Institute of Computer Science
Academy of Sciences of the Czech Republic

Some modifications of the limited-memory variable metric optimization methods

Jan Vlček[a], Ladislav Lukšan[a, b]

[a]Institute of Computer Science of the Czech Academy of Sciences,
Pod Vodárenskou věží 2, 182 07 Prague 8, Czech Republic and
[b]Technical University of Liberec, Hálkova 6, 461 17 Liberec, Czech Republic

Technical report No. V 1290

January 2023

Pod Vodárenskou věží 2, 182 07 Prague 8 phone: +420 266 052 083, fax: +420 286 585 789,
e-mail:luksan@cs.cas.cz, vlcek@cs.cas.cz

Institute of Computer Science
Academy of Sciences of the Czech Republic

Some modifications of the limited-memory variable metric optimization methods[1]

Jan Vlček[a], Ladislav Lukšan[a, b]

[a]Institute of Computer Science of the Czech Academy of Sciences,
Pod Vodárenskou věží 2, 182 07 Prague 8, Czech Republic and
[b]Technical University of Liberec, Hálkova 6, 461 17 Liberec, Czech Republic

Technical report No. V 1290

January 2023

Abstract:

Several modifications of the limited-memory variable metric (or quasi-Newton) line search methods for large scale unconstrained optimization are investigated. First the block version of the symmetric rank-one (SR1) update formula is derived in a similar way as for the block BFGS update in Vlček and Lukšan (Numerical Algorithms 2019). The block SR1 formula is then modified to obtain an update which can reduce the required number of arithmetic operations per iteration. Since it usually violates the corresponding secant conditions, this update is combined with the shifting investigated in Vlček and Lukšan (J. Comput. Appl. Math. 2006). Moreover, a new efficient way how to realize the limited-memory shifted BFGS method is proposed. For a class of methods based on the generalized shifted economy BFGS update, global convergence is established. A numerical comparison with the standard L-BFGS and BNS methods is given.

Keywords:
Unconstrained minimization, variable metric methods, limited-memory methods, variationally derived methods, arithmetic operations reduction, global convergence

[1]This work was supported by the Institute of Computer Science of the Czech Academy of Sciences (RVO: 67985807).

1 Introduction

In this report we propose some modifications of the variable metric (quasi-Newton) line search methods, see [5], [12], [15], for large scale unconstrained optimization

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

with the intention to reduce the number of arithmetic operation per iteration. We assume that the problem function $f : \mathcal{R}^N \to \mathcal{R}$ is differentiable.

The variable metric (VM) line search methods are iterative. They start with an initial point $x_0 \in \mathcal{R}^N$ and generate iterations $x_{k+1} \in \mathcal{R}^N$ by the process $x_{k+1} = x_k + s_k$, $s_k = t_k d_k$, $k \geq 0$, where d_k is the direction vector and $t_k > 0$ is a stepsize, chosen regularly in such a way that

$$f(x_{k+1}) - f(x_k) \leq \varepsilon_1 t_k g_k^T d_k, \qquad g_{k+1}^T d_k \geq \varepsilon_2 g_k^T d_k \tag{1.1}$$

(the Wolfe line search conditions [15]), $0 < \varepsilon_1 < 1/2$, $\varepsilon_1 < \varepsilon_2 < 1$ and $g_k = \nabla f(x_k)$. Usually $d_k = -H_k g_k$ with a symmetric positive definite matrix $H_k \triangleq B_k^{-1}$ (obviously this guarantees that d_k are descent directions). Typically H_0 is a multiple of I and H_{k+1} is obtained from H_k by a VM update to satisfy the secant (quasi-Newton) condition

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

with the difference vectors s_k, $y_k = g_{k+1} - g_k$, $k \geq 0$. 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 [5], [12], [15], belongs to the most efficient; the BNS [1] and L-BFGS ([8], [14]) methods represent its well-known limited-memory adaptations. We refer to Section 2 for a brief description of these methods.

To incorporate more past information to the update formula, the block (multiple secant) VM updates were proposed. The block BFGS update was derived in [16] for symmetric positive definite VM matrices, using a variational approach, further in [6] for quadratic functions, using corrections for the exact line search, and recently in [20] for general functions, using a block variant of the approach in [3]. This update satisfies the secant conditions with all used difference vectors and brings the best improvement of convergence in some sense [19, 20] for quadratic objective functions, but it usually needs some adaptations to guarantee that the corresponding direction vectors are descent directions for general functions.

In Section 3 we derive the block version of the standard SR1 formula [15] in a similar way. In Section 4 we describe some block modifications of quadratic functions and show that they can preserve a similar character, although the corresponding secant conditions and VM updates are changed. Modifying the block SR1 update in this way, we obtain an update which can reduce the required number of arithmetic operation per iteration. Since it usually violates the corresponding secant conditions, in Section 5 we combine this approach with the shifting investigated in [17] to derive the shifted economy VM updates. Moreover, we propose a new efficient way how to realize the limited-memory shifted BFGS method. For a class of methods based on the generalized shifted economy BFGS update, we establish global convergence in Section 6. In Section 7 we give a numerical comparison with the standard L-BFGS and BNS methods.

2 The L-BFGS and BNS methods

In this section we briefly describe the limited-memory VM methods L-BFGS [8, 14], implemented in [9] (subroutine PLIS), and BNS [1]. These methods are based on the BFGS update formula, mentioned in Section 1, which preserves the positive definiteness of H and can be written in the following quasi-product form

$$H_+ = (1/b)ss^T + \Big(I - (1/b)sy^T\Big)H\Big(I - (1/b)ys^T\Big), \quad b = s^Ty \tag{2.1}$$

($b > 0$ for $g \neq 0$ by (1.1)). To adapt the BFGS method for large scale optimization, we choose $H_k^I \in \mathcal{R}^{N\times N}$ in every iteration (usually $H_k^I = \zeta_k I$, $\zeta_k > 0$) and recurrently update H_k^I by the BFGS formula, using m pairs of vectors $(s_{k-\tilde{m}}, y_{k-\tilde{m}}), \dots, (s_k, y_k)$ successively, where

$$\tilde{m} = \min[k, \hat{m}-1], \quad m = \tilde{m} + 1, \quad k \geq 0 \tag{2.2}$$

and $\hat{m} > 1$ is a given parameter. To compute the direction vector, the updated matrices (approximations of the inverse Hessian matrix) need not be formed explicitly.

Here we focus mainly on the BNS update. Instead of the famous compact form [1], we utilize in this report its form (also given in [1])

$$H_+ = SR^{-T}DR^{-1}S^T + \Big(I - SR^{-T}Y^T\Big)H^I\Big(I - YR^{-1}S^T\Big), \tag{2.3}$$

where $S_k = [s_{k-\tilde{m}}, \dots, s_k]$, $Y_k = [y_{k-\tilde{m}}, \dots, y_k]$, D_k is the diagonal matrix with the diagonal entries of $S_k^TY_k$ and the matrix $R_k \triangleq [(R_k)_{ij}]_{i,j=k-\tilde{m}}^k$ is defined by $(R_k)_{ij} = (S_k^TY_k)_{ij}$ for $i \leq j$, $(R_k)_{ij} = 0$ otherwise (an upper triangular matrix), $k \geq 0$. We can see that for $H^I = \zeta I$ the direction vector $-H_+g_+$ can be calculated efficiently (without computing of H_+ explicitly) by

$$-H_+g_+ = -\zeta g_+ - S\Big[R^{-T}\Big((D + \zeta Y^TY)R^{-1}S^Tg_+ - \zeta Y^Tg_+\Big)\Big] + Y\Big[\zeta R^{-1}S^Tg_+\Big], \tag{2.4}$$

where in the square brackets we multiply by low-order matrices.

3 The block SR1 update

The approach in [20] how to derive the block BFGS update variationally, see Section 1, can be easily modified to obtain the block version of the SR1 update. In [20] we found a VM matrix H^* satisfying $(H^*)Y = S$ nearest to the given symmetric $H^I \in \mathcal{R}^{N\times N}$ in some sense, in the form

$$H^* = P_V^TH^IP_V + V(V^TY)^{-T}S^TP_V + S(V^TY)^{-1}V^T, \quad P_V = I - Y(V^TY)^{-1}V^T, \tag{3.1}$$

where V is a given $N \times m$ matrix for which V^TY is nonsingular. If $V = ST$, $T \in \mathcal{R}^{m\times m}$ nonsingular and $H_+ = H^*$, it gives the block BFGS update

$$H_+ = (I - S(Y^TS)^{-1}Y^T)H^I(I - Y(S^TY)^{-1}S^T) + S(S^TY)^{-1}S^T. \tag{3.2}$$

The relation (3.1) can also be expressed in another way. Denoting $Z = S - H^IY$, we get

$$
\begin{aligned}
H^* &= \Big(P_V^T H^I + V(V^TY)^{-T}S^T\Big)P_V + S(V^TY)^{-1}V^T \\
&= \Big(H^I - V(V^TY)^{-T}Y^TH^I + V(V^TY)^{-T}S^T\Big)P_V + S(V^TY)^{-1}V^T \\
&= \Big(H^I + V(V^TY)^{-T}Z^T\Big)P_V + S(V^TY)^{-1}V^T \\
&= H^I - H^IY(V^TY)^{-1}V^T + V(V^TY)^{-T}Z^TP_V + S(V^TY)^{-1}V^T \\
&= H^I + Z(V^TY)^{-1}V^T + V(V^TY)^{-T}Z^TP_V.
\end{aligned}
$$

Using a similar approach as for the block BFGS update, for $V = Z\,T_1$, $T_1 \in \mathcal{R}^{m\times m}$ nonsingular and $H_+ = H^*$ we obtain

$$
P_V = I - Y(T_1^TZ^TY)^{-1}T_1^TZ^T = I - Y(Z^TY)^{-1}Z^T, \qquad Z^TP_V = 0 \tag{3.3}
$$

and

$$
H_+ = H^I + Z(T_1^TZ^TY)^{-1}T_1^TZ^T = H^I + Z(Z^TY)^{-1}Z^T, \tag{3.4}
$$

which is the block SR1 update, see below. Obviously, we have $H_+Y = S$, i.e. the secant conditions are satisfied for all used difference vectors. Note that for Z^TY symmetric, the matrices H_+ are identical with the limited-memory SR1 matrices [1].

Using Woodbury formula and denoting $B_+ = H_+^{-1}$, $B^I = (H^I)^{-1}$ and $W = B^IZ = B^IS - Y$, for W^TS nonsingular we get the following formula, given in [1]:

$$
B_+ = B^I - B^IZ(Z^TY + Z^TB^IZ)^{-1}Z^TB^I = B^I - W(W^TS)^{-1}W^T.
$$

4 The block modified VM updates

Our modifications of the block secant conditions and the corresponding VM updates are based on the following lemma:

Lemma 4.1. *Let f_Q be a quadratic function $f_Q(x) = \frac{1}{2}(x-\bar{x})^T\Omega(x-\bar{x})$, $\bar{x} \in \mathcal{R}^N$, with a symmetric positive definite matrix Ω, $S_k = [s_{k-\tilde{m}}, \dots, s_k]$, $Y_k = [y_{k-\tilde{m}}, \dots, y_k]$, $\alpha \ge 0$ and let denote $\hat{\Omega}_\alpha = (\Omega^{-1} + \alpha I)^{-1}$ and $\hat{S}_\alpha = S + \alpha Y$. Then $x = \bar{x}$ minimizes also the function $\hat{f}_{Q,\alpha}(x) = \frac{1}{2}(x-\bar{x})^T\hat{\Omega}_\alpha(x-\bar{x})$ and $\hat{\Omega}_\alpha\hat{S}_\alpha = Y$ holds.*

Moreover, let $\lambda_1 \le \dots \le \lambda_N$ be the eigenvalues of Ω. Then $\lambda_1/(1+\alpha\lambda_1) \le \dots \le \lambda_N/(1+\alpha\lambda_N)$ are the corresponding eigenvalues of $\hat{\Omega}_\alpha$ and for $\lambda_1 < \lambda_N$ and $\alpha > 0$, $\hat{\Omega}_\alpha$ is always conditioned better than Ω.

Proof. Since $\hat{\Omega}_\alpha$ is also symmetric positive definite, the functions f_Q, $\hat{f}_{Q,\alpha}$ have its global minima at the same point $x = \bar{x}$. From $\Omega S = Y$ we obtain $\hat{\Omega}_\alpha^{-1}Y = (\Omega^{-1} + \alpha I)Y = \hat{S}_\alpha$, thus $\hat{\Omega}_\alpha\hat{S}_\alpha = Y$.

Let $\Omega p = \lambda p$, $p \in \mathcal{R}^N$. Then $\lambda > 0$ and $\Omega^{-1}p = (1/\lambda)p$, thus $\hat{\Omega}_\alpha^{-1}p = (\Omega^{-1} + \alpha I)p = (1/\lambda + \alpha)p$ and $\hat{\Omega}_\alpha p = \big(1/(1/\lambda+\alpha)\big)p = \big(\lambda/(1+\alpha\lambda)\big)p$, where $\lambda/(1+\alpha\lambda)$ is the ascending function of λ. Finally, let $\lambda_1 < \lambda_N$ and $\alpha > 0$. Then the condition number of $\hat{\Omega}_\alpha$ is

$$
\kappa(\hat{\Omega}_\alpha) = \frac{\lambda_N}{1+\alpha\lambda_N}\,\frac{1+\alpha\lambda_1}{\lambda_1} < \frac{\lambda_N}{\lambda_1} = \kappa(\Omega).
$$

$\square$

The lemma indicates that for S replaced by $\hat{S}_\alpha$ with small α, the character of the quadratic approximation of f can be similar, although this replacement usually violates the corresponding secant conditions. To guarantee the positive definiteness of $\hat{S}_\alpha^T Y$ (the symmetry of $S^T Y$ is not supposed), we can use the following lemma.

Lemma 4.2. *Let the columns of Y be linearly independent, U be an upper triangular matrix satisfying $Y^T Y = U^T U$ and let $\hat{\lambda} \le 0$ be the minimum eigenvalue of $M = (1/2)U^{-T}(S^T Y + Y^T S)U^{-1}$. Then $\hat{S}_\alpha Y$ is positive definite for any $\alpha > -\hat{\lambda}$.*

Proof. Let $\alpha > -\hat{\lambda}$. We can write $M = Q\Lambda Q^T$ with Q orthogonal and Λ diagonal with $\Lambda + \alpha I$ symmetric positive definite and the assertion follows from

$$U^T Q(\Lambda + \alpha I)Q^T U = U^T(M + \alpha I)U = \frac{1}{2}(S^T Y + Y^T S) + \alpha Y^T Y = \frac{1}{2}(\hat{S}_\alpha^T Y + Y^T \hat{S}_\alpha). \quad \square$$

When we use $S + H^I Y$ instead of S for the block SR1 update (3.4) with $H^I = \sigma I$, $\sigma > 0$, we have

$$H_+ = \sigma I + S(S^T Y)^{-1} S^T, \quad H_+ Y = S + \sigma Y, \tag{4.1}$$

or

$$H_+ = \sigma I + S X S^T, \tag{4.2}$$

if we replace $(S^T Y)^{-1}$ by a suitable symmetric matrix X.

We will see that (4.2) can be considered as an economy variant of the BNS update (2.3), since using the form (4.2) we can reduce the number of the required arithmetic operations to calculate the direction vector $-H_+ g_+$, in comparison with the BNS update. Suppose that all entries of X have been calculated. While (2.3) needs $(4m+1)N + O(m^2)$ multiplications, see [1], to get $-H_+ g_+$ using (4.2), we need only $(2m+1)N + O(m^2)$ multiplications. Simultaneously, similarly as for the BNS update (see [1]), we can obviously obtain all entries of the last column of R (see Section 2), thus the whole of R and D, in a negligible number of arithmetic operations for $m \ll N$. Note that in this economy variant we do not calculate $Y^T g_+$, thus nor $Y^T s_+ = -t\, Y^T H_+ g_+$, see (4.2).

To calculate X (and subsequently $H_+ g_+$), using only entries of R, we can choose e.g. $X = (R + R^T - D)^{-1}$ (motivated by (4.1)) if this matrix is symmetric positive definite (to guarantee the descent property of the direction vector) or $X = R^{-T} D R^{-1}$ (motivated by (2.3)), which is obviously always symmetric positive definite. However, these updates usually violates the corresponding secant conditions.

5 The shifted economy VM updates

The efficiency of the method based on (4.2) can be improved, if we use the shifting approach investigated in [17]. To satisfy the secant condition $H_+ y = s$, we replace s by $\tilde{s} = s - \sigma y$, $\sigma \in (0, b/|y|^2)$ (to have $\tilde{s}^T y > 0$), together with replacement (4.2) by

$$H_+ = \sigma I + \tilde{S}\tilde{X}\tilde{S}^T \tag{5.1}$$

with some $\tilde{X}$, see below, instead of X and $\tilde{S} = [S_P, \tilde{s}]$ instead of $S = [S_P, s]$. The following theorem shows that e.g. the shifted BFGS update can be expressed in the economy form (5.1), since we can write it as $A_+ = (1/\tilde{b})\tilde{s}\tilde{s}^T + \tilde{P}^T A \tilde{P}$, if we denote $A = H - \zeta I$, $A_+ = H_+ - \sigma I$, $\tilde{P} = I - (1/\tilde{b}) y \tilde{s}^T$, $\tilde{b} = \tilde{s}^T y$, see [17]. Moreover, the theorem shows the role of the secant conditions and enables us to construct further shifted economy updates (with other suitable $\tilde{X}$). We can also see that to realize the limited-memory shifted methods, it can be used the similar approach as in case of the standard BNS method [1]. In every iteration we start with $A^I = 0$ (instead of $H^I = \zeta I$ for the BNS method) and then calculate the block shifted update (5.1).

Theorem 5.1. *Let* $S = [S_P, s]$, $\tilde{S} = [S_P, \tilde{s}]$, $\tilde{s} = s - \sigma y$, $\sigma > 0$, $\tilde{b} = \tilde{s}^T y > 0$, $\tilde{X} = \begin{bmatrix} X_P & w \\ w^T & \xi \end{bmatrix} \in \mathcal{R}^{m \times m}$, X_P *symmetric positive definite,* $w \in \mathcal{R}^{\tilde{m}}$, $\xi \in \mathcal{R}$, $A = S_P X_P S_P^T$, $A_+ = \tilde{S}\tilde{X}\tilde{S}^T$ *and* $u = S_P^T y$. *Suppose that* H_+ *is defined by (5.1) and the columns of* $\tilde{S}$ *are linearly independent. Then* $A_+ y = \tilde{s}$ *(i.e.* $H_+ y = s$*) if and only if*

$$w = (-1/\tilde{b}) X_P u, \qquad \xi = (\tilde{b} + y^T A y)/\tilde{b}^2. \tag{5.2}$$

If this is the case, then

$$A_+ = (1/\tilde{b})\tilde{s}\tilde{s}^T + \tilde{P}^T A \tilde{P}, \quad \tilde{P} = I - (1/\tilde{b}) y \tilde{s}^T, \tag{5.3}$$

$\tilde{X}$ *is symmetric positive definite and it holds*

$$\tilde{X}^{-1} = \begin{bmatrix} X_P^{-1} + (1/\tilde{b}) u u^T & u \\ u^T & \tilde{b} \end{bmatrix}. \tag{5.4}$$

Proof. We get $A_+ y = \tilde{S}(\tilde{X}\tilde{S}^T y)$, where

$$\tilde{X}\tilde{S}^T y = \begin{bmatrix} X_P & w \\ w^T & \xi \end{bmatrix} \begin{bmatrix} u \\ \tilde{b} \end{bmatrix} = \begin{bmatrix} X_P u + \tilde{b} w \\ w^T u + \xi\, \tilde{b} \end{bmatrix}.$$

Thus

$$A_+ y = S_P (X_P u + \tilde{b} w) + \tilde{s}(w^T u + \xi\, \tilde{b}) \tag{5.5}$$

and $A_+ y = \tilde{s}$ is equivalent to

$$X_P u + \tilde{b} w = 0, \quad w^T u + \xi\, \tilde{b} = 1 \tag{5.6}$$

by linear independence of columns of $\tilde{S}$ and further equivalent to (5.2) by $A = S_P X_P S_P^T$ and $\tilde{b} + y^T A y = \tilde{b} + u^T X_P u = \tilde{b} - \tilde{b} w^T u = \tilde{b} - \tilde{b}(1 - \xi\tilde{b}) = \xi\tilde{b}^2$. Let $A_+ y = \tilde{s}$. From (5.2) we obtain $S_P w = (-1/\tilde{b}) A y$ and

$$\begin{aligned} A_+ &= [S_P, \tilde{s}] \begin{bmatrix} X_P & w \\ w^T & \xi \end{bmatrix} \begin{bmatrix} S_P^T \\ \tilde{s}^T \end{bmatrix} = S_P X_P S_P^T + S_P w \tilde{s}^T + \tilde{s} w^T S_P^T + \xi \tilde{s}\tilde{s}^T \\ &= A - \frac{1}{\tilde{b}} A y \tilde{s}^T - \frac{1}{\tilde{b}} \tilde{s} y^T A + \frac{\tilde{b} + y^T A y}{\tilde{b}^2} \tilde{s}\tilde{s}^T = \frac{1}{\tilde{b}} \tilde{s}\tilde{s}^T + \tilde{P}^T A \tilde{P}, \end{aligned}$$

i.e. (5.3). Now we can derive (5.4). We have

$$\left[\begin{array}{cc} X_P & w \\ w^T & \xi \end{array}\right]\left[\begin{array}{cc} X_P^{-1}+(1/\tilde{b})uu^T & u \\ u^T & \tilde{b} \end{array}\right]=\left[\begin{array}{cc} I+(1/\tilde{b})(X_Pu+\tilde{b}w)u^T & X_Pu+\tilde{b}w \\ w^TX_P^{-1}+(1/\tilde{b})(w^Tu+\xi\tilde{b})u^T & w^Tu+\xi\,\tilde{b} \end{array}\right]. \quad (5.7)$$

Since we can rewrite (5.2) as $X_Pu+\tilde{b}w=0$ and $\xi\tilde{b}=1+(1/\tilde{b})y^TAy$, we obtain

$$w^Tu+\xi\tilde{b}=w^Tu+1+\frac{1}{\tilde{b}}u^TX_Pu=w^Tu+1-w^Tu=1$$

and

$$w^TX_P^{-1}+(1/\tilde{b})(w^Tu+\xi\tilde{b})u^T=w^TX_P^{-1}+(1/\tilde{b})u^T=\left(w^T+(1/\tilde{b})u^TX_P\right)X_P^{-1}=0.$$

These relations together with (5.7) give (5.4).

Finally, since the Schur complement of entry $\tilde{b}>0$ in $\tilde{X}^{-1}$ is X_P^{-1}, symmetric positive definite by assumption, $\tilde{X}$ is also symmetric positive definite by Theorem 2.5.6 in [4]. □

In case of the shifted economy BFGS update, (5.1) can be regarded as the shifted variant of (2.3) with $H^I=0$ and the matrix $\tilde{X}$ can be expressed in the form

$$\tilde{X}=\tilde{R}^{-T}\tilde{D}\tilde{R}^{-1}, \quad (5.8)$$

where $\tilde{D}_k$ is the diagonal matrix with the diagonal entries of $\tilde{S}_k^TY_k$ and $\tilde{R}_k\triangleq[(\tilde{R}_k)_{ij}]_{i,j=k-\tilde{m}}^k$ is defined by $(\tilde{R}_k)_{ij}=(\tilde{S}_k^TY_k)_{ij}$ for $i\le j$, $(\tilde{R}_k)_{ij}=0$ otherwise, $k\ge 0$ (an upper triangular matrix). Our experiments indicate that numerical results can be slightly improved, e.g. if we replace $\tilde{b}$ by b everywhere in the shifted economy BFGS update (5.3). Thus we will investigate the generalized update (for $\beta=\gamma=\tilde{b}$ it is (5.3))

$$A_+=(1/\gamma)\tilde{s}\tilde{s}^T+P^TAP, \quad P=I-(1/\beta)y\tilde{s}^T, \quad \beta,\gamma\ge\delta_1\tilde{b}, \quad \delta_1>0. \quad (5.9)$$

The following theorem shows that this update corresponds to (5.1) with $\tilde{X}=\tilde{U}^{-T}\tilde{E}\tilde{U}^{-1}$ (see below) and that the modification of β,γ influences only the diagonal entries of $\tilde{U},\tilde{E}$.

Theorem 5.2. *Let $\tilde{s}\in\mathcal{R}^N$, $\tilde{S}=[S_P,\tilde{s}]\in\mathcal{R}^{N\times m}$, $A=S_PX_PS_P^T$ and $X_P=U_P^{-T}E_PU_P^{-1}$ with E_P diagonal and U_P upper triangular, both nonsingular of order $\tilde{m}$. Let $A_+=\tilde{S}\tilde{X}\tilde{S}^T$, where $\tilde{X}=\tilde{U}^{-T}\tilde{E}\tilde{U}^{-1}$,*

$$\tilde{E}=\left[\begin{array}{cc} E_P & 0 \\ 0^T & \beta^2/\gamma \end{array}\right], \quad \tilde{U}=\left[\begin{array}{cc} U_P & S_P^Ty \\ 0^T & \beta \end{array}\right], \quad \beta,\gamma>0.$$

Then A_+ is given by (5.9) and

$$\tilde{X}^{-1}=\left[\begin{array}{cc} X_P^{-1}+(\gamma/\beta^2)S_P^Tyy^TS_P & (\gamma/\beta)S_P^Ty \\ (\gamma/\beta)y^TS_P & \gamma \end{array}\right]. \quad (5.10)$$

Proof. We have

$$\begin{aligned}\tilde{U}^{-T}\tilde{E}\tilde{U}^{-1} &= \left[\begin{array}{cc} U_P^{-T} & 0 \\ -(1/\beta)y^TS_PU_P^{-T} & 1/\beta \end{array}\right]\left[\begin{array}{cc} E_P & 0 \\ 0^T & \beta^2/\gamma \end{array}\right]\left[\begin{array}{cc} U_P^{-1} & -(1/\beta)U_P^{-1}S_P^Ty \\ 0^T & 1/\beta \end{array}\right] \\ &= \left[\begin{array}{cc} X_P & -(1/\beta)X_PS_P^Ty \\ -(1/\beta)y^TS_PX_P & (1/\beta^2)y^TAy+1/\gamma \end{array}\right],\end{aligned}$$

$$\begin{aligned}
A_+ &= [S_P, \tilde{s}]\begin{bmatrix} X_P & -(1/\beta)X_P S_P^T y \\ -(1/\beta)y^T S_P X_P & (1/\beta^2)y^T A y + 1/\gamma \end{bmatrix}\begin{bmatrix} S_P^T \\ \tilde{s}^T \end{bmatrix} \\
&= A - \frac{1}{\beta}Ay\tilde{s}^T - \frac{1}{\beta}\tilde{s}y^T A + \frac{y^T A y + \beta^2/\gamma}{\beta^2}\tilde{s}\tilde{s}^T = \frac{1}{\gamma}\tilde{s}\tilde{s}^T + P^T A P, \\
\tilde{U}\tilde{E}^{-1}\tilde{U}^T &= \begin{bmatrix} U_P & S_P^T y \\ 0^T & \beta \end{bmatrix}\begin{bmatrix} E_P^{-1} & 0 \\ 0^T & \gamma/\beta^2 \end{bmatrix}\begin{bmatrix} U_P^T & 0 \\ y^T S_P & \beta \end{bmatrix} \\
&= \begin{bmatrix} U_P E_P^{-1} U_P^T + (\gamma/\beta^2) S_P^T y y^T S_P & (\gamma/\beta) S_P^T y \\ (\gamma/\beta) y^T S_P & \gamma \end{bmatrix}. \qquad \square
\end{aligned}$$

The efficiency of the shifted VM updates depends strongly on the shift parameter σ, see [17]. For the generalized shifted BFGS update, good results were obtained for

$$\sigma = \frac{b}{|y|^2}\,\theta^\kappa, \quad \theta = \frac{1}{1+\sqrt{1-b^2/(|s|^2|y|^2)}}, \quad \kappa \approx 2 \left(\sigma \approx \frac{b}{\left(|y|+\sqrt{|y|^2-b^2/|s|^2}\right)^2}\right) \tag{5.11}$$

(we refer to [17] for the meaning of θ). To guarantee global convergence, we can replace (5.11) by

$$\sigma = \frac{b}{|y|^2}\,\bar{\theta}^\kappa, \quad \bar{\theta} = \frac{1}{1+\sqrt{\max[\delta_0, 1 - b^2/(|s|^2|y|^2)]}}, \qquad \delta_0 \in (0,1). \tag{5.12}$$

Obviously, this implies $1 + \sqrt{\delta_0} \le 1/\bar{\theta} \le 2$, thus

$$1/2^\kappa \le \bar{\theta}^\kappa \le 1/(1+\sqrt{\delta_0})^\kappa, \tag{5.13}$$

and further

$$(b/|y|^2)/2^\kappa \le \sigma \le (b/|y|^2)/(1+\sqrt{\delta_0})^\kappa. \tag{5.14}$$

We now state the generalized shifted economy BFGS method in details. For simplicity, we do not describe stopping criteria and contingent restarts when some computed direction vector is not a sufficiently descent direction. Note that the contingent restarts have occurred very rarely in our numerical experiments. First we present an auxiliary procedure.

Procedure 1 *(Updating of basic matrices)*

Given: matrices U_P, E_P, S_P, vectors $\tilde{s}, g_+, S_P^T g$ and $\beta, \gamma > 0$.

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

(ii): Set $\tilde{S} := [S_P, \tilde{s}]$, $\tilde{S}^T g_+ := [S_P^T g_+, \tilde{s}^T g_+]$.

(iii): Set $\tilde{U} := \begin{bmatrix} U_P & S_P^T y \\ 0^T & \beta \end{bmatrix}$, $\tilde{E} := \begin{bmatrix} E_P & 0 \\ 0^T & \beta^2/\gamma \end{bmatrix}$ and return.

Algorithm 1

Data: A maximum number $\hat{m}$ of columns S, Y, line search parameters $\varepsilon_1, \varepsilon_2$, $0 < \varepsilon_1 < 1/2$, $\varepsilon_1 < \varepsilon_2 < 1$ and global convergence parameters $\delta_0 \in (0,1)$, $\delta_1 > 0$.

Step 1: Initiation. Choose starting point $x_0 \in \mathcal{R}^N$, define the starting matrix $H_0 := I$ and the direction vector $d_0 := -g_0$ and initiate the iteration counter k to zero.

Step 2: Line search. Compute $x_+ := x+td$, where t satisfies (1.1), $g_+ := \nabla f(x_+)$, $s := td$, $y := g_+ - g$ and $b := s^T y$. Define σ by (5.12), compute $\tilde{s} := s - \sigma y$ and $\tilde{b} := \tilde{s}^T y$. Define $\beta, \gamma \geq \delta_1 \tilde{b}$ and set $\tilde{m} := \min[k, \hat{m}-1]$ and $m := \tilde{m} + 1$. If $k = 0$ set $\tilde{S} := [\tilde{s}]$, $\tilde{E} := [\beta^2/\gamma]$, $\tilde{U} := [\beta]$, compute $\tilde{S}^T g_+$ and go to Step 4.

Step 3: Basic matrices updating. Using Procedure 1, form the matrices $\tilde{S}, \tilde{U}, \tilde{E}$.

Step 4: Direction vector. Define H_+ by (5.1) with $\tilde{X} = \tilde{U}^{-T} \tilde{E} \tilde{U}^{-1}$ and compute $d_+ := -H_+ g_+$. Set $k := k+1$. If $k \geq \hat{m}$ delete the first column of $\tilde{S}_-$ and the first row and column of $\tilde{U}, \tilde{E}$ to form S_P, U_P, E_P. Go to Step 2.

6 Global convergence

In this section we establish global convergence of Algorithm 1 in convex case and without restarts. Note that a suitable restarts technique can guarantee global convergence also for non-convex f, see e.g. Algorithm 6.1 and comments in the beginning of Section 7 in [21]. Besides, there are some other possibilities how to establish global convergence of VM methods for non-convex f, see e.g. [7, 22].

Assumption 6.1 and Lemma 6.1 are presented in [18]. By Theorem 5.2, instead of (5.1) we can use $H_{k+1} = \sigma_k I + A_{k+1}^{k+1}$ in Step 4 of Algorithm 1, where

$$A_{k-\tilde{m}}^{k+1} = 0, \quad A_{i+1}^{k+1} = \frac{1}{\gamma_i} \tilde{s}_i \tilde{s}_i^T + P_i^T A_i^{k+1} P_i, \;\; i = k-\tilde{m}, \ldots, k, \quad P_i = I - \frac{1}{\beta_i} y_i \tilde{s}_i^T. \qquad (6.1)$$

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. $0 < \underline{G} \leq \underline{\lambda}(G(x)) \leq \overline{\lambda}(G(x)) \leq \overline{G} < \infty$, $x \in \mathcal{R}^N$, 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 $\underline{G} \leq |y|^2/b \leq \overline{G}$ and $b/|s|^2 \geq \underline{G}$.*

Lemma 6.2. *Let A_{i+1}^{k+1} be given by (6.1) with A_i^{k+1} symmetric positive semidefinite and $\beta_i, \gamma_i > 0$. Then*

$$\operatorname{Tr} A_{i+1}^{k+1} \leq \frac{|\tilde{s}_i|^2}{\gamma_i} + \Big(1 + \frac{|\tilde{s}_i||y_i|}{\beta_i}\Big)^2 \operatorname{Tr} A_i^{k+1}, \quad i = k - \tilde{m}, \ldots, k, \quad k \geq 0. \qquad (6.2)$$

Proof. Using the Schwarz inequality and since $|Kp| \leq |p| \operatorname{Tr} K$ for $p \in \mathcal{R}^N$ and $K \in \mathcal{R}^{N \times N}$ symmetric positive semidefinite, from (6.1) we obtain

$$\begin{aligned} \operatorname{Tr} A_{i+1}^{k+1} &= \frac{|\tilde{s}_i|^2}{\gamma_i} + \operatorname{Tr} A_i^{k+1} - 2 \frac{\tilde{s}_i^T A_i^{k+1} y_i}{\beta_i} + \frac{|\tilde{s}_i|^2 \, |y_i^T A_i^{k+1} y_i|}{\beta_i^2} \\ &\leq \frac{|\tilde{s}_i|^2}{\gamma_i} + \Big(1 + 2 \frac{|\tilde{s}_i||y_i|}{\beta_i} + \frac{|\tilde{s}_i|^2 |y_i|^2}{\beta_i^2}\Big) \operatorname{Tr} A_i^{k+1}. \end{aligned} \qquad \square$$

Theorem 6.1. *Let 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. (i) First we will show

$$\operatorname{Tr} B_{k+1} \le N/\sigma_k \le N\overline{G}2^\kappa, \quad k \ge 0, \tag{6.3}$$

where we denote $B_{k+1} = H_{k+1}^{-1}$. To do it, we can use (5.1), which implies

$$\sigma_k B_{k+1} = I - \tilde{S}_k(\sigma_k \tilde{X}_k^{-1} + \tilde{S}_k^T \tilde{S}_k)^{-1} \tilde{S}_k^T.$$

Since $\tilde{X}_k$ is obviously symmetric positive definite, we have $\operatorname{Tr} B_{k+1} \le N/\sigma_k$, thus (6.3) by (5.14) and Lemma 6.1.

(ii) Denoting

$$C_1 = 1/(1+\sqrt{\delta_0})^\kappa, \;\; C_2 = \overline{G}/(\delta_1(1- C_1)), \;\; C_3 = (1/\underline{G})/(\delta_1(1- C_1)) + C_2(C_1/\underline{G})^2,$$

we will prove that for any $i > 0$

$$b_i/\tilde{b}_i \le 1/(1 - C_1), \quad |y_i|^2/\beta_i \le C_2, \quad |\tilde{s}_i|^2/\beta_i \le C_3, \quad |\tilde{s}_i|^2/\gamma_i \le C_3. \tag{6.4}$$

As regards the first inequality, we get

$$b_i/\tilde{b}_i = b_i/(b_i - \sigma_i|y_i|^2) = 1/(1 - \bar{\theta}_i^\kappa) \le 1/(1 - C_1)$$

by (5.13), observing that $1/(1 - t)$ is an increasing function of t on $(0, 1)$. The second inequality follows immediately from $\beta_i \ge \delta_1 \tilde{b}_i$ and Lemma 6.1; similarly we get $|s_i|^2/\beta_i \le (1/\underline{G})/(\delta_1(1- C_1))$; the same inequality holds for $|s_i|^2/\gamma_i$. Considering that $\sigma_i \le C_1/\underline{G}$ by (5.14) and Lemma 6.1, it suffices to use $|\tilde{s}_i|^2 = |s_i|^2 - 2\sigma_i b_i + \sigma_i^2|y_i|^2 \le |s_i|^2 + \sigma_i^2|y_i|^2$.

(iii) Denoting $C_0 = (1 + \sqrt{C_2C_3}\,)^2$, we will further prove

$$\operatorname{Tr} H_{k+1} \le NC_1/\underline{G} + (1 + C_0 + \ldots + C_0^{m-1})C_3 \triangleq C_4. \tag{6.5}$$

Using Lemma 6.2, we get $\operatorname{Tr} A_{i+1}^{k+1} \le C_3 + C_0 \operatorname{Tr} A_i^{k+1}$, $i = k-\tilde{m}, \ldots, k$, which yields

$$\operatorname{Tr} A_{k+1}^{k+1} \le (1 + C_0 + \ldots + C_0^{m-1})C_3$$

by $\operatorname{Tr} A_{k-\tilde{m}}^{k+1} = 0$. This gives (6.5) by $\sigma_i \le C_1/\underline{G}$.

(iv) Setting $q_k = H_k^{1/2} g_k$, from $s_k = -t_k H_k g_k$ we get

$$\frac{(s_k^T g_k)^2}{|s_k|^2|g_k|^2} = \frac{-t_k q_k^T q_k}{t_k^2 q_k^T H_k q_k} \frac{-t_k q_k^T q_k}{q_k^T B_k q_k} = \frac{q_k^T q_k}{q_k^T H_k q_k} \frac{q_k^T q_k}{q_k^T B_k q_k} \ge \frac{1}{\operatorname{Tr} H_k} \frac{1}{\operatorname{Tr} B_k} \ge \frac{1}{C_4} \frac{1}{N\overline{G}2^\kappa}, \tag{6.6}$$

$k > 0$. It follows from the positive definiteness of H_k that the search direction is a descent direction. Thus, (6.6) and the Zoutendijk condition (see e.g. [15]) yield $\lim_{i\to\infty}\|g_i\| = 0$, see Theorem 3.2 in [15] and relations (3.17)–(3.18) ibid. □

In the same way as in [8] one can show that (6.6) with line search conditions (2.1) and Assumption 6.1 imply that the sequence $\{x_i\}$ is at least R-linearly convergent.

7 Numerical experiments

In Table 1 we compare the total number of function evaluations (NFV) and the total computational time in seconds (Time) for the generalized shifted economy BFGS method (se-BFGS), using $\tilde{X} = \tilde{U}^{-T}\tilde{E}\tilde{U}^{-1}$, σ given by (5.12) and $\beta = \gamma = b$, with the VM methods

L-BFGS and BNS, see Section 2. We use the collections Test 25 of 67 test problems from [10] and Test 11 of 55 problems from [11] (problems from the CUTE collection [2], 8 of them modified, $N = 1000 - 5625$), $m = 5$, $\varepsilon_1 = 10^{-4}$, $\varepsilon_2 = 0.9$, $\delta_0 = 10^{-10}$, $\delta_1 = 1$, $\kappa = 2.1$ and the final precision $\|g(x^\star)\|_\infty \le 10^{-6}$.

Note that 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`.

Method	Test 11		Test 25, N: 1000		Test 25, N: 2000		Test 25, N: 5000	
	NFV	Time	NFV	Time	NFV	Time	NFV	Time
L-BFGS	79575	11.39	125348	10.89	188547	37.08	441568	209.44
BNS	76463	9.74	120328	9.39	179629	31.83	434504	187.52
se-BFGS	82103	9.14	126591	9.09	197567	30.30	489690	184.37

Table 1: Comparison of the selected methods.

8 Conclusions

In this contribution, in a similar way as for the block BFGS update in [20] we derive the block SR1 update variationally. Then we modify it to reduce the required number of arithmetic operations per iteration. Since it usually violates the corresponding secant conditions, this update is combined with the shifting investigated in [17] to derive the shifted economy VM updates. Moreover, a new efficient way how to realize the limited-memory shifted BFGS method is proposed. For a class of methods based on the generalized shifted economy BFGS update, global convergence is established. Further, a numerical comparison with the standard L-BFGS and BNS methods is given.

Our experiments indicate that this approach can improve unconstrained large-scale minimization results compared with our implementation of the frequently used L-BFGS and BNS methods as regards the computational time.

References

[1] Byrd, R.H., Nocedal, J., Schnabel, R.B.: *Representation of quasi-Newton matrices and their use in limited memory methods*, Math. Programming 63, 129-156 (1994)

[2] Bongartz, I., Conn, A.R., Gould, N., Toint, P.L.: *CUTE: constrained and unconstrained testing environment*, ACM Transactions on Mathematical Software 21, 123-160 (1995)

[3] Dennis, J.E., Jr., Schnabel, R.B.: *Least change secant updates for quasi-Newton methods*, SIAM Review 21, 443-459 (1979)

[4] Fiedler, M.: Special matrices and their applications in numerical mathematics, 2nd ed. Mineola, Dover Publications, N.Y., 2008

[5] Fletcher, R.: Practical Methods of Optimization, John Wiley & Sons, Chichester, 1987

[6] Hu, Y.F., Storey, C.: *Motivating Quasi-Newton Updates by Preconditioned Conjugate Gradient Methods*, Math. Report A 150, Department of Mathematical Sciences, Loughborough University of Technology, England (1991)

[7] Li, D., Fukushima M., *A modified BFGS method and its global convergence in nonconvex minimization*, J. Comput. Appl. Math. 129, 15-35 (2001)

[8] Liu, D.C., Nocedal, J.: *On the limited memory BFGS method for large scale optimization*, Math. Prog. 45, 503-528 (1989)

[9] Lukšan, L., Matonoha, C., Vlček, J.: *Algorithm 896: LSA - Algorithms for Large-Scale Optimization*, ACM Transactions on Mathematical Software 36, 16:1-16:29 (2009)

[10] Lukšan, L., Matonoha, C., Vlček, J.: *Sparse Test Problems for Unconstrained Optimization*, Report V-1064, Prague, ICS AS CR (2010)

[11] Lukšan, L., Matonoha, C., Vlček, J.: *Modified CUTE Problems for Sparse Unconstrained Optimization*, Report V-1081, Prague, ICS AS CR (2010)

[12] Lukšan, L., Spedicato, E.: *Variable metric methods for unconstrained optimization and nonlinear least squares*, J. Comput. Appl. Math. 124, 61-95 (2000)

[13] Lukšan, L., Vlček, J.: *Sparse and partially separable test problems for unconstrained and equality constrained optimization*, Report V-767, Prague, ICS AS CR (1998)

[14] Nocedal, J.: *Updating quasi-Newton matrices with limited storage*, Math. Comp. 35, 773-782 (1980)

[15] Nocedal, J., Wright, S.J.: Numerical optimization, Springer-Verlag, New York, 1999

[16] Schnabel, R.B.: *Quasi-Newton Methods Using Multiple Secant Equations*, Technical Report CU-CS-247-83, Department of Computer Science, University of Colorado at Boulder, USA (1983)

[17] Vlček, J., Lukšan, L.: *Shifted variable metric methods for large-scale unconstrained optimization*, J. Comput. Appl. Math. 186, 365-390 (2006)

[18] Vlček, J., Lukšan, L.: *A conjugate directions approach to improve the limited-memory BFGS method*, Report V-1120, Prague, ICS AS CR (2011)

[19] Vlček, J., Lukšan, L.: *A modified limited-memory BNS method for unconstrained minimization based on conjugate directions idea*, Optimization Methods & Software 30, 616-633 (2015)

[20] Vlček, J., Lukšan, L.: *Properties of the block BFGS update and its application to the limited-memory block BNS method for unconstrained minimization*, Numerical Algorithms 80, 957-987 (2019)

[21] Vlček, J., Lukšan, L.: *A limited-memory optimization method using the infinitely many times repeated BNS update and conjugate directions*, J. Comput. Appl. Math. 351, 14-28 (2019)

[22] Yuan, G., Sheng, Z., Wang, B., Hu, W., Li, Ch. *The global convergence of a modified BFGS method for nonconvex functions*, J. Comput. Appl. Math. 327, 274-294 (2018)