C^T+(I-S_CU_C^{-T}Y_C^T)\bar{H}_I(I-Y_CU_C^{-1}S_C^T), \tag{4.5}$$

where

$$U_C=\begin{bmatrix} U_L & S_L^TY_R \\ & S_R^TY_R \end{bmatrix},\qquad E_C=\begin{bmatrix} E_L & \\ & Y_R^TS_R\,C_R^{-1} \end{bmatrix} \tag{4.6}$$

(matrix U_C is upper block triangular, E_C block diagonal).

Proof. From (4.3) – (4.4) we obtain

$$H_C=S_R(S_R^TY_R\,C_R)^{-1}S_R^T+P_R^TS_LU_L^{-T}E_LU_L^{-1}S_L^TP_R+K^T\bar{H}_IK, \tag{4.7}$$

where

$$\begin{aligned} K &= \left(I-Y_LU_L^{-1}S_L^T\right)\left(I-Y_R(S_R^TY_R)^{-1}S_R^T\right) \\ &= I-Y_LU_L^{-1}S_L^T-Y_R(S_R^TY_R)^{-1}S_R^T+Y_LU_L^{-1}S_L^TY_R(S_R^TY_R)^{-1}S_R^T \\ &= I-\left[Y_L,Y_R\right]\begin{bmatrix} U_L^{-1} & -U_L^{-1}S_L^TY_R(S_R^TY_R)^{-1} \\ & (S_R^TY_R)^{-1} \end{bmatrix}\begin{bmatrix} S_L^T \\ S_R^T \end{bmatrix}=I-Y_C\,U_C^{-1}S_C^T\,. \end{aligned}$$

Using this representation of U_C^{-1}, we obtain $[\,I\;\;0\,]\,U_C^{-1}=[U_L^{-1},-U_L^{-1}S_L^TY_R(S_R^TY_R)^{-1}]$, therefore

$$U_L^{-1}S_L^T P_R = U_L^{-1}S_L^T - U_L^{-1}S_L^T Y_R (S_R^T Y_R)^{-1} S_R^T = [\, I \;\; 0\,]\, U_C^{-1} S_C^T \tag{4.8}$$

by (4.7). Similarly $[\,0 \;\; I\,]\,U_C^{-1} = [\,0, (S_R^T Y_R)^{-1}]$, i.e. $(S_R^T Y_R)^{-1} S_R^T = [\,0 \;\; I\,]\, U_C^{-1} S_C^T$, thus

$$\begin{aligned} S_R (S_R^T Y_R\, C_R)^{-1} S_R^T &= S_R\, (S_R^T Y_R)^{-T} Y_R^T S_R C_R^{-1} (S_R^T Y_R)^{-1} S_R^T \\ &= S_C\, U_C^{-T} [\,0 \;\; I\,]^T Y_R^T S_R\, C_R^{-1}\, [\,0 \;\; I\,]\, U_C^{-1} S_C^T \\ &= S_C U_C^{-T} \begin{bmatrix} 0 & \\ & Y_R^T S_R C_R^{-1} \end{bmatrix} U_C^{-1} S_C^T. \end{aligned} \tag{4.9}$$

To get (4.5), it suffices to use (4.6) – (4.9) together with $K = I - Y_C\, U_C^{-1} S_C^T$. □

The following theorem describes a basic version of the block BNS method.

Theorem 4.1. *Let* $S = [S_{[1]}, \dots, S_{[n]}]$, $Y = [Y_{[1]}, \dots, Y_{[n]}]$, $n \geq 1$, $S_i = [S_{[1]}, \dots, S_{[i]}]$, $Y_i = [Y_{[1]}, \dots, Y_{[i]}]$, *matrices* $S_{[i]}^T Y_{[i]}\, C_{[i]}$ *be nonsingular, matrices* $H_{[i+1]}$ *be given by (4.1),* $i = 1, \dots, n$, *and* $H_{[1]} = H_I$. *Then*

$$H_{[i+1]} = S_i U_i^{-T} E_i U_i^{-1} S_i^T + \frac{1}{2}\Big(I - S_i U_i^{-T} Y_i^T\Big)\Big(H_I + H_I^T\Big)\Big(I - Y_i U_i^{-1} S_i^T\Big), \tag{4.10}$$

where (an upper block triangular matrix)

$$U_i = \begin{bmatrix} S_{[1]}^T Y_{[1]} & \dots & S_{[1]}^T Y_{[i-1]} & S_{[1]}^T Y_{[i]} \\ & \ddots & \vdots & \vdots \\ & & S_{[i-1]}^T Y_{[i-1]} & S_{[i-1]}^T Y_{[i]} \\ & & & S_{[i]}^T Y_{[i]} \end{bmatrix}, \tag{4.11}$$

$$E_i = \operatorname{diag}\left[\frac{1}{2}\Big(\Sigma_1 + \Sigma_1^T\Big), \dots, \frac{1}{2}\Big(\Sigma_{i-1} + \Sigma_{i-1}^T\Big), \Sigma_i\right], \quad \Sigma_j = Y_{[j]}^T S_{[j]} C_{[j]}^{-1}, \tag{4.12}$$

$i, j = 1, \dots, n$.

Proof. We will proceed by induction on i. For $i = 1$, update (4.1) can be written as

$$H_{[2]} = S_{[1]} (S_{[1]}^T Y_{[1]})^{-T} (Y_{[1]}^T S_{[1]}\, C_{[1]}^{-1}) (S_{[1]}^T Y_{[1]})^{-1} S_{[1]}^T + \frac{1}{2} P_{[1]}^T \Big(H_I + H_I^T\Big) P_{[1]}\,,$$

i.e. (4.10) with $U_1 = S_{[1]}^T Y_{[1]}$, $E_1 = Y_{[1]}^T S_{[1]}\, C_{[1]}^{-1} = \Sigma_1$.

Suppose that (4.10) – (4.12) hold for some $i < n$ and set $\bar{H}_{[i+1]} = \frac{1}{2}(H_{[i+1]} + H_{[i+1]}^T)$ and

$$H_{[i+2]} = S_{[i+1]} (S_{[i+1]}^T Y_{[i+1]}\, C_{[i+1]})^{-1} S_{[i+1]}^T + P_{[i+1]}^T \bar{H}_{[i+1]} P_{[i+1]} \tag{4.13}$$

in view of (4.1). Since $\bar{H}_{[i+1]}$ can be written in the form (4.10) with E_i replaced by $\bar{E}_i = \frac{1}{2}(E_i + E_i^T)$, we can use Lemma 4.2 with $S_L = S_i$, $Y_L = Y_i$, $S_R = S_{[i+1]}$, $Y_R = Y_{[i+1]}$, $C_R = C_{[i+1]}$, $S_C = S_{i+1}$, $Y_C = Y_{i+1}$, $U_L = U_i$, $E_L = \bar{E}_i$, $\bar{H}_I = \frac{1}{2}(H_I + H_I^T)$, $H_L = \bar{H}_{[i+1]}$, $H_C = H_{[i+2]}$. Denoting $E_{i+1} = \operatorname{diag}\Big[\bar{E}_i\,, \Sigma_{i+1}\Big]$, we obtain (4.10) with $H_{[i+1]}$, S_i, Y_i, U_i, E_i replaced by $H_{[i+2]}, S_{i+1}, Y_{i+1}, U_{i+1}, E_{i+1}$ and the induction is established with $i+1$ replacing i. □

Similar representations of H_{k+1} can be derived also for update (2.21) with the choice (2.30), which we sometimes use instead of the last update (4.1), see Section 5.

Corollary 4.1. *Let* $H_{[1]} = H_I$, $n \geq 1$, $S = [S_{[1]}, \dots, S_{[n]}] \triangleq [S_P, s]$, $Y = [Y_{[1]}, \dots, Y_{[n]}] \triangleq [Y_P, y]$, $S_{[n]} \triangleq [S_{[n]}^P, s]$, $Y_{[n]} \triangleq [Y_{[n]}^P, y]$, $\hat{s} = s - \alpha s_-$, $\hat{y} = y - \beta y_-$, $\alpha = s^T y_- / b_-$, $\beta = y^T s_- / b_-$, $\hat{s}^T \hat{y} \neq 0$, $\hat{S} = [S_P, \hat{s}]$, $\hat{Y} = [Y_P, \hat{y}]$, *the matrices* $S_{[i]}^T Y_{[i]}\, C_{[i]}$, $i = 1, \dots, n-1$, $(S_{[n]}^P)^T Y_{[n]}^P C_{[n]}^P$ *be nonsingular, the matrices* $H_{[i]}$, $i = 2, \dots, n$, *be given by update (4.1) and a matrix* H_+ *by*

$$H_+ = (1/\hat{s}^T\hat{y})\,\hat{s}\hat{s}^T + \Big(I-(1/\hat{s}^T\hat{y})\,\hat{s}\hat{y}^T\Big)H_P\Big(I-(1/\hat{s}^T\hat{y})\,\hat{y}\hat{s}^T\Big), \tag{4.14}$$

$$H_P = S^P_{[n]}\Big((S^P_{[n]})^T Y^P_{[n]} C^P_{[n]}\Big)^{-1}(S^P_{[n]})^T + \frac{1}{2}(P^P_{[n]})^T\Big(H_{[n]}+H^T_{[n]}\Big)P^P_{[n]}, \tag{4.15}$$

$$P^P_{[n]} = I - Y^P_{[n]}\Big((S^P_{[n]})^T Y^P_{[n]}\Big)^{-1}(S^P_{[n]})^T. \tag{4.16}$$

Then

$$H_+ = \hat{S}\hat{U}^{-T}\hat{E}\hat{U}^{-1}\hat{S}^T + \tfrac{1}{2}\Big(I-\hat{S}\hat{U}^{-T}\hat{Y}^T\Big)\Big(H_I+H_I^T\Big)\Big(I-\hat{Y}\hat{U}^{-1}\hat{S}^T\Big) \tag{4.17}$$

$$= S\tilde{U}^{-T}\tilde{E}\tilde{U}^{-1}S^T + \tfrac{1}{2}\Big(I-S\tilde{U}^{-T}Y^T\Big)\Big(H_I+H_I^T\Big)\Big(I-Y\tilde{U}^{-1}S^T\Big), \tag{4.18}$$

where

$$\hat{U}=\begin{bmatrix} U_P & S_P^T\hat{y} \\ & s^T\hat{y}\end{bmatrix},\quad \hat{E}=\begin{bmatrix} E_P & \\ & s^T\hat{y}\end{bmatrix},\quad \tilde{U}=\begin{bmatrix} U_P & S_P^T y \\ \alpha\tilde{u}^T & s^T y\end{bmatrix},\quad \tilde{E}=\begin{bmatrix} E_P & \beta\tilde{w} \\ \beta\tilde{v}^T & \kappa\end{bmatrix}, \tag{4.19}$$

$$U_P=\begin{bmatrix} S^T_{[1]}Y_{[1]} & \dots & S^T_{[1]}Y_{[n-1]} & S^T_{[1]}Y^P_{[n]} \\ & \ddots & \vdots & \vdots \\ & & S^T_{[n-1]}Y_{[n-1]} & S^T_{[n-1]}Y^P_{[n]} \\ & & & (S^P_{[n]})^T Y^P_{[n]}\end{bmatrix},\quad E_P=\begin{bmatrix} \frac{1}{2}(\Sigma_1+\Sigma_1^T) & & \\ & \ddots & & \\ & & \frac{1}{2}(\Sigma_{n-1}+\Sigma_{n-1}^T) & \\ & & & \Sigma_n^P\end{bmatrix} \tag{4.20}$$

(matrices $\hat{U}, U_P$ are upper block triangular, $\hat{E}, E_P$ block diagonal), $\Sigma_i = Y^T_{[i]}S_{[i]}C^{-1}_{[i]}$, $i = 1,\dots,n-1$, $\Sigma^P_n = (Y^P_{[n]})^T S^P_{[n]}(C^P_{[n]})^{-1}$, $\tilde{u}^T = s_-^T Y^P_{[n]}$ is the last row of U_P, $\tilde{v}^T$ the last row of E_P, $\tilde{w}$ the last column of E_P and $\kappa = \beta^2\tilde{v}_{m-1} + s^T\hat{y}$. If $C^P_{[n]} = I$ then $\tilde{w} = \tilde{u}$, $\tilde{v}$ is the last column of $\operatorname{diag}[S^T_{[1]}Y_{[1]},\dots,S^T_{[n-1]}Y_{[n-1]},(S^P_{[n]})^T Y^P_{[n]}]$ *and $\kappa = b+\beta(\beta-\alpha)b_-$.*

Proof. We have $\hat{s}^T\hat{y} = s^T\hat{y}$ by Theorem 2.5. Using Theorem 4.1 for updates (4.1), $i=1,\dots,n-1$, followed by (4.15) (i.e. for updates (4.1), $i=1,\dots,n$, with $S_{[n]}, Y_{[n]}$ replaced by $S^P_{[n]}, Y^P_{[n]}$ or with $S=S_n, Y=Y_n$ replaced by S_P, Y_P, we get

$$H_P = S_P U_P^{-T} E_P U_P^{-1} S_P^T + \frac{1}{2}\Big(I - S_P U_P^{-T} Y_P^T\Big)\Big(H_I+H_I^T\Big)\Big(I - Y_P U_P^{-1} S_P^T\Big) \tag{4.21}$$

and to prove (4.17), it suffices to use Lemma 4.2 for update (4.14) of H_P, i.e. with $S_L = S_P$, $Y_L = Y_P$, $S_R = \hat{s}$, $Y_R = \hat{y}$, $C_R = 1$, $S_C = \hat{S}$, $Y_C = \hat{Y}$, $U_L = U_P$, $E_L = E_P$, $\bar{H}_I = \frac{1}{2}(H_I + H_I^T)$, $H_L = H_P$, $H_C = H_+$.

Since we can write $\hat{S} = [S_P, s-\alpha s_-] = ST_S$, $\hat{Y} = [Y_P, y-\beta y_-] = YT_Y$, where

$$T_S = \operatorname{diag}\left[I, \begin{bmatrix} 1 & -\alpha \\ 0 & 1\end{bmatrix}\right] \in \mathcal{R}^{m\times m},\quad T_Y = \operatorname{diag}\left[I, \begin{bmatrix} 1 & -\beta \\ 0 & 1\end{bmatrix}\right] \in \mathcal{R}^{m\times m}, \tag{4.22}$$

(4.17) yields (4.18) with $\tilde{U} = T_S^{-T}\hat{U}T_Y^{-1}$, $\tilde{E} = T_Y^{-T}\hat{E}T_Y^{-1}$. After rearrangement we obtain

$$\tilde{U} = T_S^{-T}\begin{bmatrix} U_P & S_P^T\hat{y} \\ & s^T\hat{y}\end{bmatrix}\begin{bmatrix} I & & \\ & 1 & \beta \\ & & 1\end{bmatrix} = \begin{bmatrix} I & & \\ & 1 & \\ & \alpha & 1\end{bmatrix}\begin{bmatrix} U_P & \beta S_P^T y_- + S_P^T\hat{y} \\ & s^T\hat{y}\end{bmatrix} = \begin{bmatrix} U_P & S_P^T y \\ \alpha\tilde{u}^T & s^T y\end{bmatrix},$$

$$\tilde{E} = T_Y^{-T}\begin{bmatrix} E_P & \\ & s^T\hat{y}\end{bmatrix}\begin{bmatrix} I & & \\ & 1 & \beta \\ & & 1\end{bmatrix} = \begin{bmatrix} I & & \\ & 1 & \\ & \beta & 1\end{bmatrix}\begin{bmatrix} E_P & \beta\tilde{w} \\ & s^T\hat{y}\end{bmatrix} = \begin{bmatrix} E_P & \beta\tilde{w} \\ \beta\tilde{v}^T & \beta^2\tilde{v}_{m-1} + s^T\hat{y}\end{bmatrix}$$

by $\beta S_P^T y_- + S_P^T\hat{y} = S_P^T y$, $\alpha s_-^T y + s^T\hat{y} = \alpha\beta b_- + s^T y - \alpha\beta b_- = s^T y$ and $\tilde{v}_{m-1} = \tilde{w}_{m-1}$, where obviously $\tilde{w} = \tilde{u}$ and $\tilde{v}_{m-1} = b_-$ for $C^P_{[n]} = I$. □

To estimate the benefit of the block BFGS update in Section 5, we use values $\tilde a$, $\tilde b$, see Theorem 2.4, which can be calculated with a negligible increase in the number of arithmetic operations:

Corollary 4.2. *Let* $H_{[1]} = H_I$, $n \ge 1$, $S = [S_{[1]}, \dots, S_{[n]}] \triangleq [S_P, s]$, $Y = [Y_{[1]}, \dots, Y_{[n]}] \triangleq [Y_P, y]$, $S_{[n]} \triangleq [S^P_{[n]}, s]$, $Y_{[n]} \triangleq [Y^P_{[n]}, y]$, *the matrices* $S^T_{[i]} Y_{[i]} C_{[i]}$ *be nonsingular, matrices* $H_{[i]}$ *be given by update (4.1),* $i = 2, \dots, n$, *with* $H_I = \zeta I$, $\zeta > 0$, *matrices* H_P, $P^P_{[n]}$, U_P, E_P *by (4.15), (4.16) and (4.20) and let* $\tilde y = P^P_{[n]} y$, $\tilde a = \tilde y^T H_P \tilde y$, $\tilde b = s^T \tilde y$. *Then*

$$\tilde a = \zeta |y|^2 + y^T S_P U_P^{-T}\Big(\bar E + \zeta Y_P^T Y_P\Big) U_P^{-1} S_P^T y - 2\,\zeta y^T S_P U_P^{-T} Y_P^T y\,, \tag{4.23}$$

$$\tilde b = b - s^T Y^P_{[n]}((S^P_{[n]})^T (Y^P_{[n]}))^{-1} (S^P_{[n]})^T y, \tag{4.24}$$

where

$$\bar E = \mathrm{diag}\Big[\tfrac12\Big(\Sigma_1 + \Sigma_1^T\Big), \dots, \tfrac12\Big(\Sigma_{n-1} + \Sigma_{n-1}^T\Big), 0\,\Big], \quad \Sigma_i = Y^T_{[i]} S_{[i]} C^{-1}_{[i]}, \tag{4.25}$$

$i = 1, \dots, n-1$, *and the dimension of the null matrix is equal to* $\dim((Y^P_{[n]})^T S^P_{[n]} (C^P_{[n]})^{-1})$.

Proof. In the same way as in the proof of Theorem 4.1 we get (4.21). Furthermore, since $(S^P_{[n]})^T P^P_{[n]} = 0$ and $(P^P_{[n]})^2 = P^P_{[n]}$, from (4.15) we obtain

$$(P^P_{[n]})^T H_P P^P_{[n]} = H_P - S^P_{[n]}\Big((S^P_{[n]})^T Y^P_{[n]} C^P_{[n]}\Big)^{-1} (S^P_{[n]})^T\,. \tag{4.26}$$

In a similar way as in the proof of Lemma 4.2 (relation (4.9)) we prove (the dimension of the null principal submatrix is equal to $\dim \Sigma_1 + \ldots + \dim \Sigma_{n-1}$)

$$S^P_{[n]}\Big((S^P_{[n]})^T Y^P_{[n]} C^P_{[n]}\Big)^{-1} (S^P_{[n]})^T = S_P\, U_P^{-T} \begin{bmatrix} 0 & \\ & (Y^P_{[n]})^T S^P_{[n]} (C^P_{[n]})^{-1} \end{bmatrix} U_P^{-1} S_P^T\,;$$

for $H_I = \zeta I$, $\zeta > 0$, this together with (4.20)–(4.21) and (4.26) immediately gives

$$(P^P_{[n]})^T H_P P^P_{[n]} = S_P U_P^{-T} \bar E U_P^{-1} S_P^T + \zeta\Big(I - S_P U_P^{-T} Y_P^T\Big)\Big(I - Y_P U_P^{-1} S_P^T\Big), \tag{4.27}$$

and subsequently yields (4.23) by $\tilde a = y^T\Big((P^P_{[n]})^T H_P P^P_{[n]}\Big) y$. Finally, (4.24) follows by analogy with (2.23) (for the proof of (2.23) we need not the symmetry of $S^T Y$). □

Using representation (4.10) or (4.18), the direction vector and an auxiliary vector $Y^T H_+ g_+$ (see Section 5) can be calculated effectively, similarly as for the BNS method, see [1]. E.g. for $H = \zeta I$ and matrix $H_+ = H_{[n+1]}$ given by (4.10) we have (omitting index n)

$$-H_+ g_+ = -\zeta g_+ - S\Big[U^{-T}\Big((E + \zeta Y^T Y) U^{-1} S^T g_+ - \zeta Y^T g_+\Big)\Big] + Y\Big[\zeta U^{-1} S^T g_+\Big], \tag{4.28}$$

$$Y^T H_+ g_+ = \zeta Y^T g_+ + Y^T S\Big[U^{-T}\Big((E + \zeta Y^T Y) U^{-1} S^T g_+ - \zeta Y^T g_+\Big)\Big] - Y^T Y\Big[\zeta U^{-1} S^T g_+\Big], \tag{4.29}$$

where in brackets we multiply by low-order matrices. Similarly for H_+ given by (4.18)

$$-H_+ g_+ = -\zeta g_+ - S\Big[\tilde U^{-T}\Big((\tilde E + \zeta Y^T Y) \tilde U^{-1} S^T g_+ - \zeta Y^T g_+\Big)\Big] + Y\Big[\zeta \tilde U^{-1} S^T g_+\Big]; \tag{4.30}$$

from this we easily obtain the corresponding representation of $Y^T H_+ g_+$.

In comparison with the BNS method, here $U, \tilde U$ are not triangular matrices generally, which can complicate calculations. Using factorization $S^T_{[i]} Y_{[i]} = R_{[i]} L_{[i]}$, $i = 1, \dots, n$, where $R_{[i]}$ and $L^T_{[i]}$ are upper triangular matrices, and denoting $L_D = \mathrm{diag}[\, L_{[1]}, \dots, L_{[n]}\,]$,

$E_A = L_D^{-T}(E + \zeta Y^T Y)$, we can set $U = U_T L_D$, where $U_T = U L_D^{-1}$ and L_D^T are upper triangular matrices, and rewrite (4.28) and E_A in the form

$$-H_+ g_+ = -\zeta g_+ - S\Big[U_T^{-T}\Big(E_A L_D^{-1} U_T^{-1} S^T g_+ - \zeta L_D^{-T} Y^T g_+\Big)\Big] + Y\Big[\zeta L_D^{-1} U_T^{-1} S^T g_+\Big], \quad (4.31)$$

$$E_A = \mathrm{diag}\Big[\frac{1}{2}\Big(R_{[1]}^T + L_{[1]}^{-T} S_{[1]}^T Y_{[1]}\Big), \dots, \frac{1}{2}\Big(R_{[n-1]}^T + L_{[n-1]}^{-T} S_{[n-1]}^T Y_{[n-1]}\Big), R_{[n]}^T\Big] + \zeta L_D^{-T} Y^T Y. \quad (4.32)$$

In case of matrix $\tilde{U}$ we can proceed similarly. If we denote

$$\hat{U}_{[n]} = \begin{bmatrix} (S_{[n]}^P)^T Y_{[n]}^P & S_P^T \hat{y} \\ & s^T \hat{y} \end{bmatrix}, \quad \tilde{U}_{[n]} = \begin{bmatrix} (S_{[n]}^P)^T Y_{[n]}^P & S_P^T y \\ \alpha \tilde{u}^T & s^T y \end{bmatrix}, \quad \tilde{E}_{[n]} = \begin{bmatrix} \Sigma_n^P & \beta \tilde{w} \\ \beta \tilde{v}^T & \kappa \end{bmatrix} \quad (4.33)$$

(submatrices of $\hat{U}, \tilde{U}, \tilde{E}$ in (4.19)), we can see that for $S_{[n]}^T Y_{[n]}$ positive definite (thus $s^T \hat{y} = b - s^T y_- \, y^T s_- / b_- > 0$ and $(S_{[n]}^P)^T Y_{[n]}^P$ positive definite) a RL factorization of $\hat{U}_{[n]}$ exists by Lemma 4.1, because all its principal minors are obviously nonzero. Since they do not change by adding to a row (column) a multiple of another row (column), we can also factorize matrix $\tilde{U}_{[n]}$ and write $\tilde{U}_{[n]} = \tilde{R}_{[n]} \tilde{L}_{[n]}$, where $\tilde{R}_{[n]}, \tilde{L}_{[n]}^T$ are upper triangular matrices. Denoting $\tilde{L}_D = \mathrm{diag}[\, L_{[1]}, \dots, L_{[n-1]}, \tilde{L}_{[n]}\,]$, $\tilde{E}_A = \tilde{L}_D^{-T}(\tilde{E} + \zeta Y^T Y)$, we can set $\tilde{U} = \tilde{U}_T \tilde{L}_D$, where $\tilde{U}_T = \tilde{U} \tilde{L}_D^{-1}$ and $\tilde{L}_D^T$ are upper triangular matrices, and rewrite (4.30) and $\tilde{E}_A$:

$$-H_+ g_+ = -\zeta g_+ - S\Big[\tilde{U}_T^{-T}\Big(\tilde{E}_A \tilde{L}_D^{-1} \tilde{U}_T^{-1} S^T g_+ - \zeta \tilde{L}_D^{-T} Y^T g_+\Big)\Big] + Y\Big[\zeta \tilde{L}_D^{-1} \tilde{U}_T^{-1} S^T g_+\Big], \quad (4.34)$$

$$\tilde{E}_A = \mathrm{diag}\Big[\frac{1}{2}\Big(R_{[1]}^T + L_{[1]}^{-T} S_{[1]}^T Y_{[1]}\Big), \dots, \frac{1}{2}\Big(R_{[n-1]}^T + L_{[n-1]}^{-T} S_{[n-1]}^T Y_{[n-1]}\Big), \tilde{L}_{[n]}^{-T} \tilde{E}_{[n]}\Big] + \zeta \tilde{L}_D^{-T} Y^T Y. \quad (4.35)$$

Our experiments indicate, that this approach can also improve numerical results.

5 Implementation

We will assume that $C_{[1]} = \ldots = C_{[n]} = C_{[n]}^P = I$ and $H_I = \zeta I$, $\zeta = b / y^T y > 0$, and denote $S = [\, S_P, s]$, $Y = [\, Y_P, y]$. Before we give the algorithm of the method, we will discuss the question how to split matrices S, Y into $S = [S_{[1]}, \dots, S_{[n]}]$, $Y = [Y_{[1]}, \dots, Y_{[n]}]$, $n \in [1, m]$, with suitable positive definite blocks $[S_{[i]}^T Y_{[i]}]$, $i = 1, \dots, n$, and how to choose the appropriate update from (2.28)–(2.30) for each of blocks. As we mentioned in Section 4, we start with the submatrix $S_{[n]}^T Y_{[n]}$ to have maximum of the latest QN conditions satisfied.

In this connection, from now on we denote a set of indices j of vectors s_j, y_j which form matrices $S_{[i]}, Y_{[i]}$ by $\mathcal{I}_i$, a number of columns of these matrices by $m_i \ge 1$, $i = 1, \dots, n$, and a set of indices j of vectors s_j, y_j which correspond to entries of the principal submatrix $[S^T Y]_{\underline{\nu}}^{\overline{\nu}}$ (see the end of Section 1), $1 \le \underline{\nu} \le \overline{\nu} \le m$, by $\mathcal{I}_{\underline{\nu}}^{\overline{\nu}}$. Obviously, $\sum_{i=1}^n m_i = m$.

In accordance with the theory in Sections 2, 3 we should use the block BFGS update whenever an objective function is close to a quadratic function (e.g. near to a local minimum). Taking this into consideration, we find such positive definite (to have direction vectors descent) submatrices $S_{[i]}^T Y_{[i]}$ of the largest order, for which $\Delta_i \le \delta_1$ for $i = n$, $\Delta_i \le \delta_2$ otherwise, where the numbers $\Delta_i = \max_{j_1, j_2 \in \mathcal{I}_i} \{(s_{j_1}^T y_{j_2} - s_{j_2}^T y_{j_1})^2 / (b_{j_2} b_{j_1})\}$ (zero for quadratic functions), can serve as a measure of the deviation from a quadratic function, $i = n, \dots, 1$.

On the other hand, the use of this update can deteriorate stability, which is most noticeable in case of the last block $S_{[n]}^T Y_{[n]}$ if it is almost symmetric, i.e. $\Delta_n < \delta_3$. Therefore to select the suitable choice from (2.28)–(2.30) for such a block, we estimate the benefit of the block BFGS update in comparison with the corresponding BFGS updates, see below. If we regard this benefit as sufficient or if $m_n \le 2$, we always use the choice (2.28), otherwise we denote $a_{i,j} = (S_{[n]}^T Y_{[n]})_{i,j}$, $i, j = 1, \ldots, m_n$ and calculate the value

$$\theta = \sum_{i=1}^{m_n-2} \sqrt{|a_{i,m_n} a_{m_n,i}|}/b \tag{5.1}$$

(this formula was chosen empirically), which can be also regarded as an estimate of the deviation f from a quadratic function and is equal to zero for quadratic function if $t_- = 1$, see Theorem 3.2. Subsequently, we use the choice (2.28) for $\theta < \delta_4$, (2.29) for $\theta > \delta_5$ or $\ddot{s}^T \ddot{y} > \delta_6$ and (2.30) otherwise, see Algorithm 1 and Procedure 3 for details.

It follows from the proof of Theorem 2.4 that $\|\bar{G}^{1/2} \ddot{H}_+ \bar{G}^{1/2} - I\|_F^2 = \varphi(\xi)$, $\xi = \tilde{b}/\ddot{b} \in (0,1]$ for $S^T Y$ symmetric positive definite, where the quadratic function φ given by (2.27) is nonincreasing on $[0, 1]$, all its coefficients are independent of $\sigma \in \mathcal{R}^m$, $\varphi(0) = \|M\|_F^2$ corresponds to H_P (no updating), $\varphi(\tilde{b}/b)$ to the standard BFGS update, i.e. (2.21) with the choice (2.29) and $\varphi(1)$ to the block BFGS update, i.e. (2.21) with the choice (2.28). Although we cannot calculate either $\varphi(\xi)$ or $\varphi'(\xi)$, the following lemma shows that the ratio $b/\tilde{b}$ and a suitable estimate of the decrease of φ on $[\tilde{b}/b, 1]$ can be considered as good indicators of the benefit of the block BFGS update for $S^T Y$ near to symmetric.

Lemma 5.1. *Let we denote quantities $\tilde{a}, \tilde{b}$ as in Theorem 2.4, $\tilde{w}$, M as in the proof of Theorem 2.4, $\xi_1 = \tilde{b}/b \in (0,1]$ and let the function $\varphi(\xi)$ be given by (2.27). Then*

$$\varphi(\xi_1) - \varphi(1) \;\ge\; (1 - \tilde{a}/\tilde{b})^2 (1 - \xi_1)^2, \tag{5.2}$$

$$[\varphi(0) - \varphi(\xi_1)]/[\varphi(0) - \varphi(1)] \;\le\; \xi_1(2 - \xi_1). \tag{5.3}$$

Proof. Quadratic function (2.27) can be written in the form

$$\varphi(\xi) = \bar{c}\xi^2 - 2\bar{d}\xi + \|M\|_F^2, \quad \bar{c} = (\tilde{w}^T M \tilde{w}/|\tilde{w}|^2)^2 = (1 - \tilde{a}/\tilde{b})^2, \quad \bar{d} = |M\tilde{w}|^2/|\tilde{w}|^2. \tag{5.4}$$

Since $\bar{c} \le \bar{d}$ by the Schwarz inequality, we obtain

$$\varphi(\xi_1) - \varphi(1) = \bar{c}(\xi_1^2 - 1) + 2\bar{d}(1 - \xi_1) \ge \bar{c}(1 - \xi_1)^2.$$

Denoting $\psi(t) = (t\xi_1 - \bar{c}\xi_1^2)/(t - \bar{c})$, $t \ne \bar{c}$, we have

$$[\varphi(0) - \varphi(\xi_1)]/[\varphi(0) - \varphi(1)] = (2\bar{d}\xi_1 - \bar{c}\xi_1^2)/(2\bar{d} - \bar{c}) = \psi(2\bar{d}) \le \psi(2\bar{c}) = \xi_1(2 - \xi_1)$$

by $\psi'(t) = \bar{c}(\xi_1^2 - \xi_1)/(t - \bar{c})^2 \le 0$. □

Both values $\tilde{a}$, $\tilde{b}$ can be calculated efficiently by (4.23)–(4.24), with a negligible increase in the number of arithmetic operations. Since we need this values while we create blocks $S_{[n]}, Y_{[n]}$ and thus we have not blocks $S_{[i]}, Y_{[i]}$, $i < n$, created yet (see Algorithm 1), we will calculate only an estimate of $\tilde{a}$, assuming that all matrices $S_{[i]}, Y_{[i]}$, $i < n$, have one column, i.e. that the matrix H_P given by (4.21) is calculated by the BNS method, see Section 1. In view of Lemma 5.1 we regard the benefit of the block BFGS update as sufficient, if $(1 - \tilde{b}/b)|1 - \tilde{a}/\tilde{b}| > 1$ together with $b/\tilde{b} > 1.5$ or if $b/\tilde{b} > 50$ (this criterion was found empirically).

To improve the readability of the main algorithm, we first present three auxiliary procedures. Procedure 1 serves for updating of the basic matrices S^TY, Y^TY, similar to the algorithm given in [1] for updating of the matrices D, U, Y^TY in (1.5). In comparison with the standard BNS method, where the upper triangular matrix U is used, we need the whole matrix S^TY here, therefore we use an additional vector $Y_P^T s = -t\, Y_P^T Hg$, see also Algorithm 1. Note that the number of arithmetic operations is approximately the same as for the corresponding algorithm in [1]. We present the whole procedure for completeness, although some parts of steps (ii), (iii) are contained in Step 1 of Algorithm 1.

Procedure 1 *(Updating of basic matrices)*

Given: $t > 0$, matrices S_P, Y_P, $S_P^T Y_P$, $Y_P^T Y_P$ and vectors s, y, g_+, $S_P^T g$, $Y_P^T g$, $Y_P^T Hg$.

(i): Set $S := [\,S_P, s]$, $Y := [\,Y_P, y]$.

(ii): Compute $S^T g_+ = [S_P^T g_+, s^T g_+]$, $Y^T g_+ = [Y_P^T g_+, y^T g_+]$, $Y_P^T s = -t\, Y_P^T Hg$.

(iii): Compute $S_P^T y = S_P^T g_+ - S_P^T g$, $Y_P^T y = Y_P^T g_+ - Y_P^T g$, $s^T y$, $y^T y$.

(iv): Set $S^T Y := \begin{bmatrix} S_P^T Y_P & S_P^T y \\ s^T Y_P & s^T y \end{bmatrix}$, $Y^T Y := \begin{bmatrix} Y_P^T Y_P & Y_P^T y \\ y^T Y_P & y^T y \end{bmatrix}$ and return.

Procedure 2, based on Lemma 4.1, is used for seeking out of the positive definite bottom-right-corner principal submatrix of $[S^TY]_{\underline{\nu}}^{\overline{\nu}}$ of a maximum order (with $i_D = 0$) and for its RL factorization (with $i_D = 1$), see Procedure 3.

Procedure 2 *(RL factorization of A)*

Given: A factorization indicator i_D, a global convergence parameter $\varepsilon_D \in (0, 1)$, indices bounds $\underline{\nu}$, $\overline{\nu}$, $\underline{\nu} \le \overline{\nu}$, and the matrix $[S^TY]_{\underline{\nu}}^{\overline{\nu}} \triangleq A$.

(i): If $i_D = 0$ set $A := A + A^T$. Set $\tilde{\nu} = \overline{\nu} - \underline{\nu} + 1$, $\hat{\nu} := \tilde{\nu}$.

(ii): If $i_D = 0$ and $A_{\hat{\nu},\hat{\nu}} \le \varepsilon_D \mathrm{Tr} A$ set $\underline{\nu} := \min(\underline{\nu} + \hat{\nu}, \overline{\nu})$ and go to *(iv). If $\hat{\nu} = 1$ go to (iv).*

(iii): Set $A_{\hat{\nu},j} := A_{\hat{\nu},j} / A_{\hat{\nu},\hat{\nu}}$, $j = 1, \ldots, \hat{\nu} - 1$. Set $A_{i,j} := A_{i,j} - A_{i,\hat{\nu}} A_{\hat{\nu},j}$, $i = 1, \ldots, \hat{\nu} - 1$, $j = 1, \ldots, \hat{\nu} - 1$. Set $\hat{\nu} := \hat{\nu} - 1$ and go to *(ii)*.

(iv): If $i_D = 0$ return. Set $L_{i,j} := A_{i,j}$ for $1 \le j < i \le \tilde{\nu}$, $L_{i,j} := 1$ for $1 \le j = i \le \tilde{\nu}$, $R_{i,j} := A_{i,j}$ for $1 \le i \le j \le \tilde{\nu}$, $L_{i,j} := R_{i,j} := 0$ otherwise. Return.

The following Procedure 3 is used for formation and factorization of blocks $S_{[i]}^T Y_{[i]}$, $i = 1, \ldots, n$ and selection of the suitable update formula. Note that to realize updating with the choice (2.29), we merely create block $S_{[n]}^T Y_{[n]}$ of order 1, see step *(v)*.

Procedure 3 *(Block generation)*

Given: Symmetry tolerances $\delta_1, \delta_2, \delta_3$ and update-type tolerances $\delta_4, \delta_5, \delta_6$, $\delta_i > 0$, $i = 1, \ldots, 6$, and a global convergence parameter $\varepsilon_D \in (0, 1)$.

(i): Set $\delta := \delta_1$, an indices upper bound $\overline{\nu} := m$, an auxiliary block index $i_B := 1$ and an update-type ((2.28)–(2.30)) indicator $i_U := 0$.

(ii): Find a minimum indices bound $\underline{\nu}$ such that $\max_{j_1,j_2 \in \mathcal{I}_{\underline{\nu}}^{\overline{\nu}}} \left\{ (s_{j_1}^T y_{j_2} - s_{j_2}^T y_{j_1})^2 / (b_{j_2} b_{j_1}) \right\} \le \delta$.

(iii): Using Procedure 2 with $i_D = 0$, possibly correct the indices lower bound $\underline{\nu}$. If $m \le 3$ or $\overline{\nu} < m$ or $\overline{\nu} - \underline{\nu} \le 2$ or $\max_{j_1,j_2 \in \mathcal{I}_{\underline{\nu}}^{\overline{\nu}}} \left\{ (s_{j_1}^T y_{j_2} - s_{j_2}^T y_{j_1})^2 / (b_{j_2} b_{j_1}) \right\} > \delta_3$ go to *(v)*.

(iv): Compute θ by (5.1), $\tilde{a}$ by (4.23) and $\tilde{b}$ by (4.24). If $((1-\tilde{b}/b)|1-\tilde{a}/\tilde{b}| > 1$ and $b/\tilde{b} > 1.5)$ or $b/\tilde{b} > 50$ or $\theta < \delta_4$ then go to *(v)*. If $\theta > \delta_5$ or $\hat{b}/b > \delta_6$ set $i_U := 1$, otherwise set $i_U := 2$.

(v): If $i_U = 1$ set $\underline{\nu} := \overline{\nu}$ and $i_U := 0$. Set $A_{i_B} := [S^T Y]_{\underline{\nu}}^{\overline{\nu}}$. If $i_U = 2$ and $\overline{\nu} = m$, denote by A_{i_B} matrix $\tilde{U}_{[n]}$ in (4.33). Using Procedure 2 with $i_D = 1$, find matrices $R_{i_B} = R$ and $L_{i_B} = L$ such that $A_{i_B} := R_{i_B} L_{i_B}$. Set $\overline{\nu} := \underline{\nu} - 1$. If $\overline{\nu} \ge 1$ set $\delta := \delta_2$, $i_B := i_B + 1$ and go to *(ii)*.

(vi): Set $n := i_B$, $S_{[i]}^T Y_{[i]} := A_{n-i+1}$, $R_{[i]} := R_{n-i+1}$, $L_{[i]} := L_{n-i+1}$, $i = 1, \dots, n$. If $i_U = 2$ set $\tilde{R}_{[n]} := R_{[n]}$ and $\tilde{L}_{[n]} := L_{[n]}$. Return.

We now state the method in details. For simplicity, here we omit stopping criteria and a contingent restart when some computed direction vector is not sufficiently descent.

Algorithm 1

Data: A maximum number $\hat{m} > 1$ of columns S, Y, line search parameters ε_1, ε_2, $0 < \varepsilon_1 < 1/2$, $\varepsilon_1 < \varepsilon_2 < 1$, tolerance parameters $\delta_1, \dots, \delta_6$, $\delta_i > 0$, $i \in \{1, \dots, 6\}$, $\delta_4 < \delta_5$, and a global convergence parameter $\varepsilon_D \in (0, 1)$.

Step 0: *Initiation.* Choose starting point $x_0 \in \mathcal{R}^N$, define starting matrix $H_0 = I$ and direction vector $d_0 = -g_0$ and initiate iteration counter k to zero.

Step 1: *Line search.* Compute $x_{k+1} = x_k + t_k d_k$, where t_k satisfies (1.1), $g_{k+1} = \nabla f(x_{k+1})$, $s_k = t_k d_k$, $y_k = g_{k+1} - g_k$, $b_k = s_k^T y_k$, $\zeta_k = b_k / y_k^T y_k$. If $k = 0$ set $S_k = [s_k]$, $Y_k = [y_k]$, $S_k^T Y_k = [s_k^T y_k]$, $Y_k^T Y_k = [y_k^T y_k]$, compute $S_k^T g_{k+1}$, $Y_k^T g_{k+1}$ and go to Step 4.

Step 2: *Basic matrices updating.* Using Procedure 1, form the matrices S_k, Y_k, $S_k^T Y_k$, $Y_k^T Y_k$.

Step 3: *Block generation and factorization.* Using Procedure 3, find a number of blocks n and an update indicator i_U and form and factorize positive definite blocks $S_{[i]}^T Y_{[i]} = R_{[i]} L_{[i]}$, $i = n, \dots, 1$. Form matrices $U = U_n$ by (4.11), $L_D = \operatorname{diag}[L_{[1]}, \dots, L_{[n]}]$, E_A by (4.32) and $U_T := U L_D^{-1}$ for $i_U = 0$ or $\tilde{U}$ by (4.19), $\tilde{L}_D = \operatorname{diag}[L_{[1]}, \dots, L_{[n-1]}, \tilde{L}_{[n]}]$, $\tilde{E}_A$ by (4.35) and $\tilde{U}_T := \tilde{U} \tilde{L}_D^{-1}$ for $i_U = 2$.

Step 4: *Direction vector.* Compute $d_{k+1} = -H_{k+1} g_{k+1}$ and an auxiliary vector $Y_k H_{k+1} g_{k+1}$ by (4.31) for $i_U = 0$ or by (4.34) for $i_U = 2$. Set $k := k + 1$. If $k \ge \hat{m}$ delete the first column of S_{k-1}, Y_{k-1} and the first row and column of $S_{k-1}^T Y_{k-1}$, $Y_{k-1}^T Y_{k-1}$ to form matrices $(S_P)_k$, $(Y_P)_k$, $(S_P)_k^T (Y_P)_k$, $(Y_P)_k^T (Y_P)_k$. Go to Step 1.

6 Global convergence

In this section, we establish the global convergence of Algorithm 1. The following assumption and lemma are presented in [17].

Assumption 6.1 *The objective function $f : \mathcal{R}^N \to \mathcal{R}$ is bounded from below and uniformly convex with bounded second-order derivatives (i.e. $0 < \underline{G} \le \underline{\lambda}(G(x)) \le \overline{\lambda}(G(x)) \le \overline{G} < \infty$, $x \in \mathcal{R}^N$, where $\underline{\lambda}(G(x))$ and $\overline{\lambda}(G(x))$ are the lowest and the greatest eigenvalues of the Hessian matrix $G(x)$).*

Lemma 6.1. *Let the objective function f satisfy Assumption 6.1. Then* $\underline{G} \le |y|^2/b \le \overline{G}$ *and* $b/|s|^2 \ge \underline{G}$.

Lemma 6.2. *Let* $A_1 \in \mathcal{R}^{\mu\times\mu}$, $\mu > 0$, *be a positive semidefinite matrix,* $A_2 \in \mathcal{R}^{\mu\times\mu}$ *symmetric positive semidefinite. Then* $0 \le \mathrm{Tr}(A_1A_2) \le \mathrm{Tr}\, A_1\, \mathrm{Tr}\, A_2$. *Moreover, if* A_2 *is symmetric positive definite, then* $\mathrm{Tr}(A_1A_2^{-1}) \le \mathrm{Tr}\, A_1\, (\mathrm{Tr}\, A_2)^{\mu-1}/\det A_2$.

Proof. We can write $A_2 = Q\Lambda Q^T$ with Q orthogonal and Λ diagonal with $\Lambda_{ii} \ge 0$, $i = 1,\ldots,\mu$, thus $\mathrm{Tr}(A_1A_2) = \mathrm{Tr}(A_1Q\Lambda Q^T) = \mathrm{Tr}(K\Lambda)$, where the matrix $K = Q^TA_1Q$ is obviously positive semidefinite, which immediately yields $K_{ii} \ge 0$, $i = 1,\ldots,\mu$. Since $\mathrm{Tr}(A_1A_2) = \mathrm{Tr}(K\Lambda) = \sum_{i=1}^{\mu} K_{ii}\Lambda_{ii}$, we get $0 \le \mathrm{Tr}(A_1A_2) \le \mathrm{Tr}\, K\, \mathrm{Tr}\, \Lambda = \mathrm{Tr}\, A_1\, \mathrm{Tr}\, A_2$.

If A_2 is symmetric positive definite, all eigenvalues Λ_{ii} of the matrix A_2 satisfy $\Lambda_{ii} \ge \det A_2/(\mathrm{Tr}\, A_2)^{\mu-1}$, which yields

$$\mathrm{Tr}(A_1A_2^{-1}) = \mathrm{Tr}(A_1Q\Lambda^{-1}Q^T) = \mathrm{Tr}(K\Lambda^{-1}) = \sum_{i=1}^{\mu} K_{ii}\Lambda_{ii}^{-1} \le \Big[(\mathrm{Tr}\, A_2)^{\mu-1}/\det A_2\Big]\, \mathrm{Tr}\, A_1$$

in view of $\sum_{i=1}^{\mu} K_{ii} = \mathrm{Tr}\, K = \mathrm{Tr}\, A_1$. □

Lemma 6.3. *Let matrices* $A_1, A_2 \in \mathcal{R}^{\mu\times\mu}$, $\mu > 0$, A_2 *nonsingular. Then* $(\mathrm{Tr}(A_1A_2^{-1}))^2 \le \mu\, \mathrm{Tr}(A_1^TA_1)\, (\mathrm{Tr}(A_2^TA_2))^{\mu-1}/(\det A_2)^2$.

Proof. For any $A \in \mathcal{R}^{\mu\times\mu}$ we have

$$(\mathrm{Tr}\, A)^2 = \Big(\sum_{i=1}^{\mu}(1.A_{ii})\Big)^2 \le \mu \sum_{i=1}^{\mu} A_{ii}^2 \le \mu \sum_{i=1}^{\mu}\sum_{j=1}^{\mu} A_{ij}^2 = \mu\, \mathrm{Tr}(A^TA)$$

by the Schwarz inequality and the assertion follows from Lemma 6.2 in view of

$$\Big(\mathrm{Tr}(A_1A_2^{-1})\Big)^2 \le \mu\, \mathrm{Tr}(A_2^{-T}A_1^TA_1A_2^{-1}) = \mu\, \mathrm{Tr}\Big((A_1^TA_1)(A_2^TA_2)^{-1}\Big).$$ □

Lemma 6.4. *If* $A \in \mathcal{R}^{\mu\times\mu}$, $\mu > 0$, *is a positive definite matrix, then* $\det \frac{1}{2}(A + A^T) \le \det A$.

Proof. We will proceed by induction on μ. The result is true for $\mu = 1$. Let it be true for all positive definite matrices of some order $\mu \ge 1$, let $u, v \in \mathcal{R}^{\mu}$ and the matrix $\bar{A} = \begin{bmatrix} A & u \\ v^T & \alpha \end{bmatrix}$ be positive definite. Then

$$\begin{vmatrix} A & u \\ v^T & \alpha \end{vmatrix} = \begin{vmatrix} A - uv^T/\alpha & u \\ 0^T & \alpha \end{vmatrix},$$

i.e. $\det \bar{A} = \alpha \det(A - uv^T/\alpha)$, where $\alpha > 0$ and the matrix $A - uv^T/\alpha$ is positive definite by Lemma 4.1. This also implies

$$\det \frac{1}{2}(\bar{A} + \bar{A}^T) = \alpha \det \Big(\frac{1}{2}(A + A^T) - ww^T/\alpha\Big), \tag{6.1}$$

where $w = \frac{1}{2}(u + v)$ and the matrix $\frac{1}{2}(A + A^T) - ww^T/\alpha$ is symmetric positive definite. Using the induction hypothesis and the identity $\det(K + qq^T) = (1 + q^TK^{-1}q) \det K$ (K a nonsingular matrix, q a vector), which for K positive definite yields

$$\det(K + qq^T) \ge \det K, \tag{6.2}$$

we get

$$\begin{aligned} \det \bar{A} &= \alpha \det(A - uv^T/\alpha) \ge \alpha \det\tfrac{1}{2}\Big(A - uv^T/\alpha + A^T - vu^T/\alpha\Big) \\ &= \alpha \det\Big(\tfrac{1}{2}(A + A^T) - ww^T/\alpha + (u - v)(u - v)^T/(4\alpha)\Big) \\ &\ge \alpha \det\Big(\tfrac{1}{2}(A + A^T) - ww^T/\alpha\Big) = \det \tfrac{1}{2}(\bar{A} + \bar{A}^T) \end{aligned}$$

and the induction is established with $\mu + 1$ replacing μ. □

Lemma 6.5. *Let $A \in \mathcal{R}^{\mu\times\mu}$, $w \in \mathcal{R}^{\mu}$, μ, $\delta > 0$, the matrix* $\bar{A} = \begin{bmatrix} \alpha & w \\ w^T & A \end{bmatrix}$ *be symmetric positive definite and* $\det \bar{A} \ge \delta(\mathrm{Tr}\,\bar{A})^{\mu+1}$. *Then* $\det A > \delta(\mathrm{Tr}\,A)^{\mu}$.

Proof. The matrices $A - ww^T/\alpha$, A are symmetric positive definite and $\alpha > 0$ by Lemma 4.1, thus $\mathrm{Tr}\,\bar{A} > \alpha$, $\mathrm{Tr}\,\bar{A} > \mathrm{Tr}\,A$. Using (6.2) and (6.1), we obtain

$$\det A \ge \det(A - ww^T/\alpha) = (\det \bar{A})/\alpha > \delta(\mathrm{Tr}\,\bar{A})^{\mu+1}/\mathrm{Tr}\,\bar{A} = \delta(\mathrm{Tr}\,\bar{A})^{\mu} > \delta(\mathrm{Tr}\,A)^{\mu}. \quad \square$$

Theorem 6.1. *Let the objective function f satisfy Assumption 6.1. Then Algorithm 1 generates a sequence $\{g_k\}$ that either satisfies $\lim_{k\to\infty} |g_k| = 0$ or terminates with $g_k = 0$ for some k.*

Proof. Procedure 2 with $i_D = 0$ de facto computes the RL factorization of the matrices $\frac{1}{2}(S_{[i]}^T Y_{[i]} + Y_{[i]}^T S_{[i]}) \stackrel{\Delta}{=} A_{[i]}$, where L has unit diagonal entries. For $m_i > 1$ (the number of columns of the matrices $S_{[i]}, Y_{[i]}$) all diagonal entries of R are greater than $\varepsilon_D \mathrm{Tr}\, S_{[i]}^T Y_{[i]} = \varepsilon_D \mathrm{Tr} A_{[i]}$ in view of step *(ii)* of Procedure 2 and for $m_i = 1$ the only entry of R is $\mathrm{Tr} A_{[i]} > \varepsilon_D \mathrm{Tr} A_{[i]}$ by $\varepsilon_D < 1$, thus for $i = 1, \dots, n$ and $k \ge 0$ by Lemma 6.4 we have

$$\det\left(\frac{1}{2}\left((S_{[i]}^T Y_{[i]})^{-1} + (Y_{[i]}^T S_{[i]})^{-1}\right)\right)^{-1} \ge \det S_{[i]}^T Y_{[i]} \ge \det A_{[i]} \ge \left(\varepsilon_D \mathrm{Tr}\, A_{[i]}\right)^{m_i}. \quad (6.3)$$

We assume that $C_{[i]} = I$, $i = 1, \dots, n$, (see Sectin 5) and denote $\bar{H}_{[i]} = \frac{1}{2}(H_{[i]} + H_{[i]}^T)$, $B_{[i]} = H_{[i]}^{-1}$, $\bar{B}_{[i]} = \bar{H}_{[i]}^{-1}$, $\bar{B}_k = (\frac{1}{2}(H_k + H_k^T))^{-1}$, $\tilde{B}_k = \frac{1}{2}(B_k + B_k^T)$, $i = 1, \dots, n+1$, $k \ge 0$. Since in all iterations we choose $H_{[1]} = \zeta_k I$, $\zeta_k = b_k/|y_k|^2$, i.e. $\bar{B}_{[1]} = (|y_k|^2/b_k)I$, Lemma 6.1 gives

$$\mathrm{Tr}\,\bar{B}_{[1]} = (|y_k|^2/b_k)\,\mathrm{Tr}\,I \le N\overline{G}, \quad \det \bar{B}_{[1]} = (|y_k|^2/b_k)^N \ge \underline{G}^N, \quad k \ge 0. \quad (6.4)$$

(i) Suppose first that $i_U = 0$ (i.e. in the kth iteration we use the block BFGS update for all blocks $S_{[i]}^T Y_{[i]}$ and set $H_+ = H_{k+1} = H_{[n+1]}$ with the matrices $H_{[i+1]}$ given by (4.1), $i = 1, \dots, n$). By Corollary 2.1, Theorem 2.3 (b) -(c), (6.3) and Lemma 6.4, (4.1) yields

$$\begin{aligned}
\bar{B}_{[i+1]} &= \bar{B}_{[i]} - \bar{B}_{[i]} S_{[i]} (S_{[i]}^T \bar{B}_{[i]} S_{[i]})^{-1} S_{[i]}^T \bar{B}_{[i]} + Y_{[i]} A_{[i]}^{-1} Y_{[i]}^T, && (6.5)\\
B_{[i+1]} &= \bar{B}_{[i]} - \bar{B}_{[i]} S_{[i]} (S_{[i]}^T \bar{B}_{[i]} S_{[i]})^{-1} S_{[i]}^T \bar{B}_{[i]} + Y_{[i]} (Y_{[i]}^T S_{[i]})^{-1} Y_{[i]}^T, && (6.6)\\
\det \bar{B}_{[i+1]} &\ge \det B_{[i+1]} \ge \det \frac{1}{2}(B_{[i+1]} + B_{[i+1]}^T) = \det \bar{B}_{[i]} \det A_{[i]} / \det(S_{[i]}^T \bar{B}_{[i]} S_{[i]}), && (6.7)
\end{aligned}$$

$i = 1, \dots, n$, where the matrices $S_{[i]}^T \bar{B}_{[i]} S_{[i]}$ are symmetric positive definite by Theorem 2.3 (d), since Algorithm 1 generates all blocks $S_{[i]}^T Y_{[i]}$ positive definite by Lemma 4.1 and thus all columns of matrices $S_{[i]}, Y_{[i]}$, $i = 1, \dots, n$, are linearly independent.

Relation (6.5), Lemma 6.2, relation (6.3) and Lemma 6.1 give

$$\begin{aligned}
\mathrm{Tr}\,\bar{B}_{[i+1]} - \mathrm{Tr}\,\bar{B}_{[i]} &\le \mathrm{Tr}(Y_{[i]}^T Y_{[i]} A_{[i]}^{-1}) \le \mathrm{Tr}\, Y_{[i]}^T Y_{[i]} (\mathrm{Tr} A_{[i]})^{m_i - 1} / (\varepsilon_D \mathrm{Tr} A_{[i]})^{m_i} \\
&= \varepsilon_D^{-m_i}\, \mathrm{Tr}\, Y_{[i]}^T Y_{[i]} / \mathrm{Tr}\, A_{[i]} \le \textstyle\sum_{j \in \mathcal{I}_i} (|y_j|^2/b_j)/\varepsilon_D^{m_i} \le m_i\, \overline{G}/\varepsilon_D^{m_i},
\end{aligned} \quad (6.8)$$

$i = 1, \dots, n$. Using (6.4), in view of $\varepsilon_D < 1$ and $\sum_{i=1}^n m_i = m$ this yields

$$\mathrm{Tr}\,\bar{B}_{[i]} \le (N + m/\varepsilon_D^m)\,\overline{G} \stackrel{\Delta}{=} \Theta_0, \; i = 1, \dots, n+1, \quad \mathrm{Tr}\,\bar{B}_{k+1} = \mathrm{Tr}\,\bar{B}_{[n+1]} \le \Theta_0, \quad k > 0. \quad (6.9)$$

Since $\mathrm{Tr}\, B_{[n+1]} - \mathrm{Tr}\,\bar{B}_{[n]} \le \mathrm{Tr}\left(Y_{[n]}^T Y_{[n]} (Y_{[n]}^T S_{[n]})^{-1}\right)$ by (6.6), Lemmas 6.1–6.3 and (6.3) give

$$
\begin{aligned}
\operatorname{Tr} B_{[n+1]} - \operatorname{Tr} \bar{B}_{[n]} &\leq \sqrt{m_n \operatorname{Tr}(Y_{[n]}^T Y_{[n]})^2 \Big[\operatorname{Tr}(S_{[n]}^T S_{[n]}) \operatorname{Tr}(Y_{[n]}^T Y_{[n]})\Big]^{m_n-1}} \Big/ (\varepsilon_D \operatorname{Tr} A_{[n]})^{m_n} \\
&\leq \frac{\sqrt{m_n}}{\varepsilon_D^{m_n}} \sum_{j\in\mathcal{I}_n} \frac{|y_j|^2}{b_j} \Big[\sum_{j\in\mathcal{I}_n} \frac{|s_j|^2}{b_j} \sum_{j\in\mathcal{I}_n} \frac{|y_j|^2}{b_j}\Big]^{\frac{m_n-1}{2}} \leq \frac{m}{\varepsilon_D^m} (m\overline{G})(m^2)^{\frac{m-1}{2}} \Big(\frac{\overline{G}}{\underline{G}}\Big)^m,
\end{aligned}
$$

which by (6.4) and (6.9) yields

$$
\operatorname{Tr} B_{k+1} = \operatorname{Tr} B_{[n+1]} \leq \Theta_0 + (m/\varepsilon_D^m)(m\overline{G}/\underline{G})^m\, \overline{G} \triangleq \Theta_1 > \Theta_0, \quad k > 0. \tag{6.10}
$$

Since $(\det A)^{1/\mu} \leq (1/\mu)\operatorname{Tr} A$ for $A \in \mathcal{R}^{\mu\times\mu}$ symmetric positive definite, $\mu > 0$, we have $(\det(S_{[i]}^T \bar{B}_{[i]} S_{[i]}))^{1/m_i} \leq \operatorname{Tr}(S_{[i]}^T \bar{B}_{[i]} S_{[i]})/m_i$ and relations (6.7) and (6.3), Lemma 6.2, relation (6.9) and Lemma 6.1 give

$$
\begin{aligned}
\Big(\frac{\det \bar{B}_{[i+1]}}{\det \bar{B}_{[i]}}\Big)^{1/m_i} &\geq \Big(\frac{\det \frac{1}{2}(B_{[i+1]} + B_{[i+1]}^T)}{\det \bar{B}_{[i]}}\Big)^{1/m_i} \geq \frac{m_i (\det A_{[i]})^{1/m_i}}{\operatorname{Tr}(S_{[i]}^T S_{[i]}\, \bar{B}_{[i]})} \geq \frac{m_i(\varepsilon_D \operatorname{Tr} A_{[i]})}{\operatorname{Tr} S_{[i]}^T S_{[i]}\, .\operatorname{Tr} \bar{B}_{[i]}} \\
&\geq \frac{m_i\, \varepsilon_D \operatorname{Tr} A_{[i]}}{\Theta_0 \operatorname{Tr} S_{[i]}^T S_{[i]}} = \frac{m_i\, \varepsilon_D}{\Theta_0} \frac{\sum_{j\in\mathcal{I}_i} b_j}{\sum_{j\in\mathcal{I}_i} |s_j|^2} \geq \frac{m_i\, \varepsilon_D/\Theta_0}{\sum_{j\in\mathcal{I}_i} |s_j|^2/b_j} \geq \frac{\varepsilon_D\, \underline{G}}{\Theta_0}\,,
\end{aligned} \tag{6.11}
$$

$i = 1, \ldots, n$. Using (6.4), this yields

$$
\det \bar{B}_{[n]} \geq \underline{G}^N (\varepsilon_D\, \underline{G}\, /\Theta_0)^{m-m_n}, \tag{6.12}
$$

$$
\det \tilde{B}_{k+1} = \det \frac{1}{2}(B_{[n+1]} + B_{[n+1]}^T) \geq \underline{G}^N (\varepsilon_D\, \underline{G}\, /\Theta_0)^m \triangleq \Theta_2\,, \quad k > 0. \tag{6.13}
$$

(ii) Let $i_U = 2$ in the k th iteration, i.e. we use the block BFGS update for the blocks $S_{[i]}^T Y_{[i]}$, $i = 1, \ldots, n$–1, (thus also $\operatorname{Tr} \bar{B}_{[n]} \leq \Theta_0$ (see (6.9)) and (6.12) hold) and for the block $S_{[n]}^T Y_{[n]}$ update (4.14)–(4.15) with $C_{[n]}^P = I$ and $\hat{s} = \ddot{s}$, $\hat{y} = \ddot{y}$ given by (2.30). Denoting $B_P = H_P^{-1}$ (positive definite by Theorem 2.3 (d)), $\tilde{B}_P = \frac{1}{2}(B_P + B_P^T)$, $\bar{H}_P = \frac{1}{2}(H_P + H_P^T)$, $\bar{B}_P = \bar{H}_P^{-1}$, $\hat{P} = I - (1/\hat{s}^T\hat{y})\hat{y}\hat{s}^T$ and $A_{[n]}^P = \frac{1}{2}((S_{[n]}^P)^T Y_{[n]}^P + (Y_{[n]}^P)^T S_{[n]}^P)$, from (4.15) we obtain

$$
\begin{aligned}
B_P &= \bar{B}_{[n]} - \bar{B}_{[n]} S_{[n]}^P ((S_{[n]}^P)^T \bar{B}_{[n]} S_{[n]}^P)^{-1} (S_{[n]}^P)^T \bar{B}_{[n]} + Y_{[n]}^P ((S_{[n]}^P)^T Y_{[n]}^P)^{-T} (Y_{[n]}^P)^T, && (6.14)\\
\bar{B}_P &= \bar{B}_{[n]} - \bar{B}_{[n]} S_{[n]}^P ((S_{[n]}^P)^T \bar{B}_{[n]} S_{[n]}^P)^{-1} (S_{[n]}^P)^T \bar{B}_{[n]} + Y_{[n]}^P (A_{[n]}^P)^{-1} (Y_{[n]}^P)^T, && (6.15)\\
\det \tilde{B}_P &= \det \bar{B}_{[n]}\, .\, \det A_{[n]}^P / \det((S_{[n]}^P)^T \bar{B}_{[n]} S_{[n]}^P) && (6.16)
\end{aligned}
$$

by Theorem 2.3 and Corollary 2.1. In the same way as (6.9) and (6.13) we get

$$
\operatorname{Tr} \bar{B}_P \leq \Theta_0 < \Theta_1, \quad \operatorname{Tr} \tilde{B}_P = \operatorname{Tr} B_P \leq \Theta_1, \quad \det \tilde{B}_P \geq \Theta_2. \tag{6.17}
$$

Denoting $u = B_P\hat{s}/\sqrt{\hat{s}^T B_P \hat{s}} = B_P\hat{s}/\sqrt{\hat{s}^T \tilde{B}_P \hat{s}}$, $v = B_P^T\hat{s}/\sqrt{\hat{s}^T B_P \hat{s}} = B_P^T\hat{s}/\sqrt{\hat{s}^T \tilde{B}_P \hat{s}}$, we obtain

$$
\begin{aligned}
B_{k+1} &= B_P - (1/\hat{s}^T B_P \hat{s}) B_P \hat{s}\hat{s}^T B_P + (1/\hat{s}^T\hat{y})\hat{y}\hat{y}^T = B_P - uv^T + (1/\hat{s}^T\hat{y})\hat{y}\hat{y}^T, && (6.18)\\
\tilde{B}_{k+1} &= \tilde{B}_P - (1/\hat{s}^T \tilde{B}_P \hat{s}) \tilde{B}_P \hat{s}\hat{s}^T \tilde{B}_P + (1/\hat{s}^T\hat{y})\hat{y}\hat{y}^T + (1/4)(u-v)(u-v)^T, && (6.19)\\
\bar{B}_{k+1} &= ((1/\hat{s}^T\hat{y})\hat{s}\hat{s}^T + \hat{P}^T \bar{H}_P \hat{P})^{-1} = \bar{B}_P - (1/\hat{s}^T \bar{B}_P \hat{s}) \bar{B}_P \hat{s}\hat{s}^T \bar{B}_P + (1/\hat{s}^T\hat{y})\hat{y}\hat{y}^T, && (6.20)
\end{aligned}
$$

by (4.14), Theorem 2.3 and relations $2(uv^T + vu^T) = (u+v)(u+v)^T - (u-v)(u-v)^T$ and $\frac{1}{2}(u+v) = (1/\hat{s}^T \tilde{B}_P \hat{s})\tilde{B}_P \hat{s}$. Setting $\bar{u} = \bar{B}_P^{-1/2} u$, $\bar{v} = \bar{B}_P^{-1/2} v$, we get

$$-2\,u^T v \le |u|^2 + |v|^2 = \bar u^T \bar B_P \bar u + \bar v^T \bar B_P \bar v \le 2\mathrm{Tr}\,\bar B_P \le 2\Theta_0 \tag{6.21}$$

by $\bar u^T \bar u = u^T \bar H_P u = u^T H_P u = 1 = \bar v^T \bar v$ and (6.17). Using (6.2) with $q = \frac{1}{2}(u - v)$, $K = \tilde B_P - (1/\hat s^T \tilde B_P \hat s)\tilde B_P \hat s \hat s^T \tilde B_P + (1/\hat s^T \hat y)\hat y \hat y^T$, (6.19) and Theorem 2.3, we obtain

$$\det \tilde B_{k+1} \ge \det K = (\det \tilde B_P)\, \hat s^T \hat y / \hat s^T \tilde B_P \hat s. \tag{6.22}$$

From $\hat y = \bar P y$, $\hat s = \bar P^T s$, where $\bar P = I - (1/b_-)\, y_- s_-^T$, we have

$$|\hat y| \le \|\bar P\|\,|y| = |y|(|s_-|\,|y_-|/b_-) \le |y|\sqrt{\overline{G}/\underline{G}}\,, \quad |\hat s| \le \|\bar P^T\|\,|s| \le |s|\sqrt{\overline{G}/\underline{G}} \tag{6.23}$$

by Lemma 6.1. Further, by Theorem 2.5 we have $\hat s^T \hat y = s^T \hat y = b - s^T y_-\, s_-^T y / b_-$. Applying Lemma 6.5 repeatedly $m_n - 2$ times to the inequality $\det A_{[n]} \ge \varepsilon_D^{m_n} (\mathrm{Tr}\, A_{[n]})^{m_n}$ (see (6.3)), we get $\det \frac{1}{2}([s_-, s]^T [y_-, y] + [y_-, y]^T [s_-, s]) > \varepsilon_D^{m_n} (b_- + b)^2$. Using Lemma 6.4, this yields

$$\hat s^T \hat y = \frac{1}{b_-}\begin{vmatrix} b_- & s_-^T y \\ s^T y_- & b \end{vmatrix} \ge \frac{1}{b_-}\begin{vmatrix} b_- & (s_-^T y + s^T y_-)/2 \\ (s_-^T y + s^T y_-)/2 & b \end{vmatrix} > \varepsilon_D^{m_n} \frac{(b_- + b)^2}{b_-} > \varepsilon_D^{m} b. \tag{6.24}$$

Since the matrix $\tilde B_P$ is symmetric positive definite, from (6.17) – (6.24) we obtain

$$\mathrm{Tr}\, B_{k+1} = \mathrm{Tr}\, B_P - u^T v + \frac{|\hat y|^2}{\hat s^T \hat y} < 2\Theta_1 + \frac{|y|^2\,\overline{G}}{\varepsilon_D^m\, b\, \underline{G}} \le 2\Theta_1 + \frac{\overline{G}^{\,2}}{\varepsilon_D^m \underline{G}} \triangleq \Theta_3, \quad \mathrm{Tr}\, \bar B_{k+1} < \Theta_3, \tag{6.25}$$

$$\det \tilde B_{k+1} \ge (\det \tilde B_P) \frac{\hat s^T \hat s}{\hat s^T \tilde B_P \hat s} \frac{\hat s^T \hat y}{\hat s^T \hat s} > \frac{\Theta_2}{\Theta_1} \frac{\varepsilon_D^m\, b}{|s|^2 (\overline{G}/\underline{G})} \ge \Theta_2 \frac{\varepsilon_D^m \underline{G}^2}{\Theta_1 \overline{G}} \triangleq \Theta_4, \tag{6.26}$$

$k > 0$, with $\Theta_3 > \Theta_1$ and $\Theta_4 < \Theta_2$, by Lemma 6.1, (6.13), $\varepsilon_D < 1$, $\underline{G} \le \overline{G}$ and (6.9) – (6.10).

(iii) The lowest eigenvalue $\underline{\lambda}(\tilde B_k)$ of $\tilde B_k$ satisfies $\underline{\lambda}(\tilde B_k) \ge \det \tilde B_k / (\mathrm{Tr}\, B_k)^{N-1}$ by $\mathrm{Tr}\, \tilde B_k = \mathrm{Tr}\, B_k$, $k \ge 0$. Setting $q_k = \bar H_k^{1/2} g_k$, from (6.9) – (6.10), (6.13) and (6.25) – (6.26) we get

$$\frac{(s_k^T g_k)^2}{|s_k|^2 |g_k|^2} = \frac{s_k^T B_k s_k}{s_k^T s_k} \frac{g_k^T H_k g_k}{g_k^T g_k} = \frac{s_k^T \tilde B_k s_k}{s_k^T s_k} \frac{q_k^T q_k}{q_k^T \bar B_k q_k} \ge \frac{\det \tilde B_k}{(\mathrm{Tr}\, B_k)^{N-1}} \frac{1}{\mathrm{Tr}\, \bar B_k} > \frac{\Theta_4}{\Theta_3^N} \tag{6.27}$$

by $g_k^T H_k g_k = g_k^T \bar H_k g_k$, $k > 1$, which implies $\lim_{k\to\infty} |g_k| = 0$, see Theorem 3.2 in [15] and relations (3.17) – (3.18) ibid. □

One can show in the same way as in [8] that the inequality (6.27), the line search conditions (1.1) and Assumption 6.1 imply that the sequence $\{x_k\}$ is R-linearly convergent.

7 Numerical experiments

In this section, we compare our results with the results obtained by the L-BFGS method, see [8], [14], by the BNS method [1] and by our best limited-memory methods based on vector corrections, see [17]–[18]. All methods are implemented in the optimization software system UFO [13], which can be downloaded from `www.cs.cas.cz/luksan/ufo.html`. We use the following collections of test problems (several problems from the both collections were excluded from our numerical experiments, since they were not solved by any limited-memory variable metric method):

- **Test 11** – 55 chosen problems from [11] (computed repeatedly ten times for a better comparison), which are problems from the CUTE collection [2], some of them modified; used N are given in Table 1, where the modified problems are marked with '*',
- **Test 25** – 68 chosen problems from [10], which are sparse test problems for unconstrained optimization, contained in the system UFO, $N = 10000$.

The source texts and the reports corresponding to these test collections can be downloaded from the web page `www.cs.cas.cz/luksan/test.html`.

Problem	N	Problem	N	Problem	N	Problem	N
ARWHEAD	5000	DIXMAANI	3000	EXTROSNB	1000	NONDIA	5000
BDQRTIC	5000	DIXMAANJ	3000	FLETCBV3*	1000	NONDQUAR	5000
BROYDN7D	2000	DIXMAANK	3000	FLETCBV2	1000	PENALTY3	1000
BRYBND	5000	DIXMAANL	3000	FLETCHCR	1000	POWELLSG	5000
CHAINWOO	1000	DIXMAANM	3000	FMINSRF2	5625	SCHMVETT	5000
COSINE	5000	DIXMAANN	3000	FREUROTH	5000	SINQUAD	5000
CRAGGLVY	5000	DIXMAANO	3000	GENHUMPS	1000	SPARSINE	1000
CURLY10	1000	DIXMAANP	3000	GENROSE	1000	SPARSQUR	1000
CURLY20	1000	DQRTIC	5000	INDEF*	1000	SPMSRTLS	4999
CURLY30	1000	EDENSCH	5000	LIARWHD	5000	SROSENBR	5000
DIXMAANE	3000	EG2	1000	MOREBV*	5000	TOINTGSS	5000
DIXMAANF	3000	ENGVAL1	5000	NCB20*	1010	TQUARTIC*	5000
DIXMAANG	3000	CHNROSNB*	1000	NCB20B*	1000	WOODS	4000
DIXMAANH	3000	ERRINROS*	1000	NONCVXU2	1000		

Table 1: Dimensions for Test 11 – the modified CUTE collection.

We have used $\hat{m} = 5$, $\delta_1 = 10^{-2}$, $\delta_2 = 10^{-1}$, $\delta_3 = 10^{-13}$, $\delta_4 = 10^{-10}$, $\delta_5 = 10^{-3}$, $\delta_6 = 0.5$, $\varepsilon_D = 10^{-6}$, $\varepsilon_1 = 10^{-4}$, $\varepsilon_2 = 0.8$ and the final precision $\|g(x^\star)\|_\infty \le 10^{-6}$.

Table 2 contains the total number of function and also gradient evaluations (NFV) and the total computational time in seconds (Time).

Method	Test 11		Test 25	
	NFV	Time	NFV	Time
L-BFGS	80539	13.941	501651	574.59
BNS	78704	14.344	517186	661.66
Alg. 4.1 in [17]	64395	13.038	319565	420.00
Alg. 4.2 in [18], $n = 4$	63987	13.063	309650	415.27
Algorithm 1	65228	12.211	371830	468.19

Table 2: Comparison of the selected methods.

For a better demonstration of both the efficiency and the reliability, we compare selected optimization methods by using performance profiles introduced in [4]. The performance profile $\rho_M(\tau)$ is defined by the formula

$$\rho_M(\tau) = \frac{\text{number of problems where } \log_2(\tau_{P,M}) \le \tau}{\text{total number of problems}}$$

with $\tau \geq 0$, where $\tau_{P,M}$ is the performance ratio of the number of function evaluations (or the time) required to solve problem P by method M to the lowest number of function evaluations (or the time) required to solve problem P. The ratio $\tau_{P,M}$ is set to infinity (or some large number) if method M fails to solve problem P.

The value of $\rho_M(\tau)$ at $\tau = 0$ gives the percentage of test problems for which the method M is the best and the value for τ large enough is the percentage of test problems that method M can solve. The relative efficiency and reliability of each method can be directly seen from the performance profiles: the higher is the particular curve, the better is the corresponding method. Figures 1–4, based on results in Table 2, reveal the performance profiles for tested methods graphically.

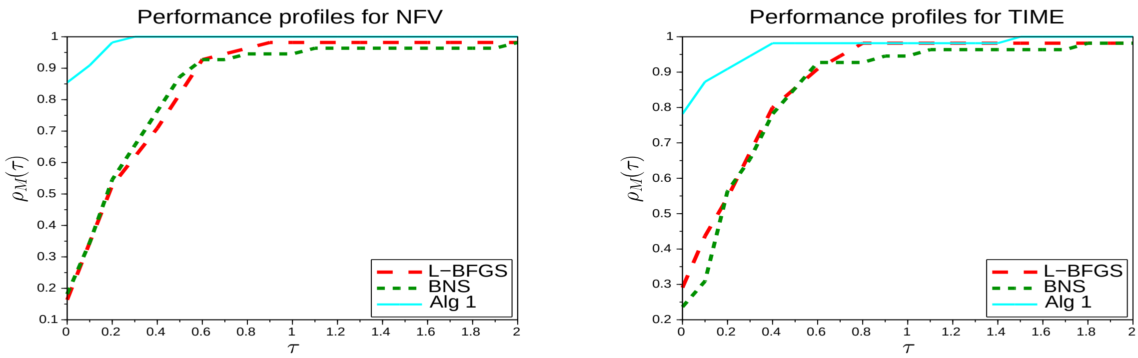

Figure 7.1: Comparison of $\rho_M(\tau)$ for Test 11 and various methods for NFV and TIME.

Figures 1–2 demonstrate the efficiency of our method in comparison with the BNS and the L-BFGS methods and from Figures 3–4 we can see that the numerical results for the new method and the results for our methods [18], [17] are comparable.

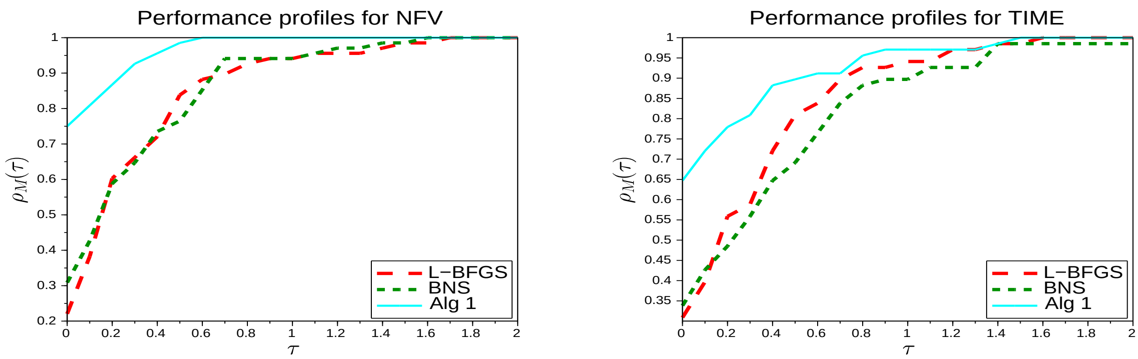

Figure 7.2: Comparison of $\rho_M(\tau)$ for Test 25 and various methods for NFV and TIME.

8 Conclusions

In this contribution, we derive a block version of the BFGS variable metric update formula for general functions and show some its positive properties and similarities to approaches based on vector corrections ([18], [17]).

In spite of the fact that this formula does not guarantee that the corresponding direction vectors are descent, we propose the block BNS method for large scale unconstrained

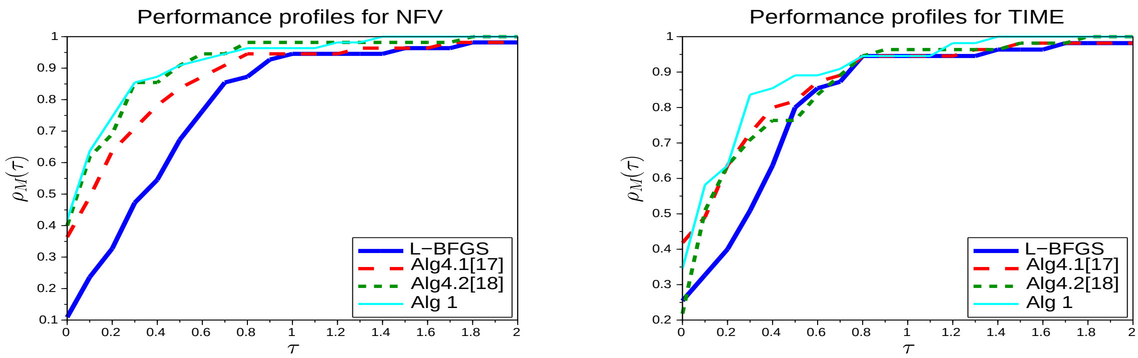

Figure 7.3: Comparison of $\rho_M(\tau)$ for Test 11 and various methods for NFV and TIME.

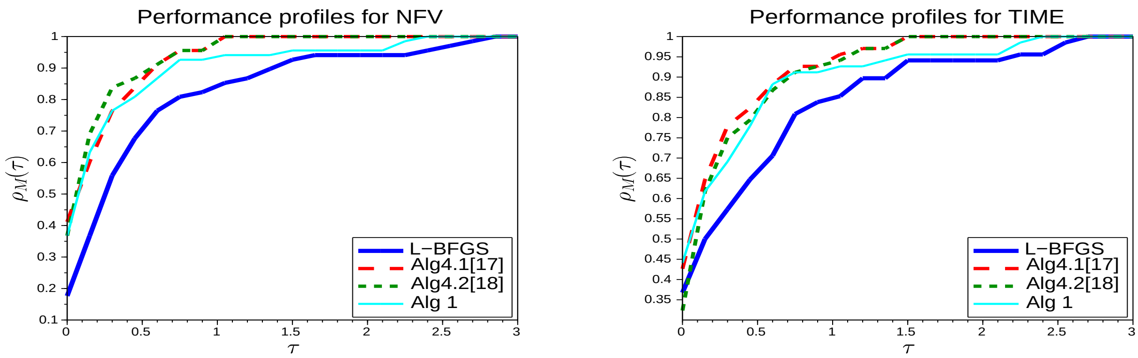

Figure 7.4: Comparison of $\rho_M(\tau)$ for Test 25 and various methods for NFV and TIME.

optimization, which utilizes the advantageous properties of the block BFGS update and is globally convergent.

Numerical results indicate that the block approach can improve unconstrained large-scale minimization results significantly compared with the frequently used L-BFGS and BNS methods.

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