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A conjugate directions approach to improve the limited-memory BFGS method[1]

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Abstract:

Simple modifications of the limited-memory BFGS method (L-BFGS) for large scale unconstrained optimization are considered, which consist in corrections (derived from the idea of conjugate directions) of the used difference vectors, utilizing information from the preceding iteration. In case of quadratic objective functions, the improvement of convergence is the best one in some sense and all stored difference vectors are conjugate for unit stepsizes. Global convergence of algorithm is established for convex sufficiently smooth functions. Numerical experiments indicate that the new method often improves the L-BFGS method significantly.

Keywords:
Unconstrained minimization, variable metric methods, limited-memory methods, the BFGS update, conjugate directions, numerical results

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1 Introduction

In this report we propose some modifications of the L-BFGS method (see [6], [11]) 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.

Similarly as in the multi-step quasi-Newton methods (see e.g. [10]), we utilize information from the preceding iteration to correct the used difference vectors a change the quasi-Newton condition correspondingly. However, while the multi-step methods derive the corrections of the difference vectors from various interpolation methods, our approach is based on the idea of conjugate directions (see e.g. [4], [12]). Note that some of these thoughts are presented in our report [14] (in the second family of methods).

The L-BFGS method belongs to the variable metric (VM) or quasi-Newton line search methods, see [4], [9]. 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, usually chosen in such a way that

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

$k \geq 0$, where $0 < \varepsilon_1 < 1/2$, $\varepsilon_1 < \varepsilon_2 < 1$, $f_k = f(x_k)$, $g_k = \nabla f(x_k)$ and $d_k = -H_k g_k$ with a symmetric positive definite matrix H_k; usually H_0 is a multiple of I and H_{k+1} is obtained from H_k by a VM update to satisfy the quasi-Newton condition

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

(see [4], [9]), where $y_k = g_{k+1} - g_k$, $k \geq 0$. For $k \geq 0$ we denote

$$b_k = s_k^T y_k, \quad V_k = I - (1/b_k) s_k y_k^T, \quad B_k = H_k^{-1}$$

(note that $b_k > 0$ for $g_k \neq 0$ by (1.1)).

Among VM methods, the BFGS method belongs to the most efficient; the update formula can be written in the following quasi-product form, see [4], [9], [12],

$$H_{k+1} = (1/b_k) s_k s_k^T + V_k H_k V_k^T, \tag{1.3}$$

$k \geq 0$, on which the L-BFGS method – a limited-memory adaptation of the BFGS method – is based. An advantage of this form consists in the fact that instead of $N \times N$ matrix H_k, only the last $\tilde{m} + 1$ couples $\{s_j, y_j\}_{j=k-\tilde{m}}^k$ can be stored, where

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

and $m \geq 1$ is a given parameter. The direction vector is computed by the Strang recurrences, see [11], and still satisfies $d_{k+1} = -H_{k+1} g_{k+1}$, $k \geq 0$, but matrix H_{k+1} has only theoretical significance here and is not formed explicitly; it can be defined by $H_{k+1} = H_{k+1}^{k+1}$, where auxiliary matrices $\{H_i^{k+1}\}_{i=k-\tilde{m}}^{k+1}$ (also not formed explicitly) satisfy

$$H_{k-\tilde{m}}^{k+1} = (b_k/|y_k|^2) I, \tag{1.5}$$

$$H_{i+1}^{k+1} = (1/b_i) s_i s_i^T + V_i H_i^{k+1} V_i^T, \qquad k - \tilde{m} \leq i \leq k\,. \tag{1.6}$$

The concept of the conjugacy plays important role in optimization methods based on quadratic models, see e.g. [4], [12]. The conjugacy of consecutive direction vectors s_k, s_{k+1} with respect to matrix B_{k+1} can be easily achieved e.g. by means of suitable vector corrections. They can be understood as corrections for exact line searches, since relation $d_{k+1} = -H_{k+1} g_{k+1}$ implies

$$s_k^T B_{k+1} s_{k+1} = -t_{k+1}\, s_k^T g_{k+1}\,,$$

$k \ge 0$, therefore unit stepsizes in corrected methods for quadratic objective functions have similar position as exact line searches in classical methods, see Section 3.

However, not every correction for the conjugacy improves efficiency. E.g. addition a multiple of y_k to g_{k+1}, before the new direction vector is computed, seems to be advantageous, since in this way we can utilize properties of the line search procedure. Setting $\tilde{g}_{k+1} = g_{k+1} - (s_k^T g_{k+1}/b_k) y_k$ and $\tilde{d}_{k+1} = -H_{k+1}\tilde{g}_{k+1}$ for some $k \ge 0$, we get $s_k^T B_{k+1} \tilde{d}_{k+1} = -s_k^T \tilde{g}_{k+1} = 0$, but also

$$-\tilde{d}_{k+1} = H_{k+1} g_{k+1} - \frac{s_k^T g_{k+1}}{b_k} H_{k+1} y_k = \Big(H_{k+1} - \frac{s_k s_k^T}{b_k} \Big) g_{k+1}$$

by (1.2), i.e. by (1.3) this direction vector corresponds to singular VM matrix $V_k H_k V_k^T$, which is inconvenient for the line search and gives bad results.

In this report we will investigate such corrections of vectors s_k, y_k which provide conjugacy of consecutive direction vectors and show that update VM matrices constructed by means of corrected vectors have some positive properties and that this approach can improve results significantly. Thus we will define corrected quantities $\bar{s}_k$, $\bar{y}_k$ and consequently $\bar{b}_k$ and $\bar{V}_k$, $k \ge 0$, by $\bar{s}_0 = s_0$, $\bar{y}_0 = y_0$, $\bar{b}_0 = b_0$, $\bar{V}_0 = V_0$ and

$$\bar{s}_k = s_k - \alpha_k \bar{s}_{k-1}, \quad \bar{y}_k = y_k - \beta_k \bar{y}_{k-1}, \quad \bar{b}_k = \bar{s}_k^T \bar{y}_k, \quad \bar{V}_k = I - (1/\bar{b}_k) \bar{s}_k \bar{y}_k^T, \tag{1.7}$$

$k > 0$, with such α_k, $\beta_k \in \mathcal{R}$ that $\bar{b}_k > 0$. Correspondingly, we will use direction vector $d_k = -\bar{H}_k g_k$, $k \ge 0$, instead of $-H_k g_k$, where $\bar{H}_0 = I$ and matrix $\bar{H}_{k+1} = \bar{H}_{k+1}^{k+1}$ is obtained by

$$\bar{H}_{k-\tilde{m}}^{k+1} = (b_k/|y_k|^2) I, \tag{1.8}$$

$$\bar{H}_{i+1}^{k+1} = (1/\bar{b}_i) \bar{s}_i \bar{s}_i^T + \bar{V}_i \bar{H}_i^{k+1} \bar{V}_i^T, \qquad k - \tilde{m} \le i \le k\,. \tag{1.9}$$

Note that matrix $\bar{H}_{k+1}$ satisfies the quasi-Newton condition $\bar{H}_{k+1}\bar{y}_k = \bar{s}_k$ and is obtained by the last BFGS update (1.9) of matrix $\bar{H}_k^{k+1}$, which satisfies $\bar{H}_k^{k+1}\bar{y}_{k-1} = \bar{s}_{k-1}$, $k \ge 1$, for $m > 1$, as we can see from (1.9) with $i = k-1$.

We will use the following notation

$$\bar{a}_i^{k+1} = \bar{y}_i^T \bar{H}_i^{k+1} \bar{y}_i, \quad \bar{c}_i^{k+1} = \bar{s}_i^T \bar{B}_i^{k+1} \bar{s}_i, \quad \bar{B}_i^{k+1} = (\bar{H}_i^{k+1})^{-1}, \quad \bar{B}_k = \bar{H}_k^{-1}, \tag{1.10}$$

$k \ge 0$, $i = k - \tilde{m}, \dots, k+1$; note that always $\bar{a}_i^{k+1} \bar{c}_i^{k+1} \ge \bar{b}_i^2$ by the the Schwarz inequality.

To analyse the particular BFGS updates (1.9) in the simplified form, we omit index i, replace index $i+1$ by symbol $+$, index $i-1$ by symbol $-$ and write $\bar{H}$, $\bar{H}_+$, $\bar{H}_-$, $\bar{a}$, $\bar{c}$ instead of $\bar{H}_i^{k+1}$, $\bar{H}_{i+1}^{k+1}$, $\bar{H}_{i-1}^{k+1}$, $\bar{a}_i^{k+1}$, $\bar{c}_i^{k+1}$.

In Section 2 we investigate the standard BFGS update (1.9) (in the simplified form)

$$\bar{H}_+ = (1/\bar{b})\bar{s}\bar{s}^T + \bar{V}\bar{H}\bar{V}^T \tag{1.11}$$

of any symmetric positive definite matrix $\bar{H}$ with corrected difference vectors from the point of view of conjugacy and discuss the choice of parameters. In Section 3 we present some interesting properties of the corrected BFGS update (1.11) and the corrected L-BFGS method for quadratic functions. Application to limited-memory methods and the corresponding algorithm are described in Section 4, and global convergence of the algorithm is established in Section 5. Numerical results are reported in Section 6.

2 The BFGS update with corrected vectors

In this section we will investigate influence of correction parameters α, β on properties of update (1.11). Using another formulation of conjugacy property, we will derive a formula for parameter α. As regards parameter β, we will discuss two basic variants of its choice and their advantages. First we reformulate conjugacy property in another form.

The following lemma shows that, under some assumptions, the conjugacy of difference vectors $\bar{s}$, $\bar{s}_-$ with respect to matrices $\bar{B}$, $\bar{B}_+$ is equivalent to the property of $\bar{H}_+$ that it satisfies not only the quasi-Newton condition $\bar{H}_+\bar{y} = \bar{s}$, but also $\bar{H}_+\bar{B}\bar{s}_- = \bar{s}_-$.

Lemma 2.1. *Let $\bar{H}$ be any symmetric positive definite matrix. If vectors $\bar{s}$, $\bar{H}\bar{y}$ are linearly independent then matrix $\bar{H}_+$ given by update (1.11) of $\bar{H}$ with $\bar{b} > 0$ satisfies $\bar{H}_+\bar{B}\bar{s}_- = \bar{s}_-$ if and only if vectors $\bar{s}$, $\bar{s}_-$ are conjugate to matrices $\bar{B}$, $\bar{B}_+$.*

Proof. Let $\bar{H}_+\bar{B}\bar{s}_- = \bar{s}_-$. By $\bar{V}^T\bar{B}\bar{s}_- = \bar{B}\bar{s}_- - (\bar{s}^T\bar{B}\bar{s}_-/\bar{b})\,\bar{y}$, from (1.11) we obtain

$$\begin{aligned}\bar{H}_+\bar{B}\bar{s}_- &= (\bar{s}^T\bar{B}\bar{s}_-/\bar{b})\,\bar{s} + \left(I - (1/\bar{b})\bar{s}\bar{y}^T\right)\left(\bar{s}_- - (\bar{s}^T\bar{B}\bar{s}_-/\bar{b})\,\bar{H}\bar{y}\right)\\ &= \bar{s}_- + \left[\frac{\bar{s}^T\bar{B}\bar{s}_- - \bar{s}_-^T\bar{y}}{\bar{b}} + \frac{\bar{a}}{\bar{b}^2}\bar{s}^T\bar{B}\bar{s}_-\right]\bar{s} - \left[\frac{\bar{s}^T\bar{B}\bar{s}_-}{\bar{b}}\right]\bar{H}\bar{y}.\end{aligned}$$

To have $\bar{H}_+\bar{B}\bar{s}_- = \bar{s}_-$, both expressions in brackets must be equal to zero in view of linear independency of $\bar{s}$, $\bar{H}\bar{y}$, i.e. $\bar{s}^T\bar{B}\bar{s}_- = \bar{s}_-^T\bar{y} = 0$; since $\bar{H}_+\bar{y} = \bar{s}$ by (1.11), this is equivalent to $\bar{s}^T\bar{B}\bar{s}_- = \bar{s}^T\bar{B}_+\bar{s}_- = 0$.

On the contrary, if $\bar{s}^T\bar{B}\bar{s}_- = \bar{s}_-^T\bar{y} = 0$ then (1.11) implies $\bar{H}_+\bar{B}\bar{s}_- = \bar{V}\bar{s}_- = \bar{s}_-$. □

We focus here on the case when the quasi-Newton condition $\bar{H}\bar{y}_- = \bar{s}_-$ is satisfied and thus we can replace condition $\bar{H}_+\bar{B}\bar{s}_- = \bar{s}_-$ in Lemma 2.1 by $\bar{H}_+\bar{y}_- = \bar{s}_-$ and write $\bar{s}^T\bar{y}_-$ instead of $\bar{s}^T\bar{B}\bar{s}_-$. Note that in case of the limited-memory methods which define matrix $\bar{H}_+$ by relations (1.8), (1.9), parameters α, β are determined during the last update. Then, considering the form (1.11), condition $\bar{H}\bar{y}_- = \bar{s}_-$ represents the quasi-Newton condition from the preceding update, which is satisfied for $m > 1$, see Section 1.

Formulation of conjugacy as in Lemma 2.1 enables us to distinguish roles of products $\bar{s}^T\bar{y}_-$, $\bar{s}_-^T\bar{y}$ (and consequently, parameters α, β).

Lemma 2.2. *Let $\bar{H}$ be any symmetric positive definite matrix with $\bar{H}\bar{y}_- = \bar{s}_-$, $\bar{H}_+$ be given by update (1.11) of $\bar{H}$ with $\bar{b} > 0$ and $\Delta_1 = (\bar{H}_+\bar{y}_- - \bar{s}_-)^T\bar{B}_+(\bar{H}_+\bar{y}_- - \bar{s}_-)$. Then*

$$\Delta_1 = \left[(\bar{s}_-^T\bar{y} - \bar{s}^T\bar{y}_-)^2 + (\bar{s}^T\bar{y}_-)^2(\bar{a}/\bar{b} - \bar{b}/\bar{c})\right]/\bar{b}\,, \tag{2.1}$$

where $\bar a/\bar b \ge \bar b/\bar c$, *with* $\bar a/\bar b = \bar b/\bar c$ *only in case of dependency of vectors* $\bar s$, $\bar H \bar y$.

Proof. Since relation (1.11) is the standard BFGS update with $\bar s$, $\bar y$ instead of s, y, it holds (see [4], [9])

$$\bar H_+ = \bar H + \Big(1 + \frac{\bar a}{\bar b}\Big)\frac{\bar s \bar s^T}{\bar b} - \frac{\bar H \bar y \bar s^T + \bar s \bar y^T \bar H}{\bar b}, \qquad \bar B_+ = \bar B + \frac{\bar y \bar y^T}{\bar b} - \frac{\bar B \bar s \bar s^T \bar B}{\bar c}, \tag{2.2}$$

which yields

$$\bar y_-^T \bar H_+ \bar y_- = \bar s_-^T \bar y_- + \big(1 + \bar a/\bar b\big)\,(\bar s^T \bar y_-)^2/\bar b - 2\bar s^T \bar y_-\, \bar s_-^T \bar y/\bar b\,, \tag{2.3}$$

$$\bar s_-^T \bar B_+ \bar s_- = \bar s_-^T \bar y_- + (\bar s_-^T \bar y)^2/\bar b - (\bar s^T \bar y_-)^2/\bar c\,. \tag{2.4}$$

Setting it to $\Delta_1 = \bar y_-^T \bar H_+ \bar y_- + \bar s_-^T \bar B_+ \bar s_- - 2\bar s_-^T \bar y_-$, we obtain (2.1). The rest follows from the Schwarz inequality. □

If function f is close to a quadratic function (e.g. in the proximity to minimum) then value $\bar s_-^T \bar y - \bar s^T \bar y_-$ is obviously close to zero, but value $\bar a/\bar b - \bar b/\bar c \ge 0$ need not be small. Therefore we can see from relation (2.1) that mainly value $\bar s^T \bar y_-$ should be close to zero, to have Δ_1 small. In view of this, the choice $\alpha = s^T \bar y_-/\bar b_-$, for which $\bar s^T \bar y_- = 0$, appears to be very suitable (which is in accordance with our numerical experiments) and is considered in the rest of this section, while the choice of β is not so straightforward.

By Lemma 2.2, the natural basic choice of parameter β is $\beta = \bar s_-^T y/\bar b_-$, which yields $\bar s_-^T \bar y = 0$ and thus $\bar H_+ \bar y_- = \bar s_-$ by $\Delta_1 = 0$. This value has additional interesting properties.

Theorem 2.1. *Let* $\bar H$ *be any symmetric positive definite matrix with* $\bar H \bar y_- = \bar s_-$ *and* $\bar H_+$ *be given by update (1.11) of* $\bar H$ *with* $\bar b > 0$. *If* $\alpha = s^T \bar y_-/\bar b_-$ *then* $\bar s^T \bar y_- = 0$, $\bar b = b - \alpha\, \bar s_-^T y$ *and both value* $\bar a$ *and the condition number of matrix* $\bar H^{1/2} \bar B_+ \bar H^{1/2}$ *as functions of* β *are minimized by the choice* $\beta = \bar s_-^T y/\bar b_-$.

Proof. If $\alpha = s^T \bar y_-/\bar b_-$ then obviously $\bar s^T \bar y_- = 0$, which yields $\bar b = \bar s^T y = b - \alpha \bar s_-^T y$.

Value $\bar a = y^T \bar H y - 2\beta \bar s_-^T y + \beta^2 \bar b_-$ is obviously minimized by $\beta = \bar s_-^T y/\bar b_-$. Denoting $A = \bar H^{1/2} \bar B_+ \bar H^{1/2}$, from (2.2) we get

$$A = I + (1/\bar b) \bar H^{1/2} \bar y \bar y^T \bar H^{1/2} - (1/\bar c) \bar B^{1/2} \bar s \bar s^T \bar B^{1/2}\,.$$

Since $\mathrm{Tr}(A) = N - 1 + \bar a/\bar b$ and $\det(A) = \bar b/\bar c$ by identity $\det(I + uu^T - vv^T) = (1 + |u|^2)(1 - |v|^2) + (u^T v)^2$, $u \in \mathcal{R}^N$, $v \in \mathcal{R}^N$, two nonunit eigenvalues $\lambda_1 \ge \lambda_2$ of A are roots of the quadratic equation $0 = \lambda^2 - (1 + \bar a/\bar b)\lambda + \bar b/\bar c \overset{\Delta}{=} \psi(\lambda)$. From $\psi(1) = \bar b/\bar c - \bar a/\bar b \le 0$ (see Lemma 2.2) and $\bar b/\bar c > 0$ we can deduce that $\lambda_1 \ge 1 \ge \lambda_2 > 0$. Values $\bar b$, $\bar c$ are independent of β and thus the condition number of A

$$\lambda_1/\lambda_2 = \lambda_1^2/(\lambda_1 \lambda_2) = \left[1 + \bar a/\bar b + \sqrt{(1 + \bar a/\bar b)^2 - 4\bar b/\bar c}\,\right]^2 \bar c/(4\bar b)$$

is minimized together with $\bar a$ by $\beta = \bar s_-^T y/\bar b_-$. □

Satisfaction of condition $\bar H_+ \bar y_- = \bar s_-$ (implied by the choice $\beta = \bar s_-^T y/\bar b_-$) also guarantees that matrix $\bar H_+$ is closer to $\bar H$ than to $\bar H_-$ in some sense, as we can see from the following theorem with $\bar H_-$, $\bar H$, $\bar s_-$, $\bar y_-$ instead of $\bar H$, $\bar H_+$, $\bar s$, $\bar y$ and $\tilde G = \bar H_+^{-1}$ ($\|.\|_F$ denotes the Frobenius matrix norm). Note that similar formulas with inverse VM matrices B_{k+1}, B_k can be found in [13] for the BFGS update or in [5] for more general updates.

Theorem 2.2. *Let $\bar{H}$ be any symmetric positive definite matrix, matrix $\bar{H}_+$ be given by update (1.11) of $\bar{H}$ with $\bar{b} > 0$, $\tilde{G}$ be any symmetric positive definite matrix satisfying $\tilde{G}\bar{s} = \bar{y}$, $W_+ = \tilde{G}^{1/2}\bar{H}_+\tilde{G}^{1/2}$ and $W = \tilde{G}^{1/2}\bar{H}\tilde{G}^{1/2}$. Then*

$$\|I - W_+\|_F^2 - \|I - W\|_F^2 = -\|W_+ - W\|_F^2 \le -\left(\bar{a}/\bar{b} - 1\right)^2 . \tag{2.5}$$

Proof. Denoting $w = \tilde{G}^{1/2}\bar{s} = \tilde{G}^{-1/2}\bar{y}$ and $M = W - I$, we can rewrite update (1.11)

$$W_+ = (1/|w|^2)ww^T + PWP = I + PMP, \quad P = I - (1/|w|^2)ww^T, \tag{2.6}$$

by $|w|^2 = \bar{b}$ and $P^2 = P$. Using $\|I - W_+\|_F^2 = \|PMP\|_F^2 = \text{Tr}(PMPM)$, we get firstly

$$\|I - W_+\|_F^2 - \|M\|_F^2 = 2\text{Tr}(PMPM) - \|PMP\|_F^2 - \|M\|_F^2 = -\|PMP - M\|_F^2 , \tag{2.7}$$

which is equality in (2.5) by $W_+ - W = W_+ - I - (W - I) = PMP - M$, and secondly

$$\begin{aligned} \|PMP - M\|_F^2 &= \|M\|_F^2 - \text{Tr}(PMPM) = \|M\|_F^2 - \text{Tr}\Big(\big[M - (1/|w|^2)ww^TM\big]^2\Big) \\ &= \text{Tr}\Big(ww^TM^2 + Mww^TM - \big[w^TMw/|w|^2\big]\, ww^TM\Big)/|w|^2 \\ &= 2|Mw|^2/|w|^2 - (w^TMw)^2/|w|^4 \ \ge\ (w^TMw)^2/|w|^4 \end{aligned}$$

by the Schwarz inequality. Since $|w|^2 = \bar{b}$ and $w^TMw = \bar{a} - \bar{b}$, we obtain (2.5). □

Although the choice $\beta = \bar{s}_-^T y/\bar{b}_-$ gives good results, it cannot be recommended generally. The following lemma indicates that β should also be near to α, if we want to have $|\bar{H}_+ y - s|$ small. Therefore value β between $\bar{s}_-^T y/\bar{b}_-$, $s^T\bar{y}_-/\bar{b}_-$ can be more suitable.

Lemma 2.3. *Let $\bar{H}$ be any symmetric positive definite matrix with $\bar{H}\bar{y}_- = \bar{s}_-$ and matrix $\bar{H}_+$ be given by update (1.11) of $\bar{H}$ with $\bar{b} > 0$. If $\alpha = s^T\bar{y}_-/\bar{b}_-$ then $\Delta_1 = (\bar{s}_-^T\bar{y})^2/\bar{b}$ and*

$$\Delta_2 \triangleq (\bar{H}_+ y - s)^T\bar{B}_+(\bar{H}_+ y - s) = \alpha^2\Delta_1 + (\alpha - \beta)^2\bar{b}_- . \tag{2.8}$$

Proof. From (2.1) we get $\Delta_1 = (\bar{s}_-^T\bar{y})^2/\bar{b}$ and (2.3) - (2.4) imply $\bar{y}_-^T\bar{H}_+\bar{y}_- = \bar{b}_-$ and $\bar{s}_-^T\bar{B}_+\bar{s}_- = \bar{b}_- + \Delta_1$. By $\bar{H}_+\bar{y} = \bar{s}$ we obtain

$$\bar{H}_+ y - s = \bar{H}_+\bar{y} + \beta\bar{H}_+\bar{y}_- - s = \beta\bar{H}_+\bar{y}_- - \alpha\bar{s}_-, \tag{2.9}$$

which yields

$$\Delta_2 = (\beta\bar{H}_+\bar{y}_- - \alpha\bar{s}_-)^T(\beta\bar{y}_- - \alpha\bar{B}_+\bar{s}_-) = \beta^2\bar{y}_-^T\bar{H}_+\bar{y}_- + \alpha^2\bar{s}_-^T\bar{B}_+\bar{s}_- - 2\alpha\beta\bar{b}_- ,$$

i.e. (2.8). □

To find a convenient value of parameter β, we can take account of our numerical experience that the initial scaling parameter $b/|y|^2$ in (1.5) (with b, y without bars) appears to be suitable also for the new methods. In classical case, choice $\gamma = b/|y|^2$ for the BFGS update can be motivated by an idea to minimize $|(H_+ - \gamma I)y|$, see [9]. Similarly, minimizing $|(\bar{H}_+ - \bar{\gamma}I)y|$ here, we get $\bar{\gamma} = y^T\bar{H}_+ y/|y|^2$. Therefore it can be advantageous to choose the value β, which satisfies $y^T\bar{H}_+ y = b$, i.e. $\bar{\gamma} = b/|y|^2$.

Lemma 2.4. *Let $\bar{H}$ be any symmetric positive definite matrix with $\bar{H}\bar{y}_- = \bar{s}_-$ and matrix $\bar{H}_+$ be given by update (1.11) of $\bar{H}$. If $\alpha = s^T\bar{y}_-/\bar{b}_-$, $\beta^2 = s^T\bar{y}_-\,\bar{s}_-^Ty/\bar{b}_-^2$ and $\bar{b} > 0$ then $y^T\bar{H}_+y = b$.*

Proof. From $\alpha = s^T\bar{y}_-/\bar{b}_-$ we get $\bar{s}^T\bar{y}_- = 0$, which implies $\bar{s}^Ty = \bar{s}^T\bar{y} = \bar{b}$. Using (2.2) and $\bar{H}\bar{y}_- = \bar{s}_-$, we obtain $\bar{H}_+\bar{y}_- = \bar{s}_- - (\bar{s}_-^T\bar{y}/\bar{b})\bar{s}$, which yields $y^T\bar{H}_+\bar{y}_- = \bar{s}_-^Ty - \bar{s}_-^T\bar{y} = \beta\bar{b}_-$. In view of (2.9) and $\beta^2\bar{b}_- = \alpha\,\bar{s}_-^Ty$, we obtain

$$y^T\bar{H}_+y - b = y^T(\bar{H}_+\bar{y} - s) = y^T(\beta\bar{H}_+\bar{y}_- - \alpha\bar{s}_-) = \beta^2\bar{b}_- - \alpha\,\bar{s}_-^Ty = 0.$$

□

3 Results for quadratic functions

In this section we suppose that f is a quadratic function with a symmetric positive definite matrix G and that $\beta = \alpha$, which is a natural choice, if we want to have $\bar{y} = G\bar{s}$. Here we consider only G-conjugacy of vectors. Since $\bar{s}^TG\bar{s}_- = \bar{s}^T\bar{y}_- = s^T\bar{y}_- - \alpha\bar{b}_-$ by (1.7), the conjugacy of $\bar{s}$, $\bar{s}_-$ can be achieved by the choice $\alpha = s^T\bar{y}_-/\bar{b}_- = \bar{s}_-^Ty/\bar{b}_-$.

The following theorem shows that for this choice the standard quasi-Newton condition $\bar{H}_+y = s$ is satisfied, value $\bar{b}$ is minimized and improvement of convergence is the best in some sense and that $\bar{b} > 0$ always holds for linearly independent direction vectors ($\|.\|_F$ denotes the Frobenius matrix norm). Note that the quasi-Newton condition $\bar{H}\bar{y}_- = \bar{s}_-$ is discussed in Section 2.

Theorem 3.1. *Let $\hat{\alpha} = s^T\bar{y}_-/\bar{b}_- = \bar{s}_-^Ty/\bar{b}_-$, $\bar{H}$ be any symmetric positive definite matrix with $\bar{H}\bar{y}_- = \bar{s}_-$ and let f be quadratic function $f(x) = \frac{1}{2}(x-x^*)^TG(x-x^*)$, $x^* \in \mathcal{R}^N$, with a symmetric positive definite matrix G. If vectors s, $\bar{s}_-$ are linearly independent, then $\bar{b} > 0$ and choice $\alpha = \hat{\alpha}$ implies $\bar{H}_+y = s$ and minimizes values $\bar{b}$, $\|G^{1/2}\bar{H}_+G^{1/2} - I\|_F$ as functions of α, where matrix $\bar{H}_+$ is given by update (1.11) of $\bar{H}$ with $\beta = \alpha$.*

Proof. Denoting $r = G^{1/2}s = G^{-1/2}y$, $\bar{r}_- = G^{1/2}\bar{s}_- = G^{-1/2}\bar{y}_-$, $\bar{r} = r - \alpha\bar{r}_-$, $R = G^{1/2}\bar{H}G^{1/2}$, $R_+ = G^{1/2}\bar{H}_+G^{1/2}$ and $E = R - I$, we can rewrite update (1.11) in the form

$$R_+ = (1/|\bar{r}|^2)\bar{r}\bar{r}^T + \bar{P}R\bar{P} = I + \bar{P}E\bar{P}, \qquad \bar{P} = I - (1/|\bar{r}|^2)\bar{r}\bar{r}^T. \tag{3.1}$$

by $|\bar{r}|^2 = \bar{b}$ and $\bar{P}^2 = \bar{P}$. As a special case, denoting by $\hat{H}_+$ matrix $\bar{H}_+$ for $\alpha = \hat{\alpha}$ and $\hat{r} = r - \hat{\alpha}\bar{r}_-$, $\hat{R}_+ = G^{1/2}\hat{H}_+G^{1/2}$, we can rewrite update (1.11) in the form

$$\hat{R}_+ = I + \hat{P}E\hat{P}, \qquad \hat{P} = I - (1/|\hat{r}|^2)\hat{r}\hat{r}^T. \tag{3.2}$$

First we see that value $\bar{b} = |\bar{r}|^2 = |r|^2 - 2\alpha r^T\bar{r}_- + \alpha^2|\bar{r}_-|^2$ is minimized by $\alpha = r^T\bar{r}_-/|\bar{r}_-|^2 = \hat{\alpha}$ and that the minimal value is $|r|^2 - (r^T\bar{r}_-)^2/|\bar{r}_-|^2 > 0$ by the Schwarz inequality and linear independency of r, $\bar{r}_-$. Thus we can use Lemma 2.3 with $\beta = \alpha$, which gives $\bar{H}_+y = s$ for $\alpha = \hat{\alpha}$ by $\bar{s}_-^T\bar{y} = \bar{s}_-^Ty - \alpha\bar{b}_- = 0$.

Further, we have $\hat{r}^T\bar{r}_- = r^T\bar{r}_- - \hat{\alpha}|\bar{r}_-|^2 = 0$, which implies $\hat{r}^T\hat{r} = \hat{r}^T\bar{r}$. Therefore

$$\bar{P}\hat{P} = \Big(I - \frac{\bar{r}\bar{r}^T}{|\bar{r}|^2}\Big)\hat{P} = \hat{P} - \frac{\bar{r}}{|\bar{r}|^2}\Big(\bar{r}^T - \frac{\bar{r}^T\hat{r}}{|\hat{r}|^2}\hat{r}^T\Big) = \hat{P} - (\hat{\alpha} - \alpha)\frac{\bar{r}\bar{r}_-^T}{|\bar{r}|^2}\,.$$

Assumption $\bar{H}\bar{y}_- = \bar{s}_-$ can be rewritten in the form $E\bar{r}_- = 0$, which yields $\bar{P}\hat{P}E = \hat{P}E$, thus $\bar{P}\hat{P}E\hat{P}\bar{P} = \hat{P}E\hat{P}$. Using this together with (3.1), (3.2) and $\hat{P}^2 = \hat{P}$, we obtain

$$\mathrm{Tr}\Big[(\hat{R}_+ - R_+)(\hat{R}_+ - I)\Big] = \mathrm{Tr}\Big[(\hat{P}E\hat{P} - \bar{P}E\bar{P})\hat{P}E\hat{P}\Big] = \mathrm{Tr}(E\hat{P}E\hat{P} - E\bar{P}\hat{P}E\hat{P}\bar{P}) = 0,$$

which immediately gives

$$\|R_+ - \hat{R}_+\|_F^2 + \|\hat{R}_+ - I\|_F^2 = \|R_+ - I\|_F^2.$$

Since $R_+ = \hat{R}_+$ holds for $\alpha = \hat{\alpha}$, value $\|R_+ - I\|_F$ is minimized by $\alpha = \hat{\alpha}$. □

It is well known (see e.g. [11]) that the L-BFGS method with exact line searches generates conjugate directions vectors and preserves $\tilde{m}$ (see (1.4)) previous quasi-Newton conditions. Similar properties also hold for update (1.11) with (the most frequent) unit stepsizes. If every stepsize is unit, then all direction vectors are conjugate. Moreover, only one unit stepsize is sufficient to ensure that for some VM matrix up to $\tilde{m}$ previous quasi-Newton conditions are preserved.

Theorem 3.2. *Let $x_0 \in \mathcal{R}^N$, $x^* \in \mathcal{R}^N$, $\bar{k} > 0$, $m \geq 1$, f be quadratic function $f(x) = \frac{1}{2}(x - x^*)^T G(x - x^*)$ with a symmetric positive definite matrix G, and let for $0 \leq k \leq \bar{k}$ iterations $x_{k+1} = x_k + s_k$ be generated by the method $s_k = -t_k \bar{H}_k g_k$, $g_k = \nabla f(x_k)$, $t_k > 0$, with matrices $\bar{H}_k$ defined in the following way: $\bar{H}_0 = I$ and matrices $\bar{H}_{k+1}$ are given by*

$$\begin{aligned} \bar{H}_{k+1} \;=\; & (s_k^T y_k/|y_k|^2)\, \bar{V}_k \cdots \bar{V}_{k-\tilde{m}}\, \bar{V}_{k-\tilde{m}}^T \cdots \bar{V}_k^T \\ & +\; (1/\bar{b}_{k-\tilde{m}})\, \bar{V}_k \cdots \bar{V}_{k-\tilde{m}+1}\, \bar{s}_{k-\tilde{m}} \bar{s}_{k-\tilde{m}}^T\, \bar{V}_{k-\tilde{m}+1}^T \cdots \bar{V}_k^T \\ & +\; \cdots \;+\; (1/\bar{b}_{k-1})\, \bar{V}_k\, \bar{s}_{k-1} \bar{s}_{k-1}^T\, \bar{V}_k^T \;+\; (1/\bar{b}_k)\, \bar{s}_k \bar{s}_k^T\,, \end{aligned} \tag{3.3}$$

$0 \leq k < \bar{k}$, where $\tilde{m} = \min(k, m-1)$, $y_k = g_{k+1} - g_k$, and quantities $\bar{s}_j$, $\bar{y}_j$, $\bar{V}_j$ and $\bar{b}_j$, $j \geq 0$, are formally defined by $\bar{s}_0 = s_0$, $\bar{y}_0 = y_0$, $\bar{s}_{j+1} = s_{j+1} - \alpha_{j+1}\bar{s}_j$, $\bar{y}_{j+1} = y_{j+1} - \alpha_{j+1}\bar{y}_j$, $\alpha_{j+1} = s_{j+1}^T \bar{y}_j / \bar{b}_j$, $\bar{V}_j = I - (1/\bar{b}_j)\bar{s}_j \bar{y}_j^T$, $\bar{b}_j = \bar{s}_j^T \bar{y}_j$. Suppose that every generated vector s_k is linearly independent of $\bar{s}_{k-1}$, $0 < k \leq \bar{k}$. Then the method is well defined.

Moreover, if $t_{k+1} = 1$ for some k, $0 \leq k < \bar{k}$, it holds

$$(a)\ \bar{H}_{k+i}\bar{y}_k = \bar{s}_k, \quad (b)\ \bar{s}_k^T G \bar{s}_{k+i} = 0, \quad (c)\ \bar{s}_k^T g_{k+i+1} = 0, \quad 1 \leq i \leq \min(\tilde{m}+1, \bar{k}-k). \tag{3.4}$$

Proof. First, independence of s_k, $\bar{s}_{k-1}$ implies $\bar{b}_k > 0$ by Theorem 3.1 for $k = 1, \ldots, \bar{k}$. Together with $\bar{b}_0 = b_0 > 0$ this yields that the method is well defined.

Let $t_{k+1} = 1$. For $i = 1$, (a) follows immediately from (3.3) by $\bar{V}_k^T \bar{y}_k = 0$, (b) from $\bar{s}_k^T G \bar{s}_{k+1} = \bar{s}_{k+1}^T \bar{y}_k = [s_{k+1} - (s_{k+1}^T \bar{y}_k / \bar{b}_k)\bar{s}_k]^T \bar{y}_k = 0$ and (c) from $\bar{s}_k^T g_{k+2} = \bar{s}_k^T y_{k+1} + \bar{s}_k^T g_{k+1} = \bar{y}_k^T s_{k+1} + \bar{y}_k^T \bar{H}_{k+1} g_{k+1} = \bar{y}_k^T (s_{k+1} + \bar{H}_{k+1} g_{k+1}) = 0$ by (a) and $t_{k+1} = 1$.

By induction, let $i < \min(\tilde{m}+1, \bar{k}-k)$ be fixed and let relations (3.4) with i replaced by j hold for $j = 1, \ldots, i$.

(α) Relation (b) can be written

$$\bar{y}_k^T \bar{s}_{k+j} = 0, \quad 1 \leq j \leq i, \tag{3.5}$$

Since $i \leq \tilde{m}$, matrix $\bar{V}_k$ is always identical with one of the matrices $\bar{V}_{k+i}, \ldots, \bar{V}_{k+i-\tilde{m}}$. Using (3.3) with $k = k+i$, by $\bar{V}_k^T \bar{y}_k = 0$ and (3.5) together with its consequence $\bar{V}_{k+j}^T \bar{y}_k = \bar{y}_k$, $1 \leq j \leq i$, we obtain $\bar{H}_{k+i+1}\bar{y}_k = \bar{s}_k$, i.e. (a) also holds for $i + 1$.

(β) From (c) and (α) we obtain $0 = \bar{s}_k^T g_{k+i+1} = \bar{y}_k^T \bar{H}_{k+i+1} g_{k+i+1} = -(1/t_{k+i+1})\, \bar{y}_k^T s_{k+i+1}$, therefore $\bar{y}_k^T \bar{s}_{k+i+1} = \bar{y}_k^T s_{k+i+1} - \alpha_{k+i+1}\, \bar{y}_k^T \bar{s}_{k+i} = 0$ by (b), i.e. (b) also holds for $i+1$.

(γ) Using (c), we get $\bar{s}_k^T g_{k+i+2} = \bar{s}_k^T y_{k+i+1} + \bar{s}_k^T g_{k+i+1} = \bar{s}_k^T \bar{y}_{k+i+1} + \alpha_{k+i+1}\, \bar{s}_k^T \bar{y}_{k+i} = 0$ by (β), i.e. (c) also holds for $i+1$. □

4 Application to limited-memory methods

In this section we use results from the previous sections to implement a method based on the quasi-product form (1.9) of update. We suppose here that $\alpha = s^T \bar{y}_- / \bar{b}_-$, see Section 2.

From theory in Section 3 we can deduce that we should use the corrected difference vectors whenever objective function is close to a quadratic function, which is confirmed by our numerical experiments. As measure of deviation from a quadratic function in points x_{k-1}, x_k, x_{k+1} can serve e.g. value $|s_k^T \bar{y}_{k-1} - \bar{s}_{k-1}^T y_k|$ (zero for quadratic functions), $k > 0$. We correct, only if it is smaller than $\bar{b}_{k-1}^2 / b_k$ and if numbers $s_k^T \bar{y}_{k-1}$, $\bar{s}_{k-1}^T y_k$ have the same sign. We tested several choices of the bound and from among them, value $\bar{b}_{k-1}^2 / b_k$ led to the most robust method.

Besides, we should not correct, if value $\bar{b}_k$ would be too small with respect to b_k or $\bar{b}_k \le 0$, i.e. if $\bar{b}_k \le \delta_1 b_k$, $0 < \delta_1 < 1$. Since

$$\bar{b}_k = b_k - \alpha_k\, \bar{s}_{k-1}^T y_k = b_k - \theta_k, \qquad \theta_k = s_k^T \bar{y}_{k-1} \bar{s}_{k-1}^T y_k / \bar{b}_{k-1}, \tag{4.1}$$

by Theorem 2.1, condition $\bar{b}_k > \delta_1 b_k$ can be written as $\theta_k < (1-\delta_1) b_k$.

Value $\beta_k = \operatorname{sgn}(\alpha_k)\sqrt{\theta_k / \bar{b}_{k-1}}$, corresponding to the choice in Lemma 2.4, appears to be suitable if value $\bar{b}_k$ is sufficiently great with respect to b_k; we use condition $\bar{b}_k > \delta_2 b_k$, $\delta_1 \le \delta_2 < 1$, i.e. $\theta_k < (1-\delta_2) b_k$ by (4.1). Since condition $\theta_k < (1-\delta_1) b_k$ implies $\theta_k < b_k$, this choice of β_k satisfies $|\beta_k| < \sqrt{b_k / \bar{b}_{k-1}}$; it is a reason why we use this value β_k also in case that $|\bar{s}_{k-1}^T y_k / \bar{b}_{k-1}| > 2\sqrt{b_k / \bar{b}_{k-1}}$ to prove global convergence (see Section 5). By our experience, this alteration has only negligible influence to numerical results.

Global convergence can be easily established (in a similar way as for the L-BFGS method, see [6]), if $|\bar{s}_k| / |s_k| < \Delta$ and $|\bar{y}_k| / |y_k| < \Delta$, $k > 0$, where $\Delta > 1$ is a given constant. If this condition is not satisfied, it suffices to replace the oldest saved vectors $\bar{s}_{k-\tilde{m}}$, $\bar{y}_{k-\tilde{m}}$ e.g. by s_k, y_k, see Section 5, where $\tilde{m}$ is defined by (1.4). It is interesting that the more natural replacement by $s_{k-\tilde{m}}$, $y_{k-\tilde{m}}$ does not give better results (and is more complicated in practice). Note that in our numerical experiments with $N = 1000$, value $|\bar{y}_k| / |y_k|$ was rarely greater than 10 and value $|\bar{s}_k| / |s_k|$ greater than 50.

We now state the method in details. Instead of matrices $\bar{H}_k$, $\tilde{m}{+}1$ couples $\{\bar{s}_j, \bar{y}_j\}_{j=k-\tilde{m}}^k$, $k \ge 0$, are stored to compute the direction vector $d_{k+1} = -\bar{H}_{k+1} g_{k+1}$, see Section 1. For simplicity, we omit stopping criteria.

Algorithm 4.1

Data: The number $m \ge 1$ of VM updates per iteration, line search parameters ε_1, ε_2, $0 < \varepsilon_1 < 1/2$, $\varepsilon_1 < \varepsilon_2 < 1$, and correction parameters δ_1, δ_2, Δ, $0 < \delta_1 \le \delta_2 < 1 < \Delta$.

Step 0: Initiation. Choose starting point $x_0 \in \mathcal{R}^N$, define starting matrix $\bar{H}_0^0 = I$ 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), $g_{k+1} = \nabla f(x_{k+1})$, $y_k = g_{k+1} - g_k$ and b_k. If $k = 0$ set $\bar{s}_k = s_k$, $\bar{y}_k = y_k$ and go to Step 4.

Step 2: Correction preparation. Set $\alpha_k = s_k^T \bar{y}_{k-1}/\bar{b}_{k-1}$, $\beta_k = \bar{s}_{k-1}^T y_k/\bar{b}_{k-1}$ and $\theta_k = \alpha_k \beta_k \bar{b}_{k-1}$. If $\alpha_k \beta_k \le 0$ or $\theta_k \ge (1-\delta_1) b_k$ or $|\alpha_k - \beta_k| \ge \bar{b}_{k-1}/b_k$, set $\alpha_k = \beta_k = 0$ and go to Step 3. If $\theta_k < (1-\delta_2) b_k$ or $|\beta_k| > 2\sqrt{b_k/\bar{b}_{k-1}}$, set $\beta_k = \beta_k \sqrt{\alpha_k/\beta_k}$.

Step 3: Correction. Set $\bar{s}_k = s_k - \alpha_k \bar{s}_{k-1}$, $\bar{y}_k = y_k - \beta_k \bar{y}_{k-1}$.

Step 4: Update definition. Set $\tilde{m} = \min(k, m-1)$, $\bar{b}_k = \bar{s}_k^T \bar{y}_k$ and define $\bar{V}_k = I - (1/\bar{b}_k) \bar{s}_k \bar{y}_k^T$ and $\bar{H}_{k-\tilde{m}}^{k+1} = (b_k/|y_k|^2) I$. If $|\bar{s}_{k-\tilde{m}}|/|s_{k-\tilde{m}}| > \Delta$ or $|\bar{y}_{k-\tilde{m}}|/|y_{k-\tilde{m}}| > \Delta$, set $\bar{s}_{k-\tilde{m}} = s_k$, $\bar{y}_{k-\tilde{m}} = y_k$ and $\bar{b}_{k-\tilde{m}} = b_k$. Define $\bar{H}_{k+1} \equiv \bar{H}_{k+1}^{k+1}$ by (1.9).

Step 5: Direction vector. Compute $d_{k+1} = -\bar{H}_{k+1} g_{k+1}$ by the Strang recurrences, using the definition of matrices $\{\bar{H}_i^{k+1}\}_{i=k-\tilde{m}}^{k+1}$, set $k := k+1$ and go to Step 1.

5 Global convergence

In this section, we establish global convergence of Algorithm 4.1. In comparison with the L-BFGS method, boundedness of $|\bar{s}_k|^2/\bar{b}_k$ and $|\bar{y}_k|^2/\bar{b}_k$ cannot be derived from properties of second-order derivatives of objective function directly here, since vectors $\bar{s}_k$, $\bar{y}_k$, $k > 0$, are defined recurrently by (1.7). We will use the following assumption.

Assumption 5.1. *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 5.1. *Let objective function f satisfy Assumption 5.1. Then $\underline{G} \le |y|^2/b \le \overline{G}$ and $b/|s|^2 \ge \underline{G}$.*

Proof. Setting $G_I = \int_0^1 G(x + \xi s) d\xi$, $q = G_I^{1/2} s$, we obtain $y = g_+ - g = G_I s$ and, thus,

$$y^T y/s^T y = q^T G_I q/q^T q = \int_0^1 q^T G(x + \xi s) q/q^T q \, d\xi \in [\underline{G}, \overline{G}]$$

by Assumption 5.1. Similarly, $b/|s|^2 = s^T G_I s/s^T s = \int_0^1 s^T G(x + \xi s) s/s^T s \, d\xi \ge \underline{G}$. □

Theorem 5.1. *Let objective function f satisfy Assumption 5.1. Then, Algorithm 4.1 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. All updates in (1.9) are the standard BFGS updates with vectors $\bar{s}_i$, $\bar{y}_i$ instead of s_i, y_i; therefore we have (see [12])

$$\mathrm{Tr}(\bar{B}_{i+1}^{k+1}) = \mathrm{Tr}(\bar{B}_i^{k+1}) + |\bar{y}_i|^2/\bar{b}_i - |\bar{B}_i^{k+1} \bar{s}_i|^2/\bar{c}_i^{k+1}, \quad (5.1)$$

$$\det(\bar{B}_{i+1}^{k+1}) = \det(\bar{B}_i^{k+1}) \, \bar{b}_i/\bar{c}_i^{k+1}, \quad (5.2)$$

$k - \tilde{m} \le i \le k$.

(i) The safeguarding technique in Step 2 of Algorithm 4.1 guarantees $\alpha_k \beta_k > 0$, $\bar{b}_k > \delta_1 b_k$ and $|\beta_k| \le 2\sqrt{b_k/\bar{b}_{k-1}}$, $k > 0$, see Section 4.

(ii) We start with the first update in (1.9). Since $\bar{B}^{k+1}_{k-\tilde{m}} = (|y_k|^2/b_k)I$, we obtain

$$\mathrm{Tr}(\bar{B}^{k+1}_{k-\tilde{m}}) = (|y_k|^2/b_k)\,\mathrm{Tr}(I) \le N\overline{G}, \quad \det(\bar{B}^{k+1}_{k-\tilde{m}}) = (|y_k|^2/b_k)^N \ge \underline{G}^N \tag{5.3}$$

by Lemma 5.1. Further, if $\max(|\bar{s}_{k-\tilde{m}}|/|s_{k-\tilde{m}}|, |\bar{y}_{k-\tilde{m}}|/|y_{k-\tilde{m}}|) \le \Delta$, $k \ge 0$, in Step 4 then, in view of $\bar{b}_{k-\tilde{m}} > \delta_1 b_{k-\tilde{m}}$ and Lemma 5.1, from (5.1), (5.2) and (5.3) we get

$$\mathrm{Tr}(\bar{B}^{k+1}_{k-\tilde{m}+1}) \le \mathrm{Tr}(\bar{B}^{k+1}_{k-\tilde{m}}) + \Delta^2|y_{k-\tilde{m}}|^2/(\delta_1 b_{k-\tilde{m}}) \le (N + \Delta^2/\delta_1)\overline{G} \stackrel{\Delta}{=} C_1, \tag{5.4}$$

$$\det(\bar{B}^{k+1}_{k-\tilde{m}+1}) = \left(\det(\bar{B}^{k+1}_{k-\tilde{m}})b_k/|y_k|^2\right)\left(\bar{b}_{k-\tilde{m}}/|\bar{s}_{k-\tilde{m}}|^2\right) \ge \left(\underline{G}^N/\overline{G}\right)\left(\underline{G}\delta_1/\Delta^2\right) \stackrel{\Delta}{=} C_2. \tag{5.5}$$

Otherwise, replacing $\bar{s}_{k-\tilde{m}}$, $\bar{y}_{k-\tilde{m}}$, $\bar{b}_{k-\tilde{m}}$ by s_k, y_k, b_k in Step 4, we similarly obtain

$$\mathrm{Tr}(\bar{B}^{k+1}_{k-\tilde{m}+1}) \le \mathrm{Tr}(\bar{B}^{k+1}_{k-\tilde{m}}) + |y_k|^2/b_k \le (N+1)\overline{G} \le C_1, \tag{5.6}$$

$$\det(\bar{B}^{k+1}_{k-\tilde{m}+1}) = \left(\det(\bar{B}^{k+1}_{k-\tilde{m}})b_k/|y_k|^2\right)\left(b_k/|s_k|^2\right) \ge \underline{G}^{N+1}/\overline{G} \ge C_2. \tag{5.7}$$

(iii) We will show that

$$\mathrm{Tr}(\bar{B}^{k+1}_i) \le C_3, \quad k - \tilde{m} \le i \le k+1, \quad k > 0, \tag{5.8}$$

where C_3 is a constant. If we replace C_3 by C_1, it is true for $i = k - \tilde{m} + 1$ by (5.4) or (5.6) and for $i = k - \tilde{m}$ by (5.3) together with $N\overline{G} < C_1$. Thus (5.8) holds for $\tilde{m} = 0$ with any $C_3 \ge C_1$.

Let $\tilde{m} > 0$. Since updates in (1.9) satisfy the quasi-Newton conditions

$$\bar{H}^{k+1}_i \bar{y}_{i-1} = \bar{s}_{i-1}, \qquad k - \tilde{m} < i \le k, \quad k > 0, \tag{5.9}$$

we can write $|\bar{y}_{i-1}|^2/\bar{b}_{i-1} = \bar{y}^T_{i-1}\bar{y}_{i-1}/\bar{y}^T_{i-1}\bar{H}^{k+1}_i\bar{y}_{i-1} \le \mathrm{Tr}(\bar{B}^{k+1}_i)$, which by (5.1), (1.7), (i) and Lemma 5.1 implies

$$\mathrm{Tr}(\bar{B}^{k+1}_{i+1}) - \mathrm{Tr}(\bar{B}^{k+1}_i) \le \frac{|y_i - \beta_i\bar{y}_{i-1}|^2}{\bar{b}_i} \le \frac{2}{\delta_1}\left(\frac{|y_i|^2}{b_i} + \beta_i^2\frac{|\bar{y}_{i-1}|^2}{b_i}\right) \le \frac{2\overline{G}}{\delta_1} + \frac{8}{\delta_1}\mathrm{Tr}(\bar{B}^{k+1}_i),$$

$k - \tilde{m} < i \le k$. Denoting $C_0 = 1 + 8/\delta_1$ and using (5.4) or (5.6), we obtain

$$\mathrm{Tr}(\bar{B}^{k+1}_{i+1}) \le (1 + C_0 + \ldots + C_0^{\tilde{m}-1})2\overline{G}/\delta_1 + C_0^{\tilde{m}}C_1 \stackrel{\Delta}{=} C_3, \quad k - \tilde{m} < i \le k,$$

which together with $C_3 > C_1$ by $C_0 > 1$ concludes the proof of (5.8). For $i = k+1$ in (5.8) we have

$$\mathrm{Tr}(\bar{B}_{k+1}) = \mathrm{Tr}(\bar{B}^{k+1}_{k+1}) \le C_3, \quad k > 0. \tag{5.10}$$

(iv) Using (5.9) and $\alpha_i = s^T_i\bar{y}_{i-1}/\bar{b}_{i-1}$, we get

$$\bar{c}^{k+1}_i = (s_i - \alpha_i\bar{s}_{i-1})^T\bar{B}^{k+1}_i(s_i - \alpha_i\bar{s}_{i-1}) = s^T_i\bar{B}^{k+1}_i s_i - (s^T_i\bar{y}_{i-1})^2/\bar{b}_{i-1} \le s^T_i\bar{B}^{k+1}_i s_i,$$

$k - \tilde{m} \le i \le k$, $k > 0$, which together with (5.2) yields

$$\det(\bar{B}^{k+1}_{i+1})/\det(\bar{B}^{k+1}_i) = \bar{b}_i/\bar{c}^{k+1}_i \ge \delta_1(b_i/|s_i|^2)(s^T_i s_i/s^T_i\bar{B}^{k+1}_i s_i) \ge \delta_1\underline{G}/C_3,$$

$k - \tilde{m} \le i \le k$, by Lemma 5.1 and (5.8). From this and (5.5) or (5.7) we conclude

$$\det(\bar{B}_{k+1}) = \det(\bar{B}^{k+1}_{\tilde{m}+1}) \ge C_2(\delta_1\underline{G}/C_3)^{\tilde{m}} \stackrel{\Delta}{=} C_4, \quad k > 0. \tag{5.11}$$

(v) The lowest eigenvalue $\underline{\lambda}(\bar{B}_k)$ of matrix $\bar{B}_k$ satisfies $\underline{\lambda}(\bar{B}_k) \ge \det(\bar{B}_k)/\mathrm{Tr}(\bar{B}_k)^{N-1}$, $k \ge 0$. Setting $q_k = \bar{B}^{1/2}_k s_k$, from (5.10) and (5.11) we get

$$\frac{(s^T_k\bar{B}_k s_k)^2}{|s_k|^2|\bar{B}_k s_k|^2} = \frac{s^T_k\bar{B}_k s_k}{s^T_k s_k}\,\frac{q^T_k q_k}{q^T_k\bar{B}_k q_k} \ge \frac{\det(\bar{B}_k)}{\mathrm{Tr}(\bar{B}_k)^{N-1}}\,\frac{1}{\mathrm{Tr}(\bar{B}_k)} \ge \frac{C_4}{C_3^N}, \quad k > 1,$$

which implies $\lim_{k\to\infty}|g_k| = 0$, see [12], Theorem 3.2 and relations (3.17)-(3.18). □

6 Numerical results

In this section, we demonstrate the influence of vectors corrections on the number of evaluations and computational time, using the following collections of test problems:

[8] - Test 11 without problems 42, 48, 50, i.e. 55 problems, which are modified problems from CUTE collection [2]; used N are given in Table 1, where problems, modified in some way, are marked with '*',

[1] - termed Test 12 here, 73 problems, $N = 5000$,

[7] - Test 25 without problems 48, 57, 58, 60, 61, 67-70, 79, i.e. 72 problems, $N = 1000$.

The source texts and reports can be downloaded from `camo.ici.ro/neculai/ansoft.htm` (Test 12) and from `www.cs.cas.cz/~luksan/test.html` (Test 11 and Test 25).

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 – modified CUTE collection.

For comparison, Table 2 contains results for the following limited-memory methods: L-BFGS – the Nocedal method based on the Strang formula, see [11], method from [14] that use the preceding vectors (Algorithm 4.5) and new Algorithm 4.1. We have used $m = 5$, $\delta_1 = 0.000\,001$, $\delta_2 = 0.01$, $\Delta = 100$ and the final precision $\|g(x^\star)\|_\infty \le 10^{-6}$.

Method	Test 11		Test 12		Test 25	
	NFE	Time	NFE	Time	NFE	Time
L-BFGS	80539	32.50	43648	46.17	126733	37.65
Alg. 4.5 in [14]	80328	34.52	43182	56.67	126289	38.35
Algorithm 4.1	64395	30.20	34472	37.57	114910	39.39

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 [3]. The performance profile $\pi_M(\tau)$ is defined by the formula

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

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 $\pi_M(\tau)$ 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. The following figures, based on results in Table 2, reveal the performance profiles for tested methods graphically.

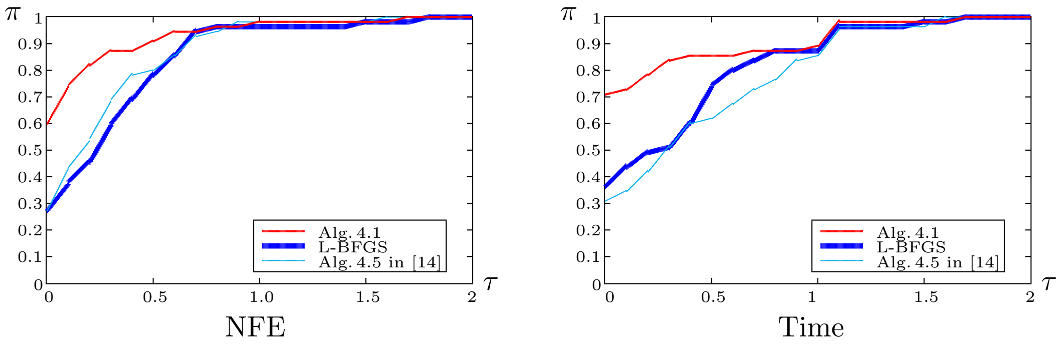

Figure 1 (Test 11, $m = 5$, 55 problems)

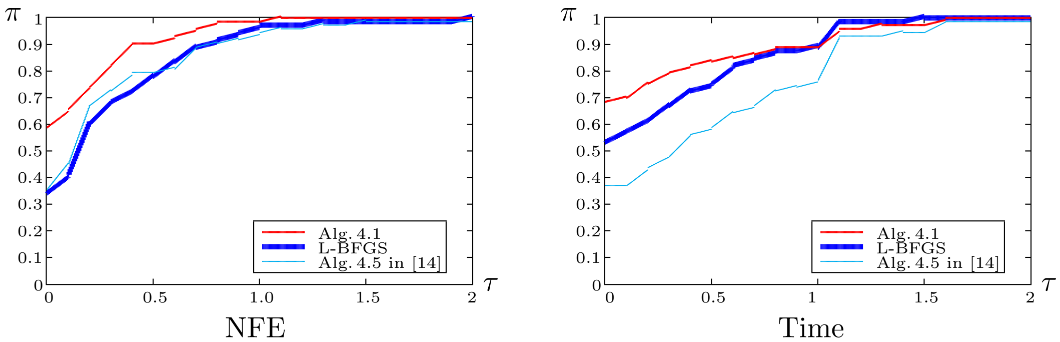

Figure 2 (Test 12, $m = 5$, 73 problems)

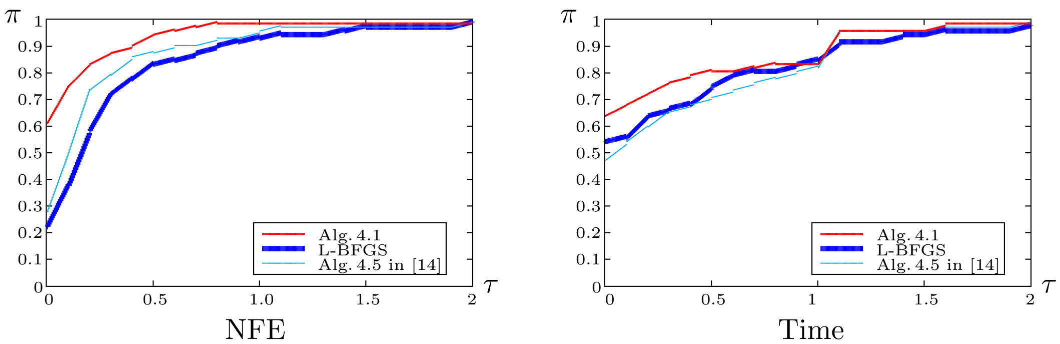

Figure 3 (Test 25, $m = 5$, 72 problems)

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