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Technical report No. V 1060

December 2009

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Generalizations of the limited-memory BFGS method based on quasi-product form of update [1]

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Abstract:

Two families of limited-memory variable metric or quasi-Newton methods for unconstrained minimization based on quasi-product form of update are derived. As for the first family, four variants how to utilize the Strang recurrences for the Broyden class of variable metric updates are investigated; three of them use the same number of stored vectors as the limited-memory BFGS method. Moreover, one of the variants does not require any additional matrix by vector multiplication. The second family uses vectors from the preceding iteration to construct a new class of variable metric updates. Resulting methods again require neither any additional matrix by vector multiplication nor any additional stored vector.

Global convergence of four of presented methods is established for convex sufficiently smooth functions. Numerical results indicate that two of the new methods can save computational time substantially for certain problems.

Keywords:
Unconstrained minimization, variable metric methods, limited-memory methods, Broyden class updates, global convergence, numerical results.

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1 Introduction

In this report we present two new families of limited-memory (LM) variable metric (VM) line search methods for unconstrained minimization which generalize the well-known LM BFGS method, see [6], [3].

VM or quasi-Newton line search methods, see [4], start with an initial point $x_0 \in \mathcal{R}^N$ and generate iterations $x_{k+1} \in \mathcal{R}^N$ by the process $x_{k+1} = x_k + s_k$, $s_k = t_k d_k$, $k \ge 0$, where d_k is the direction vector and $t_k > 0$ is a stepsize.

It is assumed that the problem function $f : \mathcal{R}^N \to \mathcal{R}$ is differentiable and stepsize t_k is chosen in such a way that

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

$k \ge 0$, 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 $H_0 = I$ and H_{k+1} is obtained from H_k by a rank-two VM update to satisfy the quasi-Newton condition $H_{k+1} y_k = s_k$ (see [2], [4]), where $y_k = g_{k+1} - g_k$, $k \ge 0$.

For $i \ge 0$ we denote (note that $s_i^T y_i > 0$ for $g_i \ne 0$ by (1.1))

$$B_i = H_i^{-1}, \quad a_i = y_i^T H_i y_i, \quad b_i = s_i^T y_i, \quad c_i = s_i^T B_i s_i, \quad V_i = I - (1/b_i) s_i y_i^T.$$

To simplify the notation we frequently omit index k and replace index $k+1$ by symbol $+$ and index $k-1$ by symbol $-$.

The LM BFGS method (see [3], [6]) is based on the following quasi-product form of the BFGS update

$$H_+ = (1/b) s s^T + V H V^T. \tag{1.2}$$

The advantage of this form consists in the fact that instead of matrices H_k, only the last $\tilde{m}+1$ couples $\{s_i, y_i\}_{i=k-\tilde{m}}^k$, where $\tilde{m} = \min(k, m-1)$ and $m \ge 1$ is a given parameter, are stored to compute the direction vector $d_{k+1} = -H_{k+1} g_{k+1}$ by the Strang recurrences, using matrices $\{H_i^{k+1}\}_{i=0}^{\tilde{m}+1}$, see [6]. Matrices H_{k+1} are not computed, only defined by $H_{k+1} = H_{\tilde{m}+1}^{k+1}$, $k \ge 0$, where

$$H_0^{k+1} = (b_k/|y_k|^2) I, \tag{1.3}$$

$$H_{i+1}^{k+1} = (1/b_j) s_j s_j^T + V_j H_i^{k+1} V_j^T, \quad j = k - \tilde{m} + i, \quad 0 \le i \le \tilde{m}. \tag{1.4}$$

Note that matrix H_k, which satisfies $d_k = -H_k g_k$, is different from matrix $H_{\tilde{m}}^{k+1}$ used in the last update (1.4) in general; among others since matrix H_k is created by updating of matrix $H_0^k = (b_{k-1}/|y_{k-1}|^2) I$, which is different from matrix $H_0^{k+1} = (b_k/|y_k|^2) I$. Thus $H_{\tilde{m}}^{k+1} g_k \ne -d_k$ generally; this fact is important for LM methods investigated in this report.

We focus here on generalization of this approach. In Section 2 we mention some problems with a such generalization for the other updates from the Broyden class, see [2], [4], and describe four methods based on the quasi-product form of the VM update resembling (1.2). In Section 3 we present a new class of variable metric updates which do not belong to the Broyden class, but which are very useful for constructing of LM methods. Corresponding algorithms for our methods are given in Section 4 and global convergence is investigated in Section 5. Numerical results are reported in Section 6.

2 The Broyden class updates in quasi-product form

Quasi-product form (1.2) of the BFGS update can be easily generalized for the Broyden class updates with $\eta \geq 0$ (see e.g. [7]):

$$H_+^{BC} = \frac{1}{b} s s^T + \tilde{V} H \tilde{V}^T, \qquad \tilde{V} = I - \left(\frac{\sqrt{\eta}}{b} s + \frac{1-\sqrt{\eta}}{a} H y \right) y^T. \tag{2.1}$$

If we proceed analogically as above, we can store the last $\tilde{m}+1$ triplets $\{s_i, y_i, H_i y_i\}_{i=k-\tilde{m}}^k$ here instead of matrix H. Besides $H_+ g_+$, also vector Hy can be computed by the slightly modified Strang recurrences which require more both arithmetic and memory operations. Nevertheless, the number of function evaluations can be reduced by the choice of η (see Section 6).

In Section 1 we mentioned the difference between matrices H_k and $H_{\tilde{m}}^{k+1}$. Similarly, VM matrices H_j occurring in the stored old vectors $H_j y_j$ contained in $\tilde{V}_j$ differ from the currently used VM matrices corresponding to H_i^{k+1} in (1.4), $j = k - \tilde{m} + i$, $0 \leq i \leq \tilde{m}$, and thus the resulting LM method with $\eta \neq 1$ (and due to similar reasons, any new LM method presented in this section) does not belong to the Broyden class.

Efficiency can be increased if we use another approach. We transform the Broyden class update with parameter η to the formal BFGS update in transformed variables, which makes possible to construct LM methods in a similar way as the BFGS update, with the same number of stored vectors. First we give the simple variant of the transformation. We denote

$$\omega = 1 + \frac{a}{b}\eta, \quad \mu = \eta + (1-\eta)\frac{b}{a}. \tag{2.2}$$

Theorem 2.1. *Let $\omega \neq 0$, $\mu \geq 0$ and denote $\alpha = (\eta \pm \sqrt{\mu})/\omega$. Then $\sqrt{\mu} \neq -\eta$ and the standard Broyden class update of symmetric positive definite matrix H with parameter η can be expressed in the form*

$$H_+^{BC} = \frac{\eta}{b} \hat{s}\hat{s}^T + \check{V} H \check{V}^T, \quad \hat{s} = s - \alpha H y, \quad \check{V} = I \pm \frac{\sqrt{\mu}}{b} \hat{s} y^T. \tag{2.3}$$

Proof. (i) First we show that $\sqrt{\mu} \neq -\eta$. From (2.2) we have

$$\eta^2 - \mu = \eta^2 - \eta - (1-\eta)b/a = (\eta - 1)(\eta + b/a) = (\eta - 1)\,\omega b/a, \tag{2.4}$$

thus $\sqrt{\mu} \neq -\eta$ for $\eta \neq 1$ by $b > 0$ and obviously also for $\eta = 1$.

(ii) Consider the Broyden class update with parameters η in the form, see [2], [4]

$$H_+^{BC} = H + \frac{\omega}{b} s s^T - \frac{\eta}{b}\left(H y s^T + s y^T H \right) + \frac{\eta - 1}{a} H y y^T H\,.$$

Setting $s = \hat{s} + \xi H y$, $\xi \in \mathcal{R}$, we obtain

$$H_+^{BC} = H + \frac{\omega}{b}\hat{s}\hat{s}^T + \frac{\xi\omega - \eta}{b}\left(H y \hat{s}^T + \hat{s} y^T H \right) + \left(\frac{\eta - 1}{a} + \frac{\xi^2 \omega - 2\xi\eta}{b} \right) H y y^T H.$$

The last term vanishes for $\xi^2\omega - 2\xi\eta + (b/a)(\eta - 1) = 0$, i.e. for $\xi = (\eta \pm \sqrt{\mu})/\omega = \alpha$; then $\xi\omega - \eta = \pm\sqrt{\mu}$ and thus

$$H_+^{BC} = H + \frac{\omega}{b}\hat{s}\hat{s}^T + \frac{\pm\sqrt{\mu}}{b}\left(H y\hat{s}^T + \hat{s}y^T H\right) = \check{V}H\check{V}^T + \frac{1}{b}\left(\omega - \frac{a}{b}\mu\right)\hat{s}\hat{s}^T.$$

In view of

$$\omega - \frac{a}{b}\,\mu = 1 + \frac{a}{b}\,\eta - \frac{a}{b}\,\eta - (1-\eta) = \eta \tag{2.5}$$

we have (2.3). □

Note that we prefer the minus sign in α and $\check{V}$, since then for $\eta = 1$ we get $\alpha = 0$, $\hat{s} = s$, $\check{V} = V$ and (2.3) represents the usual quasi-product form of the BFGS update. For $\eta \approx 1$ it is also $\sqrt{\mu} \approx 1$, therefore the formula for α above should be rewritten in another form. In view of (2.4) we obtain for $\omega \neq 0$ (thus also $\sqrt{\mu} \neq -\eta$ by Theorem 2.1)

$$\alpha = \frac{\eta - \sqrt{\mu}}{\omega} = \frac{\eta^2 - \mu}{\omega(\eta + \sqrt{\mu})} = \frac{(\eta-1)\,\omega b/a}{\omega(\eta + \sqrt{\mu})} = \frac{(\eta-1)b/a}{\eta + \sqrt{\mu}}\,. \tag{2.6}$$

For better understanding, condition $\mu \geq 0$ can be rewritten as $\eta(b-a) \leq b$, i.e. $\eta \leq \eta_{SR1}$ for $\eta_{SR1} > 0$, or $\eta \geq \eta_{SR1}$ for $\eta_{SR1} < 0$, where $\eta_{SR1} = b/(b-a)$ is the value of parameter η for the SR1 method, see [4]. For $\eta = \eta_{SR1}$ we obtain from (2.2) $\omega = b/(b-a) \neq 0$ and $\mu = 0$, therefore Theorem 2.1 can also be used for the SR1 update.

For the transformation above, the similarity to the BFGS update is relatively free. Firstly $\check{V}$ is not a projection matrix in general, secondly matrix H_+^{BC} does not satisfy the quasi-Newton condition in transformed variables. Both these properties can be obtained if we introduce an additional transformation.

Theorem 2.2. *Let matrix H be symmetric positive definite, $\omega \neq 0$, $\mu > 0$, $\alpha = (\eta - \sqrt{\mu})/\omega$, $\hat{b} = b/\sqrt{\mu}$, $\hat{s} = s - \alpha H y$, $\hat{c} = \hat{s}^T B\hat{s}$. Then $\hat{c} > 0$ and denoting $\beta = -\alpha\hat{b}/\hat{c}$ and $\hat{y} = y - \beta B\hat{s}$, we can express the standard Broyden class update of matrix H with parameter η in the form*

$$H_+^{BC} = \frac{\hat{\varrho}}{\hat{b}}\hat{s}\hat{s}^T + \hat{V}H\hat{V}^T, \quad \hat{V} = I - \frac{1}{\hat{b}}\hat{s}\hat{y}^T, \quad \hat{\varrho} = \frac{\eta}{\sqrt{\mu}} - \alpha\beta. \tag{2.7}$$

Moreover, $\hat{b} = \hat{s}^T\hat{y} > 0$ holds and if $\eta \geq 0$ then $\hat{\varrho} > 0$.

Proof. (i) First we establish $\hat{c} > 0$ and $\hat{b} = \hat{s}^T\hat{y} > 0$. From $\hat{s} = s - \alpha H y$ we get

$$\hat{c} = \hat{s}^T B\hat{s} = (s - \alpha H y)^T (Bs - \alpha y) = c - 2\alpha b + \alpha^2 a = [\,ac - b^2 + (b - \alpha a)^2]/a. \tag{2.8}$$

Since $ac \geq b^2$ by the Schwarz inequality and

$$b - \alpha a = b - b\frac{\eta - 1}{\eta + \sqrt{\mu}} = b\frac{\sqrt{\mu} + 1}{\eta + \sqrt{\mu}} \neq 0 \tag{2.9}$$

in view of (2.6) and $\sqrt{\mu} \neq -\eta$, see Theorem 2.1, we obtain $\hat{c} > 0$. Further, we can write $\hat{s}^T\hat{y} = \hat{s}^T(y - \beta B\hat{s}) = (s - \alpha Hy)^T y - \beta\hat{c}$, which gives by (2.9), (2.6) and (2.2)

$$\hat{s}^T\hat{y} = b - \alpha a + \hat{b}\alpha = b\frac{\sqrt{\mu}+1}{\eta+\sqrt{\mu}} + \frac{b}{\sqrt{\mu}}\frac{(\eta-1)b/a}{\eta+\sqrt{\mu}} = \frac{b(\mu+\sqrt{\mu}+\eta-\mu)}{\sqrt{\mu}(\eta+\sqrt{\mu})} = \hat{b} > 0.$$

(ii) Next we show that $\hat{a}/\hat{b} + 2\beta = \sqrt{\mu}(a - \beta^2\hat{c})/b$, where $\hat{a} = \hat{y}^T H\hat{y}$. From $a = y^T Hy = (\hat{y} + \beta B\hat{s})^T(H\hat{y} + \beta\hat{s}) = \hat{a} + 2\beta\hat{b} + \beta^2\hat{c}$ we obtain

$$\hat{a}/\hat{b} + 2\beta = (\hat{a} + 2\beta\hat{b})/\hat{b} = (a - \beta^2\hat{c})/\hat{b} = \sqrt{\mu}\,(a - \beta^2\hat{c})/b. \tag{2.10}$$

(iii) As in the proof of Theorem 2.1 we get

$$H_+^{BC} = H + \frac{\omega}{b}\hat{s}\hat{s}^T - \frac{\sqrt{\mu}}{b}\left(H\,y\hat{s}^T + \hat{s}y^T H\right).$$

Setting $y = \hat{y} + \beta B\hat{s}$, we obtain by $b = \hat{b}\sqrt{\mu}$

$$H_+^{BC} = H - \frac{1}{\hat{b}}\left(H\hat{y}\hat{s}^T + \hat{s}\hat{y}^T H\right) + \left(\frac{\omega}{b} - \frac{2\beta}{\hat{b}}\right)\hat{s}\hat{s}^T = \hat{V}H\hat{V}^T + \frac{1}{\hat{b}}\left[\frac{\omega}{\sqrt{\mu}} - 2\beta - \frac{\hat{a}}{\hat{b}}\right]\hat{s}\hat{s}^T.$$

To complete the proof, we rewrite the expression in brackets, using (2.10) and (2.5):

$$\frac{\omega}{\sqrt{\mu}} - \left(2\beta + \frac{\hat{a}}{\hat{b}}\right) = \left(\frac{\omega}{\sqrt{\mu}} - \frac{a}{b}\sqrt{\mu}\right) + \beta^2\frac{\hat{c}}{b}\sqrt{\mu} = \frac{\eta}{\sqrt{\mu}} + \frac{\beta\hat{c}}{\hat{b}}\beta = \frac{\eta}{\sqrt{\mu}} - \alpha\beta = \hat{\varrho}.$$

Since $\eta = \sqrt{\mu}$ for $\alpha = 0$ by $\alpha\omega = \eta - \sqrt{\mu}$, we see that $\hat{\varrho} = \eta/\sqrt{\mu} - \alpha\beta = \eta/\sqrt{\mu} + \alpha^2\hat{b}/\hat{c} > 0$ holds for $\eta \geq 0$ by $\hat{b} > 0$ and $\hat{c} > 0$. □

Obviously, the quasi-Newton condition $H_+^{BC}\hat{y} = \hat{\varrho}\hat{s}$ in transformed variables is satisfied by (2.7). Note that $\hat{c}$ can be computed e.g. by (2.8).

All these forms of the Broyden class update of matrix H with $\eta \neq 1$ need vector Hy in every iteration, but it does not mean that we must calculate two matrix by vector multiplications per iteration. If we have computed vector Hy, then the next direction vector can be expressed as a linear combination of vectors s, Hy or in the form which gives descending vector d_+ even in case that we approximate some values.

Lemma 2.1. *Consider the Broyden class update H_+ of symmetric positive definite matrix H with parameter η. If $d = -Hg$ then the direction vector $d_+ = -H_+g_+$ satisfies*

$$td_+ = \left[\eta\left(\frac{ac}{b^2} - 1\right) + 1\right]\left(s - \frac{b}{a}Hy\right) + \left(\frac{c}{b} - t\right)s. \tag{2.11}$$

Proof. Writing VM update in the form $H_+ = H + \Delta$, we get by $s = -tHg$ and the quasi-Newton condition $H_+y = s$

$$td_+ = -tH_+g_+ = -tH_+y - t(H + \Delta)g = (1 - t)s + \Delta Bs. \tag{2.12}$$

For the Broyden class update we have, see [4],

$$\Delta = \frac{1}{b}\left(1+\frac{a}{b}\eta\right) ss^T - \frac{\eta}{b}\left(H\,ys^T + sy^T H\right) + \frac{\eta-1}{a} H\,yy^T H\,.$$

Therefore

$$\Delta Bs = \left[\frac{c}{b}\left(1+\frac{a}{b}\eta\right)-\eta\right]s - \left[\frac{c}{b}\eta - \frac{b}{a}(\eta-1)\right]Hy = \frac{c}{b}s + \left[\eta\left(\frac{ac}{b^2}-1\right)+1\right]\left(s-\frac{b}{a}Hy\right) - s,$$

which together with (2.12) gives (2.11). □

Theorem 2.3. *Consider the Broyden class update H_+ of the symmetric positive definite matrix H with parameter η and let*

$$d_+ = -\frac{s^T g_+}{b}s - \frac{b+\eta\,\delta}{b+\delta}\,Vp, \qquad p = HV^T g_+ = HV^T g, \quad \delta \neq -b. \tag{2.13}$$

If $\eta \geq 0$ and $\delta \geq 0$ then $d_+^T g_+ < 0$. If $d = -Hg$ then $s^T g_+ = b - c/t$, $Hy = (tp+s)b/c$, $a = (t\,p^T y + b)b/c$ and if we set $\delta = t\,p^T y$ then vector d_+ satisfies $d_+ = -H_+ g_+$.

Proof. (i) Equivalence of the two forms of p in (2.13) follows from $V^T y = 0$.

(ii) Let $\eta \geq 0$ and $\delta \geq 0$. Then from (2.13) we have

$$d_+^T g_+ = -(s^T g_+)^2/b - [(b+\eta\,\delta)/(b+\delta)]\, g_+^T V H V^T g_+. \tag{2.14}$$

If $s^T g_+ = 0$ then $V^T g_+ = g_+$ and $d_+^T g_+ < 0$ by positive definiteness of H and $b > 0$, otherwise $d_+^T g_+ \leq -(s^T g_+)^2/b < 0$.

(iii) Let $d = -Hg$. In view of (i) we have $p = HV^T g = Hg - (s^T g/b)Hy = -(1/t)s + [c/(bt)]Hy$, i.e. $Hy = (t\,p+s)b/c$, which yields $a = (t\,p^T y + b)b/c$ and

$$s - \frac{b}{a}Hy = -\frac{b}{a}VHy = -\frac{b}{a}\frac{b}{c}V(tp+s) = -\frac{b^2 t}{ac}Vp \tag{2.15}$$

by $Vs = 0$. Further, we get $s^T g_+ = s^T y + s^T g = b - s^T Bs/t = b - c/t$.

For $t\,p^T y = \delta \neq -b$ we obtain from (2.13)

$$-d_+ = \frac{s^T g_+}{b}s + \frac{b+\eta\,t\,p^T y}{b+t\,p^T y}\,Vp = \frac{s^T g_+}{b}s + \left[1+(\eta-1)\left(1-\frac{b}{b+t\,p^T y}\right)\right]Vp\,. \tag{2.16}$$

From $a = (t\,p^T y + b)b/c \neq 0$ we get $ac/b^2 = (b + t\,p^T y)/b$, which gives

$$-d_+ = \frac{s^T g_+}{b}s + \left[1+(\eta-1)\left(1-\frac{b^2}{ac}\right)\right]Vp = \left[\eta\left(\frac{ac}{b^2}-1\right)+1\right]\frac{b^2}{ac}Vp + \frac{s^T g_+}{b}s\,,$$

i.e. (2.11) by (2.15) and $s^T g_+ = b - c/t$, therefore $d_+ = -H_+ g_+$ by Lemma 2.1. □

Although assumption $d = -Hg$ is not appropriate to LM method updates of type (1.4), see Section 1, Theorem 2.3 can be utilized to increase efficiency, see Section 4.

3 VM updates that use the preceding vectors

A drawback of methods in Section 2, consisting in the fact that for $\eta \neq 1$ we need vector Hy in every iteration, is eliminated in the following family of VM updates based on utilization of the quasi-Newton condition $Hy_- = s_-$. These updates do not belong to the Broyden class. The resulting LM methods use the same number of stored vectors and matrix by vector multiplications as the LM BFGS method, see Section 4.

Theorem 3.1. *Let matrix H be symmetric positive definite, $Hy_- = s_-$, $\sigma \in (-1, 1)$, $\bar{s} = s - \sigma\sqrt{b/b_-}\, s_-$, $\bar{y} = y - \sigma\sqrt{b/b_-}\, y_-$, $\bar{b} = \bar{s}^T y \neq 0$ and $\bar{\varrho} = (1-\sigma^2)\, b/\bar{b}$. Then update H_+^{NB} given by*

$$H_+^{NB} = (\bar{\varrho}/\,\bar{b})\, \bar{s}\bar{s}^T + \bar{V} H \bar{V}^T, \qquad \bar{V} = I - (1/\,\bar{b})\, \bar{s}\bar{y}^T, \tag{3.1}$$

with parameter σ is positive definite and satisfies the quasi-Newton condition $H_+^{NB} y = s$. If $\sigma = 0$ then (3.1) is the BFGS update. If $\sigma = s^T y_- / \sqrt{bb_-}$ then $\bar{b} = \bar{s}^T \bar{y}$ and in case that this choice satisfies $\sigma \in (-1, 1)$ and $\bar{b} > 0$, (3.1) represents the generalized BFGS update with nonquadratic correction parameter $\bar{\varrho}$ (see [4]), with vectors s and y replaced by $\bar{s}$, $\bar{y}$.

Proof. (i) Positive definiteness of H_+^{NB} follows directly from (3.1): Let $q \in \mathcal{R}^N$, $q \neq 0$. If $q^T \bar{s} \neq 0$ then $q^T H_+^{NB} q \geq (\bar{\varrho}/\,\bar{b})(q^T \bar{s})^2 > 0$, otherwise $q^T H_+^{NB} q = q^T H q > 0$.

(ii) Denoting $\tilde{\sigma} = \sigma\sqrt{b/b_-}$, we get $H\bar{V}^T y = H(y - \bar{y}) = \tilde{\sigma}\, Hy_- = \tilde{\sigma}\, s_-$ and therefore $H_+^{NB} y = \bar{\varrho}\bar{s} + \tilde{\sigma}\, \bar{V} s_- = [\bar{\varrho} - \tilde{\sigma}\, \bar{y}^T s_- /\, \bar{b}]\bar{s} + \tilde{\sigma} s_-$. The expression in brackets can be rewritten:

$$\bar{\varrho} - \tilde{\sigma}\, \bar{y}^T s_- / \bar{b} = \bar{\varrho} - \tilde{\sigma}\, y^T s_- / \bar{b} + \tilde{\sigma}^2 b_- / \bar{b} = (\bar{\varrho} + \sigma^2 b / \bar{b}) - \tilde{\sigma}\, y^T s_- / \bar{b} = (b - \tilde{\sigma}\, y^T s_-) / \bar{b} = 1,$$

which yields $H_+^{NB} y = \bar{s} + \tilde{\sigma} s_- = s$.

(iii) If $\sigma = 0$ then $\bar{s} = s$, $\bar{y} = y$, $\bar{b} = b$, $\bar{\varrho} = 1$, $\bar{V} = V$ and we have the BFGS update.

(iv) Let $\sigma = s^T y_- / \sqrt{bb_-}$. Then $\bar{s}^T y_- = s^T y_- - \sigma\sqrt{b/b_-}\, b_- = 0$ and thus $\bar{s}^T \bar{y} = \bar{s}^T y - \tilde{\sigma} \bar{s}^T y_- = \bar{b}$. If $\bar{b} > 0$ then assumption $\sigma \in (-1, 1)$ gives $\bar{\varrho} > 0$ and we have the generalized BFGS update in $\bar{s}$, $\bar{y}$. □

Our numerical experiments indicate that convergence is significantly deteriorated when $|\sigma|$ tends to unit and that all values σ satisfying $|\sigma| \leq 1/2$ with a suitable sign give very good results. We can deduce from Theorem 3.1 and the following lemma that a good choice is to use the sign of $s^T y_-$.

Lemma 3.1. *Let $Hy_- = s_-$ and let f be quadratic function $f(x) = \frac{1}{2}(x - x^*)^T G (x - x^*)$, $x^* \in \mathcal{R}^N$, with a symmetric positive definite matrix G. If vectors s, s_- are linearly independent and update H_+^{NB} of matrix H is given by (3.1) then choice $\sigma = s^T y_- / \sqrt{bb_-}$ satisfies $\bar{b} > 0$, $\sigma \in (-1, 1)$, $\bar{\varrho} = 1$ and $H_+^{NB} y_- = s_-$.*

Proof. For $\sigma = s^T y_- / \sqrt{bb_-}$ we have $b - b\,\sigma^2 = b - (s^T G s_-)^2 / b_- > 0$ by the Cauchy inequality and linear independency of s, s_-, therefore $|\sigma| < 1$. Further, we get $\bar{b} = \bar{s}^T y = b - \sigma\, s_-^T y \sqrt{b/b_-} = b - s^T y_- \cdot s_-^T y / b_- = b - (s^T G s_-)^2 / b_- = b - b\,\sigma^2$, thus $\bar{b} > 0$ and $\bar{\varrho} = 1$.

In view of $\bar{s}^T y_- = s^T y_- - \sigma\sqrt{b/b_-}\, b_- = 0$ and $\bar{s}^T y_- = \bar{s}^T G s_- = s_-^T \bar{y}$ we obtain by (3.1) $H_+^{NB} y_- = \bar{V} H \bar{V}^T y_- = \bar{V} H y_- = \bar{V} s_- = s_-$. □

Note that we need not calculate value $s^T y_-$. We use only the sign of $s^T y_-$, therefore in view of the following lemma we can utilize the value $s_-^T g$, computed during the line search procedure, in spite of the fact that assumption $d = -Hg$ is not appropriate to LM updates, see Section 1. In Section 4 we describe a choice of the sign of σ in details.

Lemma 3.2. *Let matrix H be nonsingular, $Hy_- = s_-$. If $d = -Hg$ then $s^T y_- = -t s_-^T g$.*

Proof. We obtain $s^T y_- = s^T B H y_- = s^T B s_- = -t\, s_-^T g$. □

Taking account of Theorem 3.1 and Lemma 3.1, we will choose such parameter $\sigma \in (-1, 1)$ that corresponding $\bar{b}$ is positive and not too small in comparison with b in a sense that $\bar{b} \equiv b(1 - \sigma\, s_-^T y/\sqrt{bb_-}\,) \geq b(1 - \lambda)$, $\lambda \in (0, 1)$, which is equivalent to $\sigma\, s_-^T y \leq \lambda\sqrt{bb_-}$. The following lemma shows that in case that $\bar{b} < b(1 - \lambda)$ for some $\sigma \in (-1, 1)$, we can replace this σ by a more appropriate value.

Lemma 3.3. *Let $\sigma\, s_-^T y > \lambda\sqrt{bb_-}$ for some $\lambda \in (0, 1)$. Then $s_-^T y \neq 0$ and value $\hat{\sigma} = \lambda\sqrt{bb_-}/|s_-^T y| > 0$ satisfies $\pm\hat{\sigma}\, s_-^T y \leq \lambda\sqrt{bb_-}$ (for both signs) and $\hat{\sigma} < |\sigma|$.*

Proof. Relation $s_-^T y \neq 0$ follows directly from $\sigma\, s_-^T y > \lambda\sqrt{bb_-}$ and $bb_- > 0$. Further, we have $-\hat{\sigma}|s_-^T y| \leq \hat{\sigma}|s_-^T y| = \lambda\sqrt{bb_-}$ and $\hat{\sigma}|s_-^T y| = \lambda\sqrt{bb_-} < \sigma\, s_-^T y = |\sigma|\,|s_-^T y|$. □

4 Application to limited-memory methods

In this section we use theory from the previous sections to implement five variants of methods based on the quasi-product form of update, similar to (1.2).

We again define matrices H_0^{k+1} and $H_{k+1} = H_{\tilde{m}+1}^{k+1}$, $\tilde{m} = \min(k, m-1)$, $m \geq 1$, $k \geq 0$, by relations similar to (1.3) and (1.4). Instead of matrices H_k, only $\tilde{m} + 1 \leq m$ couples (or triplets for Algorithm 4.1) of vectors are stored here, together with some auxiliary numbers, to compute the direction vector $d_{k+1} = -H_{k+1} g_{k+1}$, using the Strang recurrences, see [6] (or another vector in case of Algorithm 4.4), which requires little modifications here - using transformed nonquadratic correction parameter (see [4]) for algorithms 4.2-4.5 or more both arithmetic and memory operations for Algorithm 4.1 due to structure of matrix $\tilde{V}$. Furthermore, another vector $H_k y_k$, $k \geq 0$, is computed by the Strang recurrences (except for Algorithm 4.4 and Algorithm 4.5).

We shall now state the first three variants of methods in details. For simplicity, we omit stopping criteria. Algorithm 4.1 is based on the quasi-product form (2.1) of the Broyden class update, Algorithm 4.2 on the transformation given in Theorem 2.1, Algorithm 4.3 on the transformation given in Theorem 2.2. In Algorithm 4.2 and Algorithm 4.3, we give only two changed steps.

Algorithm 4.1 (Direct approach)

Data: The number m of VM updates per iteration, line search parameters ε_1 and ε_2, $0 < \varepsilon_1 < \frac{1}{2}$, $\varepsilon_1 < \varepsilon_2 < 1$.

Step 0: Initiation. Choose the starting point $x_0 \in \mathcal{R}^N$, define starting matrix $H_0 = H_0^0 = I$ 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), $g_{k+1} = \nabla f(x_{k+1})$, $y_k = g_{k+1} - g_k$, b_k, $H_k y_k$ (by the modified Strang recurrences, using matrices $\{H_i^k\}_{i=0}^{\min(k,m)}$) and a_k.

Step 2: Update preparation. Choose parameter $\eta_k \geq 0$ of the Broyden class update and define $\tilde{V}_k$ by (2.1).

Step 3: Update definition. Set $\tilde{m} = \min(k, m-1)$ and define $H_0^{k+1} = (b_k/|y_k|^2)\, I$ and $H_{k+1} \equiv H_{\tilde{m}+1}^{k+1}$ by

$$H_{i+1}^{k+1} = (1/b_j) s_j\, s_j^T + \tilde{V}_j H_i^{k+1} \tilde{V}_j^T, \quad j = k - \tilde{m} + i, \quad 0 \leq i \leq \tilde{m}. \tag{4.1}$$

Step 4: Direction vector. Set $k := k+1$ and compute $d_k = -H_k g_k$ by the modified Strang recurrences, using matrices $\{H_i^k\}_{i=0}^{\min(k,m)}$, and go to Step 1.

Algorithm 4.2 (Simple transformation)

Step 2: Transformation. Choose parameter $\eta_k \geq 0$ of the Broyden class update satisfying $\mu_k \geq 0$. Using Theorem 2.1, compute α_k and $\hat{s}_k$ and define $\check{V}_k$ (with the minus sign in α_k and $\check{V}_k$).

Step 3: Update definition. Set $\tilde{m} = \min(k, m-1)$ and define $H_0^{k+1} = (b_k/|y_k|^2)\, I$ and $H_{k+1} \equiv H_{\tilde{m}+1}^{k+1}$ by

$$H_{i+1}^{k+1} = (\eta_j/b_j) \hat{s}_j \hat{s}_j^T + \check{V}_j H_i^{k+1} \check{V}_j^T, \quad j = k - \tilde{m} + i, \quad 0 \leq i \leq \tilde{m}. \tag{4.2}$$

Algorithm 4.3 (Full transformation)

Step 2: Transformation. Choose parameter $\eta_k \geq 0$ of the Broyden class update satisfying $\mu_k > 0$. Using Theorem 2.2, compute α_k, $\hat{b}_k$, $\hat{c}_k$, β_k, $\hat{s}_k$, $\hat{y}_k$ and $\hat{\varrho}_k$ and define $\hat{V}_k$.

Step 3: Update definition. Set $\tilde{m} = \min(k, m-1)$ and define $H_0^{k+1} = (b_k/|y_k|^2)\, I$ and $H_{k+1} \equiv H_{\tilde{m}+1}^{k+1}$ by

$$H_{i+1}^{k+1} = (\hat{\varrho}_j/\hat{b}_j) \hat{s}_j \hat{s}_j^T + \hat{V}_j H_i^{k+1} \hat{V}_j^T, \quad j = k - \tilde{m} + i, \quad 0 \leq i \leq \tilde{m}. \tag{4.3}$$

We saw in Section 2 that one matrix by vector multiplication can be saved if we express the next direction vector d_+ as a linear combination of vectors s, Hy. But since assumption $d = -Hg$ of Lemma 2.1 is not appropriate to LM updates, see Section 1, this approach cannot be used for our methods directly. If we calculate vector Hy by the modified Strang recurrences, then (2.11) gives only a poor approximation of td_+. It is interesting that we get much better results when we instead of Hy calculate vector Hg_+ (or almost any combination of Hy, Hg_+) and use them to approximate $Hy = Hg_+ - Hg \approx Hg_+ + d$.

But it is necessary to realize that a such approximation of vector Hy and value $a = y^T Hy$ obtained in this way need not possess the same properties as true Hy and

a in VM methods, e.g. $a > 0$, $ac \geq b^2$, etc. Similarly, the value $d_+^T g_+$ could be positive occasionally. To have direction vector d_+ descending, we can use Theorem 2.3, which guarantees $d_+^T g_+ < 0$ even in case that we approximate value $p^T y$ by any positive number.

We can see from the second expression of $-d_+$ in (2.16) that value $t\,p^T y$ has influence only on the scaling of $\eta - 1$. Thus, if the calculated value of $p^T y$ is negative or near to zero, we can replace it by some suitable number. Our numerical experiments indicate that the choice of the lower bound for $t\,p^T y$ is not critical and that this approach is not suitable for Algorithm 4.3, but with Algorithm 4.2 gives very good results, see Section 6.

Efficiency of this family of methods can be increased by introducing a scaling parameter for initiation of matrix H_+. It can be readily verified that the standard Broyden class update of matrix H with parameter η can be expressed in the interesting form

$$H_+ = (1/b)ss^T + V\bar{H}V^T, \quad \bar{H} = H + [(\eta - 1)/a]Hyy^T H,$$

i.e. as the BFGS update of matrix $\bar{H}$. Since recommended scaling parameter for the BFGS update of $\bar{H}$ is (see [4]) $b/y^T\bar{H}y = (1/\eta)[\,b/y^T Hy]$, we scale H_0^k by $1/\eta_k$ in Step 3 of the next algorithm for $\eta_k \leq 1$, while for $\eta_k > 1$, value $(\eta_k + 1/\eta_k)/2$ appears to be more suitable than $1/\eta_k$.

To distinguish between approximate and true quantities, we will denote $\tilde{\tilde{H}}y$ an approximation of Hy (matrix $\tilde{\tilde{H}}$ alone is never used and need not be defined), $\tilde{\tilde{a}}$ an approximation of a and similarly as in (2.2) and Theorem 2.1

$$\tilde{\tilde{\omega}} = 1 + \frac{\tilde{\tilde{a}}}{b}\eta, \quad \tilde{\tilde{\mu}} = \eta + (1-\eta)\frac{b}{\tilde{\tilde{a}}}, \quad \tilde{\tilde{\alpha}} = \frac{\eta - \sqrt{\tilde{\tilde{\mu}}}}{\tilde{\tilde{\omega}}}, \quad \tilde{\tilde{s}} = s - \tilde{\tilde{\alpha}}\tilde{\tilde{H}}y, \quad \tilde{\tilde{V}} = I - \frac{\sqrt{\tilde{\tilde{\mu}}}}{b}\,\tilde{\tilde{s}}\,y^T. \tag{4.4}$$

Now we state the corresponding procedure in details. Note that matrix H is replaced here by $\tilde{H}$ to indicate that it is not used to calculation of the direction vector.

Algorithm 4.4 (Simple transformation, approximate direction vector)

Data: The number m of VM updates per iteration, line search parameters ε_1 and ε_2, $0 < \varepsilon_1 < \frac{1}{2}$, $\varepsilon_1 < \varepsilon_2 < 1$.

Step 0: Initiation. Choose the starting point $x_0 \in \mathcal{R}^N$, define starting matrix $\tilde{H}_0 = H_0^0 = I$ 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), $g_{k+1} = \nabla f(x_{k+1})$, $y_k = g_{k+1} - g_k$, b_k and $s_k^T g_{k+1}$.

Step 2: Approximation. Compute $p_k = \tilde{H}_k V_k^T g_{k+1}$ by the modified Strang recurrences, using matrices $\{H_i^k\}_{i=0}^{\min(k,m)}$, and set $\delta_k = \max(t_k p_k^T y_k, b_k)$. Define $\tilde{\tilde{H}}_k y_k = -(p_k + s_k/t_k)b_k/s_k^T g_k$ and $\tilde{\tilde{a}}_k = -(\delta_k + b_k)b_k/(t_k s_k^T g_k)$.

Step 3: Transformation. Choose parameter $\eta_k > 0$ of the Broyden class update satisfying $\mu_k \geq 0$. Using (4.4), compute $\tilde{\tilde{\alpha}}_k$ and $\tilde{\tilde{s}}_k$ and define $\tilde{\tilde{V}}_k$. If $\eta_k \leq 1$ set $\gamma_k = 1/\eta_k$, otherwise set $\gamma_k = (\eta_k + 1/\eta_k)/2$.

Step 4: Update definition. Set $\tilde{m} = \min(k, m-1)$ and define $H_0^{k+1} = \gamma_k(b_k/|y_k|^2)\, I$ and $\tilde{H}_{k+1} \equiv H_{\tilde{m}+1}^{k+1}$ by

$$H_{i+1}^{k+1} = (\eta_j/b_j)\ \tilde{\tilde{s}}_j\, (\tilde{\tilde{s}}_j)^T + \tilde{\tilde{V}}_j\, H_i^{k+1} (\tilde{\tilde{V}}_j)^T, \quad j = k - \tilde{m} + i, \quad 0 \le i \le \tilde{m}\,. \quad (4.5)$$

Step 5: Direction vector. Compute d_{k+1} by the first relation in (2.13) and then set $k := k+1$. Go to Step 1.

Finally we give the procedure based on Section 3. As we mentioned there, we choose the sign of σ in accordance with the sign of $-ts_-^T g \approx s^T y_-$, see Lemma 3.1 and Lemma 3.2. Since $s^T y_- = s_-^T y$ for f quadratic, see the proof of Lemma 3.1, we prefer the sign of $s_-^T y$ in case that $|ts_-^T g|$ is too small in comparison with $|s_-^T y|$ (constant 20 in Step 2 was found empirically). Using Lemma 3.3, we bound $|\sigma|$ to have $\bar{b}$ not too small, compared with b.

Algorithm 4.5 (Preceding vectors used)

Data: The number m of VM updates per iteration, upper bound $\overline{\sigma} \in (0,1)$ for $|\sigma_k|$, safeguard parameter $\lambda \in (0,1)$ and line search parameters ε_1 and ε_2, $0 < \varepsilon_1 < \frac{1}{2}$, $\varepsilon_1 < \varepsilon_2 < 1$.

Step 0: Initiation. Choose the starting point $x_0 \in \mathcal{R}^N$, define 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.

Step 2: Update preparation. If $|s_-^T y| > 20t|s_-^T g|$ set $\nu_k = \mathrm{sgn}(s_-^T y)$, otherwise set $\nu_k = -\mathrm{sgn}(s_-^T g)$. Choose parameter $\check{\sigma}_k \in [0, \overline{\sigma}]$ and set $\sigma_k = \nu_k\, \check{\sigma}_k$. If $\sigma_k\, s_-^T y > \lambda\sqrt{bb_-}$ set $\sigma_k = \lambda\nu_k\sqrt{bb_-}/|s_-^T y|$. Using Theorem 3.1, compute $\bar{b}_k$, $\bar{s}_k$ and $\bar{\varrho}_k$ and define $\bar{V}_k$.

Step 3: Update definition. Set $\tilde{m} = \min(k, m-1)$ and define $H_0^{k+1} = (b_k/|y_k|^2)\, I$ and $H_{k+1} \equiv H_{\tilde{m}+1}^{k+1}$ by

$$H_{i+1}^{k+1} = (\bar{\varrho}_j/\bar{b}_j)\bar{s}_j\, \bar{s}_j^T + \bar{V}_j H_i^{k+1} \bar{V}_j^T, \quad j = k - \tilde{m} + i, \quad 0 \le i \le \tilde{m}\,. \qquad (4.6)$$

Step 4: Direction vector. Set $k := k+1$ and compute $d_k = -H_k g_k$ by the modified Strang recurrences, using matrices $\{H_i^k\}_{i=0}^{\min(k,m)}$, and go to Step 1.

5 Global convergence

In this section we establish global convergence of our methods, excepting Algorithm 4.1, which is the least efficient, see Section 6. Note that no our new LM method belongs to the Broyden class, see Section 2 and Section 3, therefore the usual approach must be modified. The following general lemma plays basic role.

Lemma 5.1. *Let matrix A be symmetric positive definite, $\vartheta > 0$, $\tau \neq 0$, $u \in \mathcal{R}^N$ and $v \in \mathcal{R}^N$. Then update A_+ given by*

$$A_+ = \tau^2 \vartheta\, uu^T + \left(I - \tau\, uv^T\right) A \left(I - \tau\, vu^T\right) \qquad (5.1)$$

is positive definite and satisfies

$$\mathrm{Tr}(A_+) \;\leq\; \tau^2\vartheta|u|^2 + \mathrm{Tr}(A)\Big(1+|\tau|(|u||v|)\Big)^2, \tag{5.2}$$

$$\mathrm{Tr}(A_+^{-1}) \;\leq\; \mathrm{Tr}(A^{-1}) + |v|^2/\vartheta. \tag{5.3}$$

Proof. (i) Positive definiteness of A_+ follows directly from (5.1): Let $q \in \mathcal{R}^N$, $q \neq 0$. If $q^T u \neq 0$ then $q^T A_+ q \geq \tau^2\vartheta(q^T u)^2 > 0$, otherwise $q^T A_+ q = q^T A q > 0$.

(ii) Relation (5.1) can be rewritten in the form

$$A_+ \;=\; A + \tau^2\left(\vartheta + v^T A v\right) uu^T - \tau\left(Avu^T + uv^T A\right) \tag{5.4}$$

$$\;=\; A + (\tau/\phi)\left[(\phi u - Av)(\phi u - Av)^T - Avv^T A\right], \tag{5.5}$$

where $\phi = \tau(\vartheta + v^T A v)$. From (5.4) we get (5.2) by

$$\mathrm{Tr}(A_+) \leq \mathrm{Tr}(A) + \tau^2(\vartheta + \mathrm{Tr}(A)|v|^2)|u|^2 + 2|\tau|\mathrm{Tr}(A)(|u||v|).$$

(iii) The form (5.5) of update enables us to use identity

$$\Big(I + (\bar u - \bar v)(\bar u - \bar v)^T - \bar v\bar v^T\Big)^{-1} = I + \frac{\bar v \bar v^T}{1-|\bar v|^2} - \frac{(\bar u - \theta\bar v)(\bar u - \theta\bar v)^T}{|\bar u|^2 + \theta^2(1-|\bar v|^2)}, \quad \theta = \frac{1-\bar u^T\bar v}{1-|\bar v|^2}, \tag{5.6}$$

for $|\bar v| \neq 1$, $|\bar u|^2 + \theta^2(1-|\bar v|^2) \neq 0$. Setting $\bar u = \sqrt{\tau\phi}\,A^{-1/2}u$ and $\bar v = \sqrt{\tau/\phi}\,A^{1/2}v$, we have $1 - |\bar v|^2 = 1 - (\tau/\phi)v^T A v = (\tau/\phi)(\phi/\tau - v^T A v) = (\tau/\phi)\vartheta > 0$, therefore we can see from (5.6) that $\mathrm{Tr}(A_+^{-1}) - \mathrm{Tr}(A^{-1})$ consists of one positive and one negative term, which leads to $\mathrm{Tr}(A_+^{-1}) - \mathrm{Tr}(A^{-1}) \leq |A^{-1/2}\bar v|^2/(1-|\bar v|^2) = (\tau/\phi)|v|^2/[(\tau/\phi)\vartheta] = |v|^2/\vartheta$. □

First we will investigate update (4.2) with the minus sign in α and $\check V$, see Theorem 2.1, in the simplified form - we omit index j and write $\ddot H$ and $\ddot H_+$ instead of H_i^{k+1} and H_{i+1}^{k+1}:

$$\ddot H_+ = (\eta/b)\hat s\hat s^T + \Big[I - \Big(\sqrt{\mu}/b\Big)\hat s y^T\Big]\ddot H\Big[I - \Big(\sqrt{\mu}/b\Big)y\hat s^T\Big], \quad \hat s = s - \alpha H y. \tag{5.7}$$

We will use the following assumptions, where $\bar\eta > 1$ and $\Delta > 1$ are given constants and $\eta_{SR1} = b/(b-a)$ is the value of the Broyden class parameter for the SR1 method, see [4].

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. $0 < \underline{G} \leq \underline{\lambda}(G(x)) \leq \overline{\lambda}(G(x)) \leq \overline{G} < \infty$, $x \in \mathcal{R}^N$, where $\underline{\lambda}(G(x))$ and $\overline{\lambda}(G(x))$ are the lowest and the greatest eigenvalues of the Hessian matrix $G(x)$).*

Assumption 5.2. *Parameter η of the Broyden class update is always chosen in such a way that $\eta \in [\eta_{min}, \eta_{max}]$ and*

$$|\hat s| \leq |s|\,\Delta\,, \tag{5.8}$$

where $\eta_{min} = \max(1/\bar\eta, 1/[1 + (\bar\eta - 1)a/b]) \in (0,1)$, $\eta_{max} = \bar\eta$ for $b \leq a$, $\eta_{max} = \min(\bar\eta, \eta_{SR1})$ otherwise.

Note that we can always choose η such that (5.8) is satisfied, e.g. by the choice $\eta = 1$, when we have $\hat{s} = s$. Our numerical experiments indicate that condition (5.8) has only negligible influence in practice - we have tested a great number of updates, using a collection of relatively difficult problems with $N = 1000$, and found that value $|\hat{s}|/|s|$ was very rarely greater than 10.

Lemma 5.2. *Let objective function f satisfy Assumption 5.1. Then* $\underline{G} \le b/|s|^2 \le |y|^2/b \le \overline{G}$.

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

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

by Assumption 5.1. Similarly, $b/|s|^2 = s^T G_I s/s^T s = \int_0^1 s^T G(x+\xi s)s/s^T s\, d\xi \in [\,\underline{G}, \overline{G}\,]$ and the rest follows from the Schwarz inequality. □

Lemma 5.3. *Let parameter η satisfy Assumption 5.2. Then* $\mu/\eta \in [\,0, \bar{\eta}\,]$.

Proof. Let $b > a$. From $\eta \in [\eta_{min}, \eta_{max}] \subset [1/(1+(\bar{\eta}-1)a/b), b/(b-a)]$ we obtain

$$\frac{\mu}{\eta} = 1 - \frac{b}{a} + \frac{b/a}{\eta} \in \left[1 - \frac{b}{a} + \frac{b-a}{a}, 1 - \frac{b}{a} + \frac{b}{a}\left(1 + (\bar{\eta}-1)\frac{a}{b}\right)\right] = [\,0, \bar{\eta}\,]$$

by (2.2). If $b \le a$ then obviously $\mu/\eta > 0$ and in the same way as above we get $\mu/\eta \le \bar{\eta}$. □

Theorem 5.1. *Let objective function f satisfy Assumption 5.1 and parameter η satisfy Assumption 5.2. Then Algorithm 4.2 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) By Assumption 5.2, Lemma 5.2 and Lemma 5.3 we get $|\hat{s}|^2/b \le \Delta^2/\underline{G}$, $\mu = (\mu/\eta)\eta \le \bar{\eta}^2$, $|y|^2/b \le \overline{G}$. Applying Lemma 5.1 to (5.7) with $A = \ddot{H}$, $u = \hat{s}$, $v = y$, $\tau = \sqrt{\mu}/b$ and $\vartheta = \eta b/\mu$, we obtain

$$\mathrm{Tr}(\ddot{H}_+) \le \frac{\eta|\hat{s}|^2}{b} + \mathrm{Tr}(\ddot{H})\Big(1 + \sqrt{\mu}(|\hat{s}||y|)/b\Big)^2 \le \frac{\bar{\eta}}{\underline{G}}\Delta^2 + \mathrm{Tr}(\ddot{H})\Big(1 + \bar{\eta}\,\Delta\sqrt{\overline{G}/\underline{G}}\,\Big)^2, \quad (5.9)$$

$$\mathrm{Tr}(\ddot{H}_+^{-1}) \le \mathrm{Tr}(\ddot{H}^{-1}) + (|y|^2/b)(\mu/\eta) \le \mathrm{Tr}(\ddot{H}^{-1}) + \bar{\eta}\overline{G}. \quad (5.10)$$

(ii) Let $g_k \ne 0$ and $B_i^{k+1} = (H_i^{k+1})^{-1}$, $k \ge 0$, $0 \le i \le \tilde{m}+1$, where $\tilde{m} = \min(k, m-1)$. Since $B_0^{k+1} = (|y|_k^2/b_k)I$ and $|y|_k^2/b_k \le \overline{G}$ by Lemma 5.2, we get by (5.10)

$$\mathrm{Tr}(B_{k+1}) = \mathrm{Tr}(B_{\tilde{m}+1}^{k+1}) \le (N + m\bar{\eta})\,\overline{G} \triangleq C_1, \quad k \ge 0. \quad (5.11)$$

Similarly, denoting $C_0 = \Big(1 + \bar{\eta}\,\Delta\sqrt{\overline{G}/\underline{G}}\Big)^2$, $C_3 = \bar{\eta}\Delta^2/\underline{G}$ and $C_4 = N/\underline{G}$, we have $\mathrm{Tr}(H_0^{k+1}) = \mathrm{Tr}\Big((b_k/|y|_k^2)I\Big) \le C_4$ by Lemma 5.2, therefore by (5.9) we obtain

$$\mathrm{Tr}(H_{k+1}) = \mathrm{Tr}(H_{\tilde{m}+1}^{k+1}) \le C_4 C_0^m + C_3(1 + C_0 + \ldots + C_0^{m-1}) \triangleq C_2,$$

$k \geq 0$. From this and (5.11) we get

$$\frac{(s_k^T B_k s_k)^2}{|s_k|^2 |B s_k|^2} = \frac{s_k^T B_k s_k}{|s_k|^2} \frac{s_k^T B_k s_k}{|B s_k|^2} \geq \frac{1}{C_2 C_1}, \tag{5.12}$$

$k > 0$, which implies $\lim_{k\to\infty} |g_k| = 0$, see [2]. □

As regards Algorithm 4.3, we investigate update (4.3) also in the simplified form, which respects the fact that matrix H contained in $\hat{s}$ differs from current VM matrix $\ddot{H}$ (and similarly for B in $\hat{y}$ and $\ddot{H}^{-1}$)

$$\ddot{H}_+ = \frac{\hat{\varrho}}{\hat{b}} \hat{s}\hat{s}^T + \left(I - \frac{1}{\hat{b}}\hat{s}\hat{y}^T\right) \ddot{H} \left(I - \frac{1}{\hat{b}}\hat{y}\hat{s}^T\right), \quad \hat{s} = s - \alpha H y, \quad \hat{y} = y - \beta B \hat{s}, \tag{5.13}$$

where α, β, $\hat{b}$ and $\hat{\varrho}$ are defined in Theorem 2.2. To establish global convergence, we use an additional assumption.

Assumption 5.3. *Parameter η of the Broyden class update always satisfies*

$$|\hat{y}| \leq |y|\Delta\,. \tag{5.14}$$

Note that condition (5.14) is satisfied e.g. for $\eta = 1$, when $\hat{y} = y$. Using a collection of relatively difficult problems with $N = 1000$, our numerical experiments indicate that influence of condition (5.14) in practice will be even smaller than for condition (5.8).

Theorem 5.2. *Let objective function f satisfy Assumption 5.1 and parameter η satisfy Assumption 5.3 and Assumption 5.2. Then Algorithm 4.3 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 find the bound for $\sqrt{\mu}\hat{\varrho}$. From (2.7) we get by the Schwarz inequality

$$\sqrt{\mu}\hat{\varrho} = \eta - \sqrt{\mu}\alpha\beta = \eta + \alpha^2 b/\hat{c} \leq \eta + \alpha^2 ba/(\hat{s}^T y)^2 = \eta + (b/a)\left[\alpha a/(b - \alpha a)\right]^2. \tag{5.15}$$

Using relations (2.6) and (2.9), we obtain $\alpha a/(b - \alpha a) = (\eta - 1)/(1 + \sqrt{\mu})$. Since we always have $|\eta - 1| < \bar{\eta}$ (for $\eta < 1$ by $\bar{\eta} > 1$), we can use Lemma 5.2 to get from (5.15)

$$\sqrt{\mu}\hat{\varrho} \leq \eta + (b/a)\,(\eta - 1)^2 \leq \bar{\eta} + (|y|^2/a)(b/|y|^2)\bar{\eta}^2 \leq \bar{\eta} + \bar{\eta}^2 \mathrm{Tr}(B)/\underline{G}\,. \tag{5.16}$$

(ii) By Lemma 5.2, Assumption 5.2, Lemma 5.3 and Assumption 5.3 we get $|\hat{s}|^2/b \leq \Delta^2/\underline{G}$, $\mu = (\mu/\eta)\eta \leq \bar{\eta}^2$ and $|\hat{y}|^2/b \leq \Delta^2 \overline{G}$. Applying Lemma 5.1 to (5.13) with $A = \ddot{H}$, $u = \hat{s}$, $v = \hat{y}$, $\tau = 1/\hat{b} = \sqrt{\mu}/b$ and $\vartheta = \hat{\varrho}\hat{b} = (\sqrt{\mu}\hat{\varrho})b/\mu \geq \eta b/\mu$ by (5.15), we obtain by (5.16) and Lemma 5.3

$$\begin{aligned} \mathrm{Tr}(\ddot{H}_+) &\leq \sqrt{\mu}\hat{\varrho}|\hat{s}|^2/b + \mathrm{Tr}(\ddot{H})\Big(1 + \sqrt{\mu}(|\hat{s}||\hat{y}|)/b\Big)^2 \\ &\leq \Big(\bar{\eta} + \bar{\eta}^2\,\mathrm{Tr}(B)/\underline{G}\Big)\,\Delta^2/\underline{G} + \mathrm{Tr}(\ddot{H})\Big(1 + \bar{\eta}\,\Delta^2\sqrt{\overline{G}/\underline{G}}\,\Big)^2, \end{aligned} \tag{5.17}$$

$$\mathrm{Tr}(\ddot{H}_+^{-1}) \leq \mathrm{Tr}(\ddot{H}^{-1}) + \frac{|\hat{y}|^2}{\hat{\varrho}\hat{b}} \leq \mathrm{Tr}(\ddot{H}^{-1}) + \frac{\mu}{\eta}\frac{|\hat{y}|^2}{b} \leq \mathrm{Tr}(\ddot{H}^{-1}) + \bar{\eta}\Delta^2\overline{G}. \tag{5.18}$$

(iii) Let $g_k \neq 0$ and $B_i^{k+1} = (H_i^{k+1})^{-1}$, $k \geq 0$, $0 \leq i \leq \tilde{m}+1$, where $\tilde{m} = \min(k, m-1)$. In view of (5.18), $B_0^{k+1} = (|y|_k^2/b_k)I$ and $|y|_k^2/b_k \leq \overline{G}$ by Lemma 5.2 we have

$$\mathrm{Tr}(B_{k+1}) = \mathrm{Tr}(B_{\tilde{m}+1}^{k+1}) \leq \Big(N + m\overline{\eta}\Delta^2\Big)\,\overline{G} \triangleq C_1, \quad k \geq 0. \tag{5.19}$$

Similarly, denoting $C_0 = \Big(1 + \overline{\eta}\,\Delta^2\sqrt{\overline{G}/\underline{G}}\,\Big)^2$, $C_3 = \Big(\overline{\eta} + \overline{\eta}^2\,C_1/\underline{G}\Big)\Delta^2/\underline{G}$ and $C_4 = N/\underline{G}$, we have $\mathrm{Tr}(H_0^{k+1}) = \mathrm{Tr}\Big((b_k/|y|_k^2)I\Big) \leq C_4$ by Lemma 5.2. Using (5.17) together with (5.19), we get $\lim\limits_{k\to\infty} |g_k| = 0$ as in the proof of Theorem 5.1. □

In case of Algorithm 4.4, we will first investigate update (4.5) in the form

$$\ddot{H}_+ = (\eta/b)\,\tilde{\tilde{s}}\,(\tilde{\tilde{s}})^T + \Big[I - \Big(\sqrt{\tilde{\tilde{\mu}}}/b\Big)\,\tilde{\tilde{s}}\,y^T\Big]\ddot{H}\Big[I - \Big(\sqrt{\tilde{\tilde{\mu}}}/b\Big)\,\tilde{\tilde{s}}\,y^T\Big]^T, \tag{5.20}$$

which is update (5.7) with μ, $\hat{s}$ replaced by $\tilde{\tilde{\mu}}$, $\tilde{\tilde{s}}$, see (4.4). Besides, the direction vector d_+ is computed by the first relation in (2.13) with $p = \tilde{H}V^Tg_+$, which we can be interpreted as

$$d_+ = -H_+g_+, \quad H_+ = (1/b)ss^T + [(b+\eta\delta)/(b+\delta)]\,V\tilde{H}V^T, \tag{5.21}$$

i.e. d_+ can be obtained from the scaled BFGS update of $\tilde{H}$, see [4] (note that Theorem 2.3 implies that the direction vector for every update of H from the Broyden class can be obtained from the suitable scaled BFGS update of H, if condition $d = -Hg$ is satisfied).

Theorem 5.3. *Let objective function f satisfy Assumption 5.1 and parameter η satisfy Assumption 5.2 with $\tilde{\tilde{a}}$ and $\tilde{\tilde{s}}$ instead of a and $\hat{s}$. Then Algorithm 4.4 generates a sequence $\{g_k\}$ that either satisfies $\lim\limits_{k\to\infty}|g_k| = 0$ or terminates with $g_k = 0$ for some k.*

Proof. (i) Obviously $\tilde{\tilde{a}} > 0$. Since $\gamma = 1/\eta$ for $\eta \leq 1$, $\gamma = (\eta + 1/\eta)/2$ for $\eta > 1$ and $1/\overline{\eta} \leq \eta \leq \overline{\eta}$ by Assumption 5.2, we always have $1/\overline{\eta} \leq \gamma \leq \overline{\eta}$.

(ii) By Lemma 5.2, Assumption 5.2 and Lemma 5.3 with $\tilde{\tilde{a}}$, $\tilde{\tilde{\mu}}$ and $\tilde{\tilde{s}}$ instead of a, μ and $\hat{s}$ we get $|\tilde{\tilde{s}}|^2/b \leq \Delta^2/\underline{G}$, $\tilde{\tilde{\mu}} = (\tilde{\tilde{\mu}}/\eta)\eta \leq \overline{\eta}^2$, $|y|^2/b \leq \overline{G}$. Applying Lemma 5.1 to (5.20) with $A = \ddot{H}$, $u = \tilde{\tilde{s}}$, $v = y$, $\tau = \sqrt{\tilde{\tilde{\mu}}}/b$ and $\vartheta = \eta b/\tilde{\tilde{\mu}}$, we obtain

$$\mathrm{Tr}(\ddot{H}_+) \leq \frac{\eta|\tilde{\tilde{s}}|^2}{b} + \mathrm{Tr}(\ddot{H})\Big(1 + \sqrt{\tilde{\tilde{\mu}}}(|\tilde{\tilde{s}}||y|)/b\Big)^2 \leq \frac{\overline{\eta}}{\underline{G}}\Delta^2 + \mathrm{Tr}(\ddot{H})\Big(1 + \overline{\eta}\,\Delta\sqrt{\overline{G}/\underline{G}}\,\Big)^2, \tag{5.22}$$

$$\mathrm{Tr}(\ddot{H}_+^{-1}) \leq \mathrm{Tr}(\ddot{H}^{-1}) + (|y|^2/b)(\tilde{\tilde{\mu}}/\eta) \leq \mathrm{Tr}(\ddot{H}^{-1}) + \overline{\eta}\overline{G}. \tag{5.23}$$

(iii) Let $g_k \neq 0$, $B_i^{k+1} = (H_i^{k+1})^{-1}$ and $\tilde{B}_{k+1} = \tilde{H}_{k+1}^{-1}$, $k \geq 0$, $0 \leq i \leq \tilde{m}+1$, where $\tilde{m} = \min(k, m-1)$. Since $\gamma_k B_0^{k+1} = (|y|_k^2/b_k)I$ and $|y|_k^2/(\gamma_k b_k) \leq \overline{\eta}\overline{G}$ by Lemma 5.2 and (i), we get by (5.23)

$$\mathrm{Tr}(\tilde{B}_{k+1}) = \mathrm{Tr}(B_{\tilde{m}+1}^{k+1}) \leq (N+m)\,\overline{\eta}\overline{G} \triangleq \tilde{C}_1, \quad k \geq 0. \tag{5.24}$$

Similarly, denoting $C_0 = \Big(1 + \overline{\eta}\,\Delta\sqrt{\overline{G}/\underline{G}}\,\Big)^2$, $C_3 = \overline{\eta}\Delta^2/\underline{G}$ and $C_4 = N\overline{\eta}/\underline{G}$, we have $\mathrm{Tr}(H_0^{k+1}) = \mathrm{Tr}\Big(\gamma_k(b_k/|y|_k^2)I\Big) \leq C_4$ by Lemma 5.2 and (i), therefore by (5.22) we obtain

$$\mathrm{Tr}(\tilde{H}_{k+1}) = \mathrm{Tr}(H_{\tilde{m}+1}^{k+1}) \leq C_4C_0^m + C_3(1 + C_0 + \ldots + C_0^{m-1}) \triangleq \tilde{C}_2, \quad k \geq 0. \tag{5.25}$$

(iv) Denote $\tilde{\gamma} = (b+\eta\delta)/(b+\delta)$. By Assumption 5.2 and $\bar{\eta} > 1$ we have $\eta \in [1/\bar{\eta}, \bar{\eta}]$ and in view of $\delta \geq b > 0$ we obtain $\tilde{\gamma} \leq \bar{\eta}$ and $1/\tilde{\gamma} \leq \bar{\eta}$. Applying Lemma 5.1 to (5.21) with $A = \tilde{\gamma}\tilde{\tilde{H}}$, $u = s$, $v = y$, $\tau = 1/b$ and $\vartheta = b$, we obtain by (5.24), (5.25) and Lemma 5.2

$$\mathrm{Tr}(B_+) \leq \mathrm{Tr}(\tilde{B})/\tilde{\gamma} + |y|^2/b \leq \bar{\eta}\tilde{C}_1 + \overline{G} \triangleq C_1,$$

$$\mathrm{Tr}(H_+) \leq \frac{|s|^2}{b} + \tilde{\gamma}\mathrm{Tr}(\tilde{H})\Big(1+|s||y|/b\Big)^2 \leq \frac{1}{\underline{G}} + \bar{\eta}\tilde{C}_2\Big(1+\sqrt{\overline{G}/\underline{G}}\,\Big)^2 \triangleq C_2,$$

i.e. $\mathrm{Tr}(B_k) \leq C_1$, $\mathrm{Tr}(H_k) \leq C_2$, $k > 0$, and we get $\lim_{k\to\infty} |g_k| = 0$ as in the proof of Theorem 5.1. □

Finally we will investigate update (4.6), again in the simplified form ($\bar{s}$, $\bar{y}$ and $\bar{b}$ are defined in Theorem 3.1)

$$\ddot{H}_+ = (\bar{\varrho}/\bar{b})\,\bar{s}\bar{s}^T + \bar{V}\ddot{H}\bar{V}^T, \quad \bar{V} = I - (1/\bar{b})\,\bar{s}\bar{y}^T, \quad \bar{\varrho} = (1-\sigma^2)\,b/\bar{b}. \tag{5.26}$$

Theorem 5.4. *Let objective function f satisfy Assumption 5.1. Then Algorithm 4.5 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) In Section 3 it was shown that safeguarding technique in Step 2 of Algorithm 4.5 according to Lemma 3.3 guarantees $\bar{b} \geq b(1-\lambda)$, which yields $\bar{\varrho} \leq 1/(1-\lambda)$, and also $|\sigma| \leq \check{\sigma}$, thus we always have $|\sigma| \leq \overline{\sigma}$. Using Lemma 5.2, we obtain

$$\begin{aligned}
|\bar{y}|^2/b &= \Big|y - \sigma\sqrt{b/b_-}\,y_-\Big|^2/b \leq 2\Big(|y|^2/b + \sigma^2|y_-|^2/b_-\Big) \leq 2\overline{G}(1+\overline{\sigma}^2)\,, \\
|\bar{s}|^2/b &= \Big|s - \sigma\sqrt{b/b_-}\,s_-\Big|^2/b \leq 2\Big(|s|^2/b + \sigma^2|s_-|^2/b_-\Big) \leq 2(1+\overline{\sigma}^2)/\underline{G}\,.
\end{aligned}$$

(ii) Applying Lemma 5.1 to (5.26) with $A = \ddot{H}$, $u = \bar{s}$, $v = \bar{y}$, $\tau = 1/\bar{b}$ and $\vartheta = \bar{\varrho}\bar{b} = b(1-\sigma^2)$, we obtain by (i)

$$\begin{aligned}
\mathrm{Tr}(\ddot{H}_+) &\leq \bar{\varrho}|\bar{s}|^2/\bar{b} + \mathrm{Tr}(\ddot{H})\Big(1+(|\bar{s}||\bar{y}|)/\bar{b}\Big)^2 \\
&\leq \frac{2(1+\overline{\sigma}^2)}{\underline{G}(1-\lambda)^2} + \mathrm{Tr}(\ddot{H})\left(1+2\frac{1+\overline{\sigma}^2}{1-\lambda}\sqrt{\overline{G}/\underline{G}}\,\right)^2, && (5.27)\\
\mathrm{Tr}(\ddot{H}_+^{-1}) &\leq \mathrm{Tr}(\ddot{H}^{-1}) + |\bar{y}|^2/[b(1-\sigma^2)] \leq \mathrm{Tr}(\ddot{H}^{-1}) + 2\overline{G}(1+\overline{\sigma}^2)/(1-\overline{\sigma}^2) && (5.28)
\end{aligned}$$

(iii) Let $g_k \neq 0$ and $B_i^{k+1} = (H_i^{k+1})^{-1}$, $k \geq 0$, $0 \leq i \leq \tilde{m}+1$, where $\tilde{m} = \min(k, m-1)$. In view of (5.28), $B_0^{k+1} = (|y|_k^2/b_k)I$ and $|y|_k^2/b_k \leq \overline{G}$ by Lemma 5.2, this yields

$$\mathrm{Tr}(B_{k+1}) = \mathrm{Tr}(B_{\tilde{m}+1}^{k+1}) \leq \Big(N + 2m(1+\overline{\sigma}^2)/(1-\overline{\sigma}^2)\Big)\,\overline{G} \triangleq C_1, \quad k \geq 0. \tag{5.29}$$

Similarly, denoting

$$C_0 = \left(1+2\frac{1+\overline{\sigma}^2}{1-\lambda}\sqrt{\overline{G}/\underline{G}}\,\right)^2, \quad C_3 = \frac{2(1+\overline{\sigma}^2)}{\underline{G}(1-\lambda)^2}, \quad C_4 = N/\underline{G},$$

we have $\mathrm{Tr}(H_0^{k+1}) = \mathrm{Tr}\Big((b_k/|y|_k^2)I\Big) \leq C_4$ by Lemma 5.2. Using (5.27) together with (5.29), we get $\lim_{k\to\infty} |g_k| = 0$ as in the proof of Theorem 5.1. □

6 Computational experiments

In this section we demonstrate the influence of parameters η and σ on the number of evaluations and computational time, using the collection of sparse and partially separable test problems from [5] (Test 14, 22 problems each) with $N = 1000$, $m = 10$, $\lambda = 1/2$ and the final precision $\|g(x^\star)\|_\infty \leq 10^{-6}$.

Results for all algorithms are given in Table 1, where 'NFE' is the total numbers of function and also gradient evaluations over all problems, 'Time' the total computational time in seconds and ϕ is the arithmetic mean of all values for each column.

η	Alg. 4.1		Alg. 4.2		Alg. 4.3		Alg. 4.4		Alg. 4.5		30σ
	NFE	Time	NFE	Time	NFE	Time	NFE	Time	NFE	Time	
0.4	24922	15.39	25571	12.20	26648	12.34	22400	8.72	22522	8.36	0
0.5	24331	14.76	24997	11.73	24951	11.56	22442	8.64	22185	8.25	1
0.6	22024	13.37	23538	11.08	23224	10.84	22654	8.78	21121	7.80	2
0.7	22688	13.73	23010	10.75	23378	10.75	21372	8.37	20751	7.72	3
0.8	22720	13.69	22850	10.61	23057	10.56	22454	8.69	20940	7.82	4
0.9	22590	13.55	22597	10.30	23705	10.93	20806	8.07	20929	7.77	5
1.0	22857	13.46	23034	10.49	22535	10.17	22219	8.64	20144	7.55	6
1.1	21608	12.84	20893	9.54	22530	10.14	21526	8.36	20579	7.62	7
1.2	22301	13.22	21611	9.72	21043	9.36	22131	8.60	22064	8.08	8
1.3	21462	12.55	21183	9.64	22528	10.07	20781	8.02	19854	7.42	9
1.4	22798	13.20	22222	9.99	20741	9.08	21423	8.00	19865	7.36	10
1.5	23139	13.43	20299	9.14	21620	9.39	22393	8.14	20068	7.49	11
1.6	22448	12.80	21074	9.40	21301	9.36	21778	7.94	21359	7.81	12
1.7	21927	12.55	22399	10.00	22757	10.03	22608	8.24	21250	7.82	13
1.8	22022	12.42	22427	9.85	21130	9.38	22073	8.03	20779	7.71	14
1.9	23155	13.07	22590	10.11	22150	9.66	21986	7.99	19754	7.28	15
2.0	21936	12.38	22766	10.07	22129	9.72	22278	8.08	20207	7.39	16
ϕ	22643	13.32	22533	10.27	22672	10.20	21960	8.31	20845	7.72	ϕ
L-BFGS: NFE= 22092 Time= 8.91											

Table 1. Influence of parameters η, σ for Test 14.

For a better comparison of two the most efficient algorithms with the L-BFGS method, we performed additional tests with problems from the widely used CUTE collection [1] with various dimensions N, $m = 10$, $\lambda = 1/2$ and the final precision $\|g(x^\star)\|_\infty \leq 10^{-6}$. The percentage increase of NFV for various values of parameters η or σ against NFV for the L-BFGS (negative values indicate that our results are better than for the L-BFGS) is given in Table 2 for Algorithm 4.4 and in Table 3 for Algorithm 4.5, where NFV is the number of function and also gradient evaluations. In the last line, the total values over all problems and their percentage increase are given.

Problem	N	NFV L-BFGS	Percentage increase of NFV for $\eta =$									
			0.5	0.6	0.7	0.8	1.2	1.3	1.4	1.5	1.6	1.7
BDQRTIC	5000	248	17	6	5	-15	-4	-34	-52	-18	-31	-39
BROYDN7D	2000	3029	-1	-2	-1	-1	1	2	3	6	8	9
CHAINWOO	1000	515	-15	-12	-13	-12	-17	-14	-17	-20	-14	-10
CURLY10	1000	5628	2	7	-1	6	3	-2	14	14	9	14
CURLY20	1000	6852	-4	-7	-4	-6	-8	-4	-6	-3	-7	-1
CURLY30	1000	7222	-4	-5	-4	-2	-3	-2	-3	-5	-5	-2
DIXMAANE	3000	249	-23	-12	-8	1	-6	-4	-3	-6	-6	-7
DIXMAANF	3000	189	79	4	-3	15	3	14	12	3	39	63
DIXMAANG	3000	188	100	2	-9	2	-1	1	0	-3	80	98
DIXMAANH	3000	185	-10	-7	7	-1	8	-4	-1	-8	-8	41
DIXMAANI	3000	881	-37	-38	-44	-62	-19	-29	-36	-42	-43	-34
DIXMAANJ	3000	317	-11	-56	0	-7	-7	9	18	16	1	-57
DIXMAANK	3000	270	16	20	0	10	5	0	-8	3	24	0
DIXMAANL	3000	263	-5	10	13	15	-12	-9	-5	-15	-5	-4
FLETCBV2	1000	944	31	-4	-2	-2	7	0	-2	28	34	-2
FMINSRF2	5625	305	3	-2	-3	1	3	-2	4	5	4	3
FMINSURF	5625	460	-3	11	-4	-3	0	-19	7	3	3	6
GENHUMPS	1000	2223	13	25	19	-7	17	6	2	28	15	7
GENROSE	1000	2393	1	0	0	-1	3	6	8	10	13	15
MOREBV	5000	116	6	6	9	11	2	1	8	1	6	-4
MSQRTALS	529	3622	-7	-8	-8	-8	-17	-6	-7	-11	-22	-10
NCB20	1010	497	2	4	-12	15	16	-6	6	2	-3	11
NCB20B	1000	1792	-9	-5	-11	-22	-8	-9	-4	-11	-12	-9
NONCVXU2	1000	3902	-10	-6	1	4	-14	-15	5	-6	4	-19
NONDQUAR	5000	4244	17	18	7	12	-7	-1	1	-9	2	2
POWER	500	110	-9	-11	-10	-9	-9	-3	-2	-5	-9	-6
QUARTC	5000	236	7	0	0	0	0	0	0	0	2	4
SINQUAD	5000	339	16	5	3	3	-8	0	11	6	14	6
SPARSINE	1000	10680	-19	-21	-13	-12	-11	-24	-18	-17	-11	-17
SPMSRTLS	4999	224	-5	-3	-2	5	0	2	3	2	0	-3
VAREIGVL	500	168	-10	-11	-9	-4	1	-4	-11	-10	-18	-13
All problems		58291	-3.6	-4.4	-4.0	-3.8	-5.3	-7.3	-3.4	-3.6	-2.3	-3.1

Table 2: CUTE - Percentage increase of NFV against L-BFGS for Algorithm 4.4.

Problem	N	NFV L-BFGS	Percentage increase of NFV for $\sigma =$									
			.05	.10	.15	.20	.25	.30	.35	.40	.45	.50
BDQRTIC	5000	248	-29	-10	-19	-43	-33	-16	-8	-18	5	-26
BROYDN7D	2000	3029	-1	-2	-3	-3	-3	-3	-2	0	2	6
CHAINWOO	1000	515	-8	-13	-19	-14	-18	-13	-20	-17	-15	-14
CURLY10	1000	5628	4	8	8	5	-5	2	-1	3	-7	-3
CURLY20	1000	6852	-6	-7	-6	-9	-9	-7	-10	-9	-7	-10
CURLY30	1000	7222	-3	-5	-5	-7	-10	-10	-5	-9	-13	-7
DIXMAANE	3000	249	-4	-3	-4	6	-4	-4	-10	2	-11	-10
DIXMAANF	3000	189	1	2	14	14	16	14	11	-2	-4	13
DIXMAANG	3000	188	11	17	9	5	10	6	13	6	6	-7
DIXMAANH	3000	185	7	12	15	10	10	7	-6	5	-4	5
DIXMAANI	3000	881	-9	-12	-17	-14	-27	-33	-40	-64	-77	-35
DIXMAANJ	3000	317	-3	-3	-4	-5	0	-9	-6	-16	17	20
DIXMAANK	3000	270	9	-5	-11	-7	7	4	16	7	37	28
DIXMAANL	3000	263	0	-8	-10	-3	-10	-13	-9	8	8	14
FLETCBV2	1000	944	28	1	-6	26	35	35	23	54	37	-4
FMINSRF2	5625	305	5	1	2	2	2	1	2	8	6	3
FMINSURF	5625	460	0	-2	4	13	-6	-18	-4	3	-3	-13
GENHUMPS	1000	2223	8	26	14	17	41	19	27	47	52	48
GENROSE	1000	2393	-2	-2	0	0	2	3	5	8	10	13
MOREBV	5000	116	3	3	-10	-7	-1	-3	-5	-2	0	5
MSQRTALS	529	3622	-22	-9	-22	3	-7	-10	-4	-12	-27	-12
NCB20	1010	497	3	33	28	7	48	10	-5	25	4	3
NCB20B	1000	1792	-5	-23	-5	-5	-8	-9	-9	-12	-9	-6
NONCVXU2	1000	3902	-11	-17	-4	4	-2	-13	-9	0	-16	-39
NONDQUAR	5000	4244	-17	3	1	3	-1	-11	3	13	-16	-10
POWER	500	110	-5	-7	-7	-5	-12	-13	-14	-13	-11	-13
QUARTC	5000	236	0	0	0	0	0	0	0	0	0	0
SINQUAD	5000	339	5	3	3	-3	10	0	1	11	-3	7
SPARSINE	1000	10680	-10	-8	-8	-4	-12	-9	-11	-15	-26	-19
SPMSRTLS	4999	224	1	0	-1	0	-5	-2	1	-2	-2	-3
VAREIGVL	500	168	-3	-4	-3	-10	-10	-15	-5	-8	-9	-11
All problems		58291	-5.6	-3.5	-3.8	-1.2	-4.0	-5.7	-4.2	-2.6	-10.2	-8.1

Table 2: CUTE - Percentage increase of NFV against L-BFGS for Algorithm 4.5.

Our limited numerical experiments indicate that

- the efficiency of Algorithm 4.2 and Algorithm 4.3 is practically the same, Algorithm 4.1 is the least efficient,
- it is possible to generalize limited-memory BFGS method with the same number both of matrix by vector multiplications and stored vectors,
- the suitable choice of parameter η (or σ) can improve efficiency of limited-memory methods, substantially for some problems.

References

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