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A modified limited-memory BNS method for unconstrained minimization based on the conjugate directions idea.[1]

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Abstract:

A modification of the limited-memory variable metric BNS method for large scale unconstrained optimization is proposed, which consist in corrections (derived from the idea of conjugate directions) of the used difference vectors for better satisfaction of previous quasi-Newton conditions. In comparison with [16], where a similar approach is used, correction vectors from more previous iterations can be applied here. For quadratic objective functions, the improvement of convergence is the best one in some sense, all stored corrected difference vectors are conjugate and the quasi-Newton conditions with these vectors are satisfied. Global convergence of the algorithm is established for convex sufficiently smooth functions. Numerical experiments demonstrate the efficiency of the new method.

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 BNS method (see [2]) 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 (QN) methods (see e.g. [13]), we utilize information from previous iterations to correct the used difference vectors and change QN conditions 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. [5], [15]).

The BNS method belongs to the variable metric (VM) or QN line search iterative methods, see [5], [10]. 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 $x_{k+1} = x_k + s_k$, $s_k = t_k d_k$, $k \ge 0$, where usually the direction vector $d_k \in \mathcal{R}^N$ is $d_k = -H_k g_k$ with a symmetric positive definite matrix H_k and stepsize $t_k > 0$ is chosen in such a way that

$$f_{k+1} - f_k \le \varepsilon_1 t_k g_k^T d_k, \qquad g_{k+1}^T d_k \ge \varepsilon_2 g_k^T d_k, \qquad k \ge 0 \tag{1.1}$$

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

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

(see [5], [10]), where $y_k = g_{k+1} - g_k$, $k \ge 0$. For $k \ge 0$ we denote

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

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

Among VM methods, the BFGS method, see [5], [10], [15], belongs to the most efficient; the update formula preserves positive definite VM matrices and can be written in the following quasi-product form

$$H_+ = (1/b) s s^T + V H V^T. \tag{1.3}$$

The BFGS method can be easily modified for large-scale optimization; the BNS and L-BFGS (see [6], [14], [7] - subroutine PLIS) methods represent its well-known limited-memory adaptations. In every iteration, we recurrently update matrix $\zeta_k I$, $\zeta_k > 0$, (without forming an approximation of the inverse Hessian matrix explicitly) by the BFGS method, using $\tilde{m}+1$ couples of vectors $(s_{k-\tilde{m}}, y_{k-\tilde{m}}), \ldots, (s_k, y_k)$ successively, where

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

and $m>1$ is a given parameter. In case of the BNS method, matrix H_+ can be explicitly expressed either in the form, see [2],

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

where $S_k = [s_{k-\tilde{m}}, \ldots, s_k]$, $Y_k = [y_{k-\tilde{m}}, \ldots, y_k]$, $D_k = \mathrm{diag}[b_{k-\tilde{m}}, \ldots, b_k]$, $(U_k)_{i,j} = (S_k^T Y_k)_{i,j}$ for $i \le j$, $(U_k)_{i,j} = 0$ otherwise (an upper triangular matrix), $k \ge 0$, or in the form, also given in [2]

$$H_+ = SU^{-T}DU^{-1}S^T + \zeta(I - SU^{-T}Y^T)(I - YU^{-1}S^T)\,, \tag{1.5}$$

thus direction vector can be efficiently calculated (without computing of matrix H_+) by

$$-H_+g_+ = -\zeta g_+ - S\Big[U^{-T}\Big((D + \zeta Y^TY)U^{-1}S^Tg_+ - \zeta Y^Tg_+\Big)\Big] + Y\Big[\zeta U^{-1}S^Tg_+\Big]\,, \tag{1.6}$$

where in brackets we multiply by low-order matrices.

The concept of conjugacy plays an important role in optimization methods based on quadratic models, see e.g. [5], [15]. It was shown in [16] that the conjugacy of consecutive vectors s, s_+ with respect to matrices B_+ can be achieved by means of suitable vector corrections, which can be understood as corrections for exact line searches, and that this approach can improve efficiency of the L-BFGS method. The used corrected difference vectors $\bar{s}_k$, $\bar{y}_k$, $k \ge 0$, are defined by $\bar{s}_0 = s_0$, $\bar{y}_0 = y_0$ and $\bar{s}_k = s_k - \alpha_k\bar{s}_{k-1}$, $\bar{y}_k = y_k - \beta_k\bar{y}_{k-1}$, $k > 0$, with suitable chosen parameters α_k, $\beta_k \in \mathcal{R}$, i.e. one correction vector from the previous iteration is used for each of difference vectors.

In this report we generalize this approach, using vectors from more previous iterations to correct vectors s, y. Unlike [16], we use here the BNS concept to calculate the direction vector, since then the increase in total number of required arithmetic operations can be relatively small compared to the BNS or L-BFGS method. We use corrected quantities $\tilde{s}_k$, $\tilde{y}_k$, $\tilde{b}_k$, $\tilde{V}_k$ and $\tilde{H}_k$, $k \ge 0$, defined by $\tilde{s}_0 = s_0$, $\tilde{y}_0 = y_0$, $\tilde{b}_0 = b_0$, $\tilde{V}_0 = V_0$, $\tilde{H}_0 = I$ and

$$\tilde{s}_k = s_k + \underline{\tilde{S}}_k\tilde{\sigma}_k, \quad \tilde{y}_k = y_k + \underline{\tilde{Y}}_k\tilde{\eta}_k, \quad \tilde{b}_k = \tilde{s}_k^T\tilde{y}_k, \quad \tilde{V}_k = I - (1/\tilde{b}_k)\tilde{s}_k\tilde{y}_k^T, \tag{1.7}$$

$k > 0$, where $\underline{\tilde{S}}_k = [\tilde{s}_{k-\tilde{m}}, \ldots, \tilde{s}_{k-1}]$, $\underline{\tilde{Y}}_k = [\tilde{y}_{k-\tilde{m}}, \ldots, \tilde{y}_{k-1}]$ and $\tilde{\sigma}_k, \tilde{\eta}_k \in \mathcal{R}^{\tilde{m}}$ are chosen in such a way that $\tilde{b}_k > 0$. Positive definite matrix $\tilde{H}_{k+1} = \tilde{H}_{k+1}^{k+1}$, $k \ge 0$, is obtained by

$$\tilde{H}_{k-\tilde{m}}^{k+1} = \zeta_k I, \qquad \zeta_k = b_k/y_k^Ty_k > 0, \tag{1.8}$$

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

i.e. by the repeated BFGS updating of matrix $\zeta_k I$ with vectors $(\tilde{s}_{k-\tilde{m}}, \tilde{y}_{k-\tilde{m}}), \ldots, (\tilde{s}_k, \tilde{y}_k)$ (columns of $\tilde{S}_k = [\underline{\tilde{S}}_k, \tilde{s}_k]$, $\tilde{Y}_k = [\underline{\tilde{Y}}_k, \tilde{y}_k]$ for $k > 0$). Matrix $\tilde{H}_{k+1}$ and auxiliary matrices $\{\tilde{H}_i^{k+1}\}_{i=k-\tilde{m}}^k$ have only the theoretical significance and are not formed explicitly.

We propose how to choose the parameters $\tilde{\sigma}_k$, $\tilde{\eta}_k$ and show that VM matrices constructed by means of difference vectors corrected in this way have some positive properties. Numerical results indicate that additional correction vectors can improve results significantly, although they can deteriorate stability, require extra arithmetic operations and have no influence on $\tilde{s}_+, \tilde{y}_+$ for quadratic functions and (the most frequent) unit stepsizes, see Sections 3 and 4. Obviously, the choice of parameters $\tilde{\sigma}_k$, $\tilde{\eta}_k$ can affect properties of matrix $\tilde{H}_{k+1}$ only within the last update in (1.9), i.e. for $i = k$.

Note that matrix $\tilde{H}_+$ satisfies the QN condition $\tilde{H}_+\tilde{y} = \tilde{s}$ and that direction vector $\tilde{d}_+ = -\tilde{H}_+g_+$ and an auxiliary vector $\tilde{Y}^TH_+g_+$ can be calculated by analogy to (1.6) by

$$-\tilde{H}_+g_+ = -\zeta g_+ - \tilde{S}\Big[\tilde{U}^{-T}\Big((\tilde{D} + \zeta\tilde{Y}^T\tilde{Y})\tilde{U}^{-1}\tilde{S}^Tg_+ - \zeta\tilde{Y}^Tg_+\Big)\Big] + \tilde{Y}\Big[\zeta\tilde{U}^{-1}\tilde{S}^Tg_+\Big], \tag{1.10}$$

$$\tilde{Y}^T\tilde{H}_+g_+ = \zeta\tilde{Y}^Tg_+ + \tilde{Y}^T\tilde{S}\Big[\tilde{U}^{-T}\Big((\tilde{D} + \zeta\tilde{Y}^T\tilde{Y})\tilde{U}^{-1}\tilde{S}^Tg_+ - \zeta\tilde{Y}^Tg_+\Big)\Big] - \tilde{Y}^T\tilde{Y}\Big[\zeta\tilde{U}^{-1}\tilde{S}^Tg_+\Big], \tag{1.11}$$

where $\tilde{D}_k = \mathrm{diag}[\tilde{b}_{k-\tilde{m}}, \dots, \tilde{b}_k]$, $(\tilde{U}_k)_{i,j} = (\tilde{S}_k^T \tilde{Y}_k)_{i,j}$ for $i \le j$, $(\tilde{U}_k)_{i,j} = 0$ otherwise (an upper triangular matrix), $k \ge 0$.

In Section 2 we investigate the last standard BFGS update in (1.9) with corrected difference vectors $\tilde{s}, \tilde{y}$ in the more general form

$$\ddot{H}_+ = (1/\tilde{b})\tilde{s}\tilde{s}^T + \tilde{V}\ddot{H}\tilde{V}^T, \tag{1.12}$$

where $\ddot{H}$ is any symmetric positive definite matrix and discuss the choice of parameters $\tilde{\sigma}_k$, $\tilde{\eta}_k$. In Section 3 we focus on quadratic functions and show optimality of our choice of parameters and a role of unit stepsizes. Application to the corrected BNS method and the corresponding algorithm are described in Section 4. Global convergence of the algorithm is established in Section 5 and numerical results are reported in Section 6. We will denote by $\|\cdot\|_F$ the Frobenius matrix norm and by $\|\cdot\|$ the spectral matrix norm.

2 Derivation of the method

Using another formulation of the conjugacy property, we give some variational and hereditary properties of the corrected BFGS update for general functions which indicate that we can expect an improvement of convergence properties also for functions near to quadratic.

If some columns of $\underline{\tilde{S}}$, $\underline{\tilde{Y}}$ are used as correction vectors in (1.7) (i.e. if some components of vector $\tilde{\sigma}$ and corresponding components of $\tilde{\eta}$ are nonzero), we denote a matrix with these selected columns of $\underline{\tilde{S}}$, $\underline{\tilde{Y}}$ by $\underline{\hat{S}}$, $\underline{\hat{Y}}$, vectors with corresponding selected (nonzero) components of $\tilde{\sigma}$, $\tilde{\eta}$ by $\hat{\sigma}$, $\hat{\eta}$ and $\hat{S} = [\underline{\hat{S}}, \tilde{s}]$, $\hat{Y} = [\underline{\hat{Y}}, \tilde{y}]$, otherwise we define $\hat{S} = [\tilde{s}]$, $\hat{Y} = [\tilde{y}]$. In this connection, we denote a set of indices i of vectors $\tilde{s}_i, \tilde{y}_i$ which form matrices $\underline{\hat{S}}_k, \underline{\hat{Y}}_k$ by $\underline{\mathcal{I}}_k$ and $\mathcal{I}_k = \underline{\mathcal{I}}_k \cup \{k\}$, $k \ge 0$.

In Section 2.2 we present some conditions and a strategy for the choice of $\underline{\hat{S}}$, $\underline{\hat{Y}}$.

2.1 The BFGS update with corrected vectors

Assuming set $\underline{\mathcal{I}}$ to be non-empty, in this section we will investigate the influence of the correction parameters $\tilde{\sigma}$, $\tilde{\eta}$ on properties of matrix $\ddot{H}_+$, given by the BFGS update (1.12) of any symmetric positive definite matrix $\ddot{H}$. For our purpose, the satisfaction of the QN conditions $\ddot{H}_+\hat{Y} = \hat{S}$ plays a crucial role (obviously, the QN condition $\ddot{H}_+\tilde{y} = \tilde{s}$ is satisfied). In this connection we will suppose that the auxiliary QN conditions $\ddot{H}\underline{\hat{Y}} = \underline{\hat{S}}$ are satisfied (therefore matrix $\underline{\hat{S}}^T\underline{\hat{Y}} = \underline{\hat{Y}}^T\ddot{H}\underline{\hat{Y}}$ is symmetric). A technique which guarantees the satisfaction of these conditions for matrices $\tilde{H}_k^{k+1}$, $k > 0$, will be presented in Section 2.2. We denote $\ddot{B} = \ddot{H}^{-1}$, $\ddot{B}_+ = \ddot{H}_+^{-1}$, $\ddot{a} = \tilde{y}^T\ddot{H}\tilde{y}$, $\ddot{c} = \tilde{s}^T\ddot{B}\tilde{s}$.

We will consider here only a case, when the possible extra components of $\tilde{\sigma}$, $\tilde{\eta}$ compared to $\hat{\sigma}$, $\hat{\eta}$ are zero. In view of (1.7) we can then write

$$\tilde{s} = s + \underline{\tilde{S}}\,\tilde{\sigma} = s + \underline{\hat{S}}\,\hat{\sigma}, \qquad \tilde{y} = y + \underline{\tilde{Y}}\,\tilde{\eta} = y + \underline{\hat{Y}}\,\hat{\eta}. \tag{2.1}$$

The following lemma shows that, under some assumptions, conditions $\ddot{H}_+\tilde{y}_i = \tilde{s}_i$, $i \in \underline{\mathcal{I}}$, are equivalent to the conjugacy of vector $\tilde{s}$ with vectors $\tilde{s}_i$ with respect to matrices $\ddot{B}, \ddot{B}_+$, i.e. $\tilde{s}^T\ddot{B}\tilde{s}_i = \tilde{s}^T\tilde{y}_i = 0$, $\tilde{s}^T\ddot{B}_+\tilde{s}_i = \tilde{s}_i^T\tilde{y} = 0$, $i \in \underline{\mathcal{I}}$, or

$$\underline{\hat{S}}^T\tilde{y} = \underline{\hat{Y}}^T\tilde{s} = 0. \tag{2.2}$$

Besides, the lemma also gives an influence of corrections on the QN conditions.

Lemma 2.1. *Let $\ddot{H}$ be any symmetric positive definite matrix satisfying $\ddot{H}\underline{\hat{Y}} = \underline{\hat{S}}$ and matrix $\ddot{H}_+$ be given by update (1.12) of $\ddot{H}$ with $\tilde{b} > 0$. Then $\ddot{H}_+$ is symmetric positive definite and*

$$\tilde{b}\,(\ddot{H}_+\tilde{y}_i - \tilde{s}_i)^T \ddot{B}_+(\ddot{H}_+\tilde{y}_i - \tilde{s}_i) = (\tilde{s}_i^T\tilde{y} - \tilde{s}^T\tilde{y}_i)^2 + (\ddot{a}/\tilde{b} - \tilde{b}/\ddot{c})\,(\tilde{s}^T\tilde{y}_i)^2, \quad i \in \underline{\mathcal{I}}, \tag{2.3}$$

where $\ddot{a}/\tilde{b} \geq \tilde{b}/\ddot{c}$, with $\ddot{a}/\tilde{b} = \tilde{b}/\ddot{c}$ in and only in the case of dependency of vectors $\tilde{s}$, $\ddot{H}\tilde{y}$.

Moreover, if $\underline{\hat{S}}^T\tilde{y} = \underline{\hat{Y}}^T\tilde{s} = 0$, then the QN condition $\ddot{H}_+\hat{Y} = \hat{S}$ is satisfied and

$$(\ddot{H}_+y - s)^T\ddot{B}_+(\ddot{H}_+y - s) = (\hat{\sigma} - \hat{\eta})^T\underline{\hat{S}}^T\underline{\hat{Y}}(\hat{\sigma} - \hat{\eta})\,. \tag{2.4}$$

Proof. (i) Since relation (1.12) is the standard BFGS update with $\tilde{s}$, $\tilde{y}$ instead of s, y, matrix $\ddot{H}_+$ is symmetric positive definite and it holds (see [5], [10])

$$\ddot{H}_+ = \ddot{H} + \left(1 + \frac{\ddot{a}}{\tilde{b}}\right)\frac{\tilde{s}\tilde{s}^T}{\tilde{b}} - \frac{\ddot{H}\tilde{y}\tilde{s}^T + \tilde{s}\tilde{y}^T\ddot{H}}{\tilde{b}}, \qquad \ddot{B}_+ = \ddot{B} + \frac{\tilde{y}\tilde{y}^T}{\tilde{b}} - \frac{\ddot{B}\tilde{s}\tilde{s}^T\ddot{B}}{\ddot{c}}\,, \tag{2.5}$$

which for $i \in \underline{\mathcal{I}}$ yields

$$\begin{aligned} \tilde{y}_i^T\ddot{H}_+\tilde{y}_i &= \tilde{b}_i + [\,(1 + \ddot{a}/\tilde{b})/\tilde{b}\,](\tilde{s}^T\tilde{y}_i)^2 - 2\,\tilde{s}_i^T\tilde{y}\,\tilde{s}^T\tilde{y}_i/\tilde{b}\,, & (2.6)\\ \tilde{s}_i^T\ddot{B}_+\tilde{s}_i &= \tilde{b}_i + (\tilde{s}_i^T\tilde{y})^2/\tilde{b} - (\tilde{s}^T\tilde{y}_i)^2/\ddot{c} & (2.7) \end{aligned}$$

by $\ddot{H}\tilde{y}_i = \tilde{s}_i$, $i \in \underline{\mathcal{I}}$. Setting it to $(\ddot{H}_+\tilde{y}_i - \tilde{s}_i)^T\ddot{B}_+(\ddot{H}_+\tilde{y}_i - \tilde{s}_i) = \tilde{y}_i^T\ddot{H}_+\tilde{y}_i + \tilde{s}_i^T\ddot{B}_+\tilde{s}_i - 2\tilde{b}_i$, we obtain (2.3). The rest of the first part follows from the Schwarz inequality.

(ii) Let $\underline{\hat{S}}^T\tilde{y} = \underline{\hat{Y}}^T\tilde{s} = 0$. Then $\ddot{H}_+\hat{Y} = \hat{S}$ by (2.3) and (1.12). From $\ddot{H}_+\tilde{y} = \tilde{s}$ we obtain

$$\begin{aligned} \ddot{H}_+y - s &= \ddot{H}_+\tilde{y} - \tilde{s} + (\tilde{s} - s) - \ddot{H}_+(\tilde{y} - y) = \underline{\hat{S}}\hat{\sigma} - \ddot{H}_+\underline{\hat{Y}}\hat{\eta} = \underline{\hat{S}}(\hat{\sigma} - \hat{\eta}),\\ \ddot{B}_+(\ddot{H}_+y - s) &= \ddot{B}_+\underline{\hat{S}}(\hat{\sigma} - \hat{\eta}) = \underline{\hat{Y}}(\hat{\sigma} - \hat{\eta}), \end{aligned}$$

which gives (2.4). □

In the sequel, we describe the solution to equations (2.2) and some its properties.

Lemma 2.2. *Let matrix $\underline{\hat{S}}^T\underline{\hat{Y}}$ be nonsingular and let*

$$\sigma^* = -\left(\underline{\hat{Y}}^T\underline{\hat{S}}\right)^{-1}\underline{\hat{Y}}^Ts, \qquad \eta^* = -\left(\underline{\hat{S}}^T\underline{\hat{Y}}\right)^{-1}\underline{\hat{S}}^Ty. \tag{2.8}$$

Then the unique solution $(\hat{\sigma}, \hat{\eta})$ to (2.2) is (σ^*, η^*). Moreover, for any $\hat{\sigma}, \hat{\eta}$ it holds

$$\tilde{b} = (\hat{\sigma} - \sigma^*)^T\underline{\hat{S}}^T\underline{\hat{Y}}(\hat{\eta} - \eta^*) + b^*, \qquad b^* = (s^*)^Ty^* = b - s^T\underline{\hat{Y}}\left(\underline{\hat{S}}^T\underline{\hat{Y}}\right)^{-1}\underline{\hat{S}}^Ty, \tag{2.9}$$

where s^*, y^* are vectors $\tilde{s}$, $\tilde{y}$ for $\hat{\sigma} = \sigma^*$, $\hat{\eta} = \eta^*$.

Proof. From (2.8) we have $\underline{\hat{Y}}^T\underline{\hat{S}}\,\sigma^* = -\underline{\hat{Y}}^Ts$ and $\underline{\hat{S}}^T\underline{\hat{Y}}\,\eta^* = -\underline{\hat{S}}^Ty$. This yields firstly $\underline{\hat{Y}}^T\underline{\hat{S}}(\hat{\sigma} - \sigma^*) = \underline{\hat{Y}}^T(\underline{\hat{S}}\hat{\sigma} + s) = \underline{\hat{Y}}^T\tilde{s}$ and $\underline{\hat{S}}^T\underline{\hat{Y}}(\hat{\eta} - \eta^*) = \underline{\hat{S}}^T(\underline{\hat{Y}}\hat{\eta} + y) = \underline{\hat{S}}^T\tilde{y}$ by (2.1), which gives the first part, and secondly

$$\begin{aligned} (\hat{\sigma} - \sigma^*)^T\underline{\hat{S}}^T\underline{\hat{Y}}(\hat{\eta} - \eta^*) &= \hat{\sigma}^T\underline{\hat{S}}^T\underline{\hat{Y}}\hat{\eta} - \hat{\sigma}^T\left(\underline{\hat{S}}^T\underline{\hat{Y}}\eta^*\right) - \left((\sigma^*)^T\underline{\hat{S}}^T\underline{\hat{Y}}\right)\hat{\eta} + \left((\sigma^*)^T\underline{\hat{S}}^T\underline{\hat{Y}}\right)\eta^*\\ &= \left(\hat{\sigma}^T\underline{\hat{S}}^T\underline{\hat{Y}}\hat{\eta} + \hat{\sigma}^T\underline{\hat{S}}^Ty + s^T\underline{\hat{Y}}\hat{\eta}\right) + s^T\underline{\hat{Y}}(\underline{\hat{S}}^T\underline{\hat{Y}})^{-1}\underline{\hat{S}}^Ty\,, \end{aligned}$$

which yields

$$\begin{aligned}\tilde b &= (\underline{\hat S}\hat\sigma+s)^T(\underline{\hat Y}\hat\eta+y) = \Big(\hat\sigma^T\underline{\hat S}^T\underline{\hat Y}\hat\eta + \hat\sigma^T\underline{\hat S}^T y + s^T\underline{\hat Y}\hat\eta\Big) + b\\ &= (\hat\sigma-\sigma^*)^T\underline{\hat S}^T\underline{\hat Y}(\hat\eta-\eta^*) + b - s^T\underline{\hat Y}(\underline{\hat S}^T\underline{\hat Y})^{-1}\underline{\hat S}^T y\end{aligned}$$

and concludes the proof. □

Since we intend to satisfy the QN condition $\ddot H_+\hat Y = \hat S$ (this condition holds for $\ddot H\underline{\hat Y} = \underline{\hat S}$ and $\underline{\hat S}^T\tilde y = \underline{\hat Y}^T\tilde s = 0$ by Lemma 2.1), which obviously implies the symmetry of matrix

$$\hat S^T\hat Y = \left[\begin{array}{cc}\underline{\hat S}^T\underline{\hat Y} & \underline{\hat S}^T\tilde y\\ \tilde s^T\underline{\hat Y} & \tilde s^T\tilde y\end{array}\right],$$

for given $\underline{\hat S}$, $\underline{\hat Y}$ we define the set $\mathcal{S}(\underline{\hat S},\underline{\hat Y}) = \{(\hat\sigma,\hat\eta):\ \underline{\hat S}^T\tilde y = \underline{\hat Y}^T\tilde s\}$. Obviously, we have $(\sigma^*,\eta^*)\in\mathcal{S}(\underline{\hat S},\underline{\hat Y})$ by Lemma 2.2 and (2.2). The following lemmas describe some basic properties of $\mathcal{S}(\underline{\hat S},\underline{\hat Y})$.

Lemma 2.3. *Let matrix $\underline{\hat S}^T\underline{\hat Y}$ be symmetric nonsingular and $(\hat\sigma,\hat\eta)\in\mathcal{S}(\underline{\hat S},\underline{\hat Y})$. Then*

$$\underline{\hat S}^T\underline{\hat Y}(\hat\sigma-\hat\eta) = \underline{\hat S}^T y - \underline{\hat Y}^T s, \tag{2.10}$$

thus the difference $\hat\sigma$–$\hat\eta$ is firmly determined by matrices $\underline{\hat S}, \underline{\hat Y}$ and vectors s, y. Moreover, if $\underline{\hat S}^T\underline{\hat Y}$ is positive definite, value $\tilde b$ is minimized by the choice $\hat\sigma=\sigma^*$, $\hat\eta=\eta^*$, given by (2.8).

Proof. From $(\hat\sigma,\hat\eta)\in\mathcal{S}(\underline{\hat S},\underline{\hat Y})$ and (2.1) we get $\underline{\hat S}^T(y+\underline{\hat Y}\,\hat\eta) = \underline{\hat Y}^T(s+\underline{\hat S}\,\hat\sigma)$, i.e. (2.10), which gives the first assertion. Further, this implies $\hat\sigma-\hat\eta = \sigma^*-\eta^*$, i.e. $\hat\sigma-\sigma^* = \hat\eta-\eta^*$. Thus for $\underline{\hat S}^T\underline{\hat Y}$ positive definite we get the second assertion by the first relation in (2.9). □

Lemma 2.4. *Let $\ddot H$ be any symmetric positive definite matrix satisfying $\ddot H\underline{\hat Y} = \underline{\hat S}$, matrix $\underline{\hat S}^T\underline{\hat Y}$ be nonsingular and $(\hat\sigma,\hat\eta)\in\mathcal{S}(\underline{\hat S},\underline{\hat Y})$. Then*

- *(a) $\underline{\hat S}^T\underline{\hat Y}$ is symmetric positive definite,*
- *(b) the differences $\tilde s - \ddot H\tilde y$, $\ddot B\tilde s - \tilde y$, $\tilde b - \ddot a$, $\ddot c - \tilde b$ are firmly determined by matrices $\underline{\hat S}$, $\underline{\hat Y}$, $\ddot H$ plus vectors s, y,*
- *(c) values $\ddot a$, $\ddot c$ are minimized by the choice $\hat\sigma=\sigma^*$, $\hat\eta=\eta^*$, given by (2.8).*

Proof. Matrix $\underline{\hat S}^T\underline{\hat Y}$ is symmetric positive definite by its nonsingularity and by $\ddot H\underline{\hat Y}=\underline{\hat S}$, i.e. (a) holds. Using (2.1) and $\ddot H\underline{\hat Y}=\underline{\hat S}$, we can write

$$\begin{aligned}\tilde b - \ddot a &= \tilde y^T(\tilde s - \ddot H\tilde y) = y^T(\tilde s - \ddot H\tilde y) + \hat\eta^T\underline{\hat Y}^T(\tilde s - \ddot H\tilde y) = y^T(\tilde s - \ddot H\tilde y) + \hat\eta^T(\underline{\hat Y}^T\tilde s - \underline{\hat S}^T\tilde y),\\ \ddot c - \tilde b &= \tilde s^T(\ddot B\tilde s - \tilde y) = s^T(\ddot B\tilde s - \tilde y) + \hat\sigma^T\underline{\hat S}^T(\ddot B\tilde s - \tilde y) = s^T(\ddot B\tilde s - \tilde y) + \hat\sigma^T(\underline{\hat Y}^T\tilde s - \underline{\hat S}^T\tilde y).\end{aligned}$$

Observing that $\tilde s - \ddot H\tilde y = s - \ddot H y + \underline{\hat S}(\hat\sigma-\hat\eta)$ by $\ddot H\underline{\hat Y} = \underline{\hat S}$, $\ddot B\tilde s - \tilde y = \ddot B(\tilde s - \ddot H\tilde y)$ and using Lemma 2.3, we get (b) by $(\hat\sigma,\hat\eta)\in\mathcal{S}(\underline{\hat S},\underline{\hat Y})$. From (a), Lemma 2.3, $\ddot a = \tilde b - (\tilde b - \ddot a)$, $\ddot c = \tilde b + (\ddot c - \tilde b)$ and (b) we obtain (c). □

Note that this lemma has an interesting implication. Since the SR1 VM method with $\tilde s, \tilde y$ instead of s, y adds to $\ddot H$ a symmetric rank one matrix which contains only expressions $\tilde s - \ddot H\tilde y$, $\tilde b - \ddot a$, see [5], [15], matrix $\ddot H_+$ is independent of the choice $(\hat\sigma,\hat\eta)\in\mathcal{S}(\underline{\hat S},\underline{\hat Y})$ for the corrected SR1 method.

Although variational characterizations of the choice $\hat{\sigma} = \sigma^*$, $\hat{\eta} = \eta^*$ are significant mainly for quadratic functions, see Section 3, the following theorem indicates that we can expect good convergence properties of this choice also for functions near to quadratic.

Theorem 2.1. *Let $\ddot{H}$ be any symmetric positive definite matrix satisfying $\ddot{H}\underline{\hat{Y}} = \underline{\hat{S}}$, matrix $\ddot{H}_+$ be given by update (1.12) of $\ddot{H}$, matrix $\underline{\hat{S}}^T\underline{\hat{Y}}$ be nonsingular and $b^* > 0$. Then $\tilde{b} > 0$ for any $(\hat{\sigma}, \hat{\eta}) \in \mathcal{S}(\underline{\hat{S}}, \underline{\hat{Y}})$. Moreover, if we have a symmetric positive definite matrix $\ddot{G}$ such that $\ddot{G}\underline{\hat{S}} = \underline{\hat{Y}}$ and $\ddot{G}(s + \underline{\hat{S}}\ddot{\sigma}) = y + \underline{\hat{Y}}\ddot{\eta}$ for some $(\ddot{\sigma}, \ddot{\eta}) \in \mathcal{S}(\underline{\hat{S}}, \underline{\hat{Y}})$, then*

(a) $\ddot{G}\tilde{s} = \tilde{y}$ for all $(\hat{\sigma}, \hat{\eta}) \in \mathcal{S}(\underline{\hat{S}}, \underline{\hat{Y}})$,

(b) within $(\hat{\sigma}, \hat{\eta}) \in \mathcal{S}(\underline{\hat{S}}, \underline{\hat{Y}})$ it holds

$$\|\ddot{G}^{1/2}\ddot{H}_+\ddot{G}^{1/2} - I\|_F^2 = (\tilde{b} - \ddot{a})^2/\tilde{b}^2 - 2\left|\ddot{G}^{1/2}(\tilde{s} - \ddot{H}\tilde{y})\right|^2/\tilde{b} + \|\ddot{G}^{1/2}\ddot{H}\ddot{G}^{1/2} - I\|_F^2, \qquad (2.11)$$

(c) value (2.11) is minimized by the choice $\hat{\sigma} = \sigma^*$, $\hat{\eta} = \eta^*$, given by (2.8).

Proof. (i) Let $(\hat{\sigma}, \hat{\eta}) \in \mathcal{S}(\underline{\hat{S}}, \underline{\hat{Y}})$. In view of Lemma 2.4, matrix $\underline{\hat{S}}^T\underline{\hat{Y}}$ is symmetric positive definite and we can use Lemma 2.3 and assumption $b^* > 0$ to obtain $\tilde{b} \geq b^* > 0$.

(ii) Let $\ddot{G}(s + \underline{\hat{S}}\ddot{\sigma}) = y + \underline{\hat{Y}}\ddot{\eta}$. Using Lemma 2.4 with $\ddot{G}^{-1}$ instead of $\ddot{H}$, we see that the difference $\ddot{G}\tilde{s} - \tilde{y}$ is independent of $(\hat{\sigma}, \hat{\eta}) \in \mathcal{S}(\underline{\hat{S}}, \underline{\hat{Y}})$, thus equal to zero for $(\hat{\sigma}, \hat{\eta}) \in \mathcal{S}(\underline{\hat{S}}, \underline{\hat{Y}})$ by $\ddot{G}(s + \underline{\hat{S}}\ddot{\sigma}) = y + \underline{\hat{Y}}\ddot{\eta}$, i.e. (a) holds.

Denoting $w = \ddot{G}^{1/2}\tilde{s}$, $w_* = \ddot{G}^{1/2}s^*$, $W = \ddot{G}^{1/2}\ddot{H}\ddot{G}^{1/2}$, $W_+ = \ddot{G}^{1/2}\ddot{H}_+\ddot{G}^{1/2}$ and $M = I - W$, we have $|w|^2 = \tilde{b} \geq b^* = |w_*|^2 > 0$ and (1.12) can be written in the form

$$W_+ = (1/|w|^2)ww^T + PWP = I - PMP, \qquad P = I - (1/|w|^2)ww^T, \qquad (2.12)$$

by $\ddot{G}\tilde{s} = \tilde{y}$ and $P^2 = P$. In view of the fact that the trace of a product of two square matrices is independent of the order of the multiplication, from (2.12) we obtain

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

i.e. (b) by $Mw = \ddot{G}^{1/2}(\tilde{s} - \ddot{H}\tilde{y})$ and $w^TMw = \tilde{b} - \ddot{a}$. Function

$$\varphi(\xi) = (w_*^TMw_*)^2/|w_*|^4\xi^2 - 2|Mw_*|^2/|w_*|^2\xi + \|M\|_F^2 \qquad (2.13)$$

is nonincreasing on $[0, 1]$, since $\varphi'(\xi) = 2[(w_*^TMw_*)^2/|w_*|^4\xi - |Mw_*|^2/|w_*|^2] \leq 0$ for $\xi \in [0, 1]$ by the Schwarz inequality. Using Lemma 2.4, we can write $\|I - W_+\|_F^2 = \varphi(|w_*|^2/|w|^2)$ and this value is minimized for such $(\hat{\sigma}, \hat{\eta})$ which maximizes $|w_*|/|w|$, i.e. for $\hat{\sigma} = \sigma^*$, $\hat{\eta} = \eta^*$, thus (c) holds. □

2.2 The choice of correction difference vectors

Applying theory from Section 2.1 to matrices $\tilde{H}_{k+1}$, $\tilde{H}_k^{k+1}$, $k > 0$, in the last update (1.9), assumptions of Theorem 2.2 give a simple strategy for choosing matrices $\hat{S}, \hat{Y}$ which guarantees the satisfaction of the QN conditions $\tilde{H}_{k+1}\hat{Y}_k = \hat{S}_k$ and the auxiliary QN conditions $\tilde{H}_k^{k+1}\underline{\hat{Y}}_k = \underline{\hat{S}}_k$ ($\ddot{H}_+\hat{Y} = \hat{S}$ and $\ddot{H}\underline{\hat{Y}} = \underline{\hat{S}}$ in Section 2.1) in all iterations. Note that assertion (a) of the following theorem implies that matrices $\hat{S}_k^T\hat{Y}_k$ are diagonal, $k > 0$.

Theorem 2.2. *Suppose that each set $\underline{\mathcal{I}}_k$, $k>0$, is chosen in such a way that $\underline{\mathcal{I}}_k \subset \mathcal{I}_{k-1}$, $\tilde{b}_k > 0$ and $\hat{\underline{S}}_k^T \tilde{y}_k = \hat{\underline{Y}}_k^T \tilde{s}_k = 0$ in case that $\underline{\mathcal{I}}_k \neq \emptyset$. Then for $k>0$*

(a) $\tilde{s}_i^T \tilde{y}_j = \tilde{y}_i^T \tilde{s}_j = 0$ for $i \in \underline{\mathcal{I}}_k$, $i < j \le k$,

(b) the QN conditions $\tilde{H}_{k+1} \hat{Y}_k = \hat{S}_k$ are satisfied,

(c) the auxiliary QN conditions $\tilde{H}_k^{k+1} \hat{\underline{Y}}_k = \hat{\underline{S}}_k$ are satisfied for $\underline{\mathcal{I}}_k \neq \emptyset$.

Here matrices $\tilde{H}_{k+1} = \tilde{H}_{k+1}^{k+1}$, $\tilde{H}_k^{k+1}$ are defined by the repeated BFGS updating (1.9) of matrix $\tilde{H}_{k-\tilde{m}}^{k+1} = \zeta_k I$, $\zeta_k > 0$, with columns of $\tilde{S}_k, \tilde{Y}_k$.

Proof. Let $k>0$. (i) Suppose that $i \in \underline{\mathcal{I}}_k$, $i<j\le k$. For $j=k$ we have $i \in \underline{\mathcal{I}}_j$, otherwise we obtain $i \in \underline{\mathcal{I}}_k \subset \mathcal{I}_{k-1} = \underline{\mathcal{I}}_{k-1} \cup \{k-1\} \subset \ldots \subset \underline{\mathcal{I}}_j \cup \{j,\ldots,k-1\}$ by assumption, thus again $i \in \underline{\mathcal{I}}_j$ by $i<j$. This implies $\hat{\underline{S}}_j^T \tilde{y}_j = \hat{\underline{Y}}_j^T \tilde{s}_j = 0$ by assumption, therefore $\tilde{s}_i^T \tilde{y}_j = \tilde{y}_i^T \tilde{s}_j = 0$, i.e. (a) holds.

(ii) Let $i \in \mathcal{I}_k$. We will prove

$$\tilde{H}_j^{k+1} \tilde{y}_i = \tilde{s}_i, \qquad i<j\le k+1, \tag{2.14}$$

hence (b) for $j=k+1$ and (c) for $j=k$, $i<k$. For $j=i+1$ we have $\tilde{H}_j^{k+1}\tilde{y}_i = \tilde{s}_i$ by (1.9).

By induction, let

$$\tilde{H}_j^{k+1} \tilde{y}_i = \tilde{s}_i \tag{2.15}$$

for some j, $i<j\le k$. By (1.7) and (a) we get $\tilde{V}_j^T \tilde{y}_i = \tilde{y}_i$ and $\tilde{V}_j \tilde{s}_i = \tilde{s}_i$, which yields $\tilde{H}_{j+1}^{k+1} \tilde{y}_i = \tilde{V}_j \tilde{H}_j^{k+1} \tilde{y}_i = \tilde{s}_i$ by (1.9), (2.15) and (a), i.e. (2.15) with $j+1$ instead of j. $\square$

If matrix $\hat{\underline{S}}^T \hat{\underline{Y}}$ is diagonal, many results can be simplified. E.g. components of vectors σ^*, η^* in (2.8) are numbers $-s^T \tilde{y}_i / \tilde{b}_i$, $-\tilde{s}_i^T y / \tilde{b}_i$, $i \in \underline{\mathcal{I}}$, thus relation (2.4) and formula (2.9) for b^* can be written in the form

$$(\ddot{H}_+ y - s)^T \ddot{B}_+ (\ddot{H}_+ y - s) = b \sum\nolimits_{i\in\underline{\mathcal{I}}} (\tilde{s}_i^T y - s^T \tilde{y}_i)^2 / (b \tilde{b}_i), \tag{2.16}$$

$$b^* = b - \sum\nolimits_{i\in\underline{\mathcal{I}}} s^T \tilde{y}_i \, \tilde{s}_i^T y / \tilde{b}_i. \tag{2.17}$$

These representations are advantageous when we select columns of $\hat{\underline{S}}$, $\hat{\underline{Y}}$, since an influence of particular columns of $\tilde{\underline{S}}$, $\tilde{\underline{Y}}$ can be considered separately for each $i \in \underline{\mathcal{I}}$. Therefore, if value $(\ddot{H}_+ y - s)^T \ddot{B}_+ (\ddot{H}_+ y - s)$ is too great, i.e. if the QN condition with corrected difference vectors is not a good substitute for the QN condition with non-corrected vectors or if value b^* is too small or negative, we should exclude a suitable index from $\underline{\mathcal{I}}$ (see Section 4 for details).

Theorem 2.2 also enables us to express $\tilde{s}, \tilde{y}$ by means of a projection matrix as

$$\tilde{s} = Ps, \quad \tilde{y} = P^T y, \quad P^2 = P = I - \sum\nolimits_{i\in\underline{\mathcal{I}}} \tilde{s}_i \, \tilde{y}_i^T / \tilde{b}_i = \prod\nolimits_{i\in\underline{\mathcal{I}}} (I - \tilde{s}_i \, \tilde{y}_i^T / \tilde{b}_i) \tag{2.18}$$

by (2.1) and the simplified form of (2.8) mentioned above; these representations of $\tilde{s}, \tilde{y}$ are used in Section 5 and further implies $P_k \tilde{H}_k^{k+1} = \tilde{H}_k^{k+1} - \sum_{i\in\underline{\mathcal{I}}_k} \tilde{s}_i \tilde{s}_i^T / \tilde{b}_i = P_k \tilde{H}_k^{k+1} P_k^T$ after arrangement and $P_k^T \tilde{B}_k P_k = \tilde{B}_k - \sum_{i\in\underline{\mathcal{I}}_k} \tilde{y}_i \tilde{y}_i^T / \tilde{b}_i$, $k>0$, which yields formulas

$$\tilde{y}_k^T \tilde{H}_k^{k+1} \tilde{y}_k \;=\; y_k^T P_k \tilde{H}_k^{k+1} P^T y_k = y_k^T \tilde{H}_k^{k+1} y_k - \sum\nolimits_{i\in\underline{\mathcal{I}}_k} (\tilde{s}_i^T y_k)^2 / \tilde{b}_i \,, \tag{2.19}$$

$$\tilde{s}_k^T \tilde{B}_k \tilde{s}_k \;=\; s_k^T \tilde{B}_k s_k - \sum\nolimits_{i\in\underline{\mathcal{I}}_k} (s_k^T \tilde{y}_i)^2 / \tilde{b}_i = -t_k s_k^T g_k - \sum\nolimits_{i\in\underline{\mathcal{I}}_k} (s_k^T \tilde{y}_i)^2 / \tilde{b}_i \,, \tag{2.20}$$

used in Section 4.

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 $\tilde{\eta}_k = \tilde{\sigma}_k$, $k > 0$, which is a natural choice, enabling us to have $\tilde{y}_k = G\tilde{s}_k$ (and thus $\underline{\tilde{Y}}_k = G\underline{\tilde{S}}_k$), $k > 0$, in view of (1.7), similarly as for non-corrected vectors. Here we consider only G-conjugacy of vectors.

Condition $\tilde{b} > 0$ related to (1.7) can be obviously satisfied by the choice $\tilde{\sigma} = \tilde{\eta} = 0$ due to $b > 0$. For linearly independent columns of $[\underline{\tilde{S}}, s]$, the following lemma guarantees that $\tilde{b} > 0$ for any $\tilde{\sigma} = \tilde{\eta}$ and that we can always calculate values $\sigma^* = \eta^*$, which solve equations $\underline{\hat{S}}^T\tilde{y} = \underline{\hat{S}}^T G\tilde{s} = \underline{\hat{Y}}^T\tilde{s} = 0$, i.e. provide the conjugacy of vector $\tilde{s}$ with columns of $\underline{\hat{S}}$.

Lemma 3.1. *Let f be a quadratic function $f(x) = \frac{1}{2}(x-\bar{x})^T G(x-\bar{x})$, $\bar{x} \in \mathcal{R}^N$, with a symmetric positive definite matrix G and columns of $[\underline{\tilde{S}}, s]$ be linearly independent. Then for any selection of $\underline{\hat{S}}$, $\underline{\hat{Y}}$ from $\underline{\tilde{S}}$, $\underline{\tilde{Y}}$, matrix $\underline{\hat{S}}^T\underline{\hat{Y}}$ is symmetric positive definite, values $\sigma^* = \eta^*$ are well defined by (2.8) and $\tilde{b} > 0$ for any $\hat{\sigma} = \hat{\eta}$.*

Proof. Since columns of $[\underline{\hat{S}}, s]$ are linearly independent, matrix $K = [\underline{\hat{S}}, s]^T G[\underline{\hat{S}}, s]$ is symmetric positive definite, therefore also submatrix $\underline{\hat{S}}^T G\underline{\hat{S}} = \underline{\hat{S}}^T\underline{\hat{Y}}$ has this property and

$$(u^T, -1)K(u^T, -1)^T = u^T\underline{\hat{S}}^T\underline{\hat{Y}}u - 2u^T\underline{\hat{S}}^T y + b > 0$$

for any vector u of the proper dimension. For the choice $u = (\underline{\hat{S}}^T\underline{\hat{Y}})^{-1}\underline{\hat{S}}^T y$ we obtain $b - y^T\underline{\hat{S}}(\underline{\hat{S}}^T\underline{\hat{Y}})^{-1}\underline{\hat{S}}^T y > 0$, i.e. $b^* > 0$ by (2.9) and $\underline{\hat{S}}^T y = \underline{\hat{S}}^T Gs = \underline{\hat{Y}}^T s$. Thus values $\sigma^* = \eta^*$ are well defined by (2.8) and $\tilde{b} > 0$ by (2.9). □

The following theorem shows that for the choice $\hat{\sigma} = \sigma^*$, also the QN condition $\ddot{H}_+ y = s$ with non-corrected difference vectors is satisfied and improvement of convergence is the best in some sense for linearly independent direction vectors.

Theorem 3.1. *Let $\ddot{H}$ be any symmetric positive definite matrix satisfying $\ddot{H}\underline{\hat{Y}} = \underline{\hat{S}}$ and suppose that $\hat{\sigma} = \hat{\eta}$ and that the assumptions of Lemma 3.1 are satisfied. Then $\tilde{b} > 0$ and the choice $\hat{\sigma} = \sigma^*$, given by (2.8), implies $\ddot{H}_+ y = s$ and minimizes value $\|G^{1/2}\ddot{H}_+ G^{1/2} - I\|_F$ as a function of $\hat{\sigma}$, where matrix $\ddot{H}_+$ is defined by update (1.12) of $\ddot{H}$.*

Proof. Inequality $\tilde{b} > 0$, established in Lemma 3.1 for any $\hat{\sigma} = \hat{\eta}$, justifies representation (1.12) of $\ddot{H}_+$ and thus satisfaction of the QN condition $\ddot{H}_+\tilde{y} = \tilde{s}$. The choice $\hat{\sigma} = \sigma^*$ implies (2.2) by Lemma 2.2, therefore $\ddot{H}_+\underline{\hat{Y}} = \underline{\hat{S}}$ by Lemma 2.1, which yields $s = \ddot{H}_+\tilde{y} - \underline{\hat{S}}\hat{\sigma} = \ddot{H}_+ y + \ddot{H}_+\underline{\hat{Y}}\hat{\eta} - \underline{\hat{S}}\hat{\eta} = \ddot{H}_+ y$ by (1.7) and $\hat{\sigma} = \hat{\eta}$. Since matrix $\underline{\hat{S}}^T\underline{\hat{Y}}$ is symmetric positive definite by Lemma 3.1, it suffices to use Theorem 2.1 with $\ddot{G} = G$, $\hat{\sigma} = \hat{\eta}$ and e.g. $\ddot{\sigma} = \ddot{\eta} = 0$. □

In view of Lemma 3.1 we can always set $\underline{\hat{S}} = \underline{\tilde{S}}$, $\underline{\hat{Y}} = \underline{\tilde{Y}}$ and $\hat{\sigma} = \sigma^*$ for linearly independent direction vectors. The following theorem describes a situation when such a case occurs in all iterations of the corrected BNS method, proposed in Section 1.

Theorem 3.2. *Let f be quadratic function $f(x) = \frac{1}{2}(x-\bar{x})^T G(x-\bar{x})$, $\bar{x} \in \mathcal{R}^N$, with a symmetric positive definite matrix G, columns of every matrix $[\underline{\tilde{S}}_k, s_k]$ be linearly independent and we always choose $\underline{\hat{S}}_k = \underline{\tilde{S}}_k$, $\underline{\hat{Y}}_k = \underline{\tilde{Y}}_k$, $\tilde{\sigma}_k = \tilde{\eta}_k = \sigma_k^*$, $k > 0$. Then columns of $\tilde{S}_k$*

are conjugate, i.e. matrices $\tilde{S}_k^T \tilde{Y}_k = \tilde{U}_k = \tilde{D}_k$ *are diagonal,* $k > 0$*, and all QN conditions* $\tilde{H}_{k+1} \tilde{Y}_k = \tilde{S}_k$*,* $\tilde{H}_k^{k+1} \underline{\tilde{Y}}_k = \underline{\tilde{S}}_k$*,* $k \ge 0$*, are satisfied, where matrices* $\tilde{H}_{k+1}$*,* $\tilde{H}_k^{k+1}$ *are defined by the repeated BFGS updating (1.9) of matrix* $\zeta_k I$*,* $\zeta_k > 0$*, with columns of* $\tilde{S}_k, \tilde{Y}_k$*.*

Proof. We have $\underline{\tilde{S}}_k^T \tilde{y}_k = \underline{\tilde{Y}}_k^T \tilde{s}_k = 0$, $k > 0$, by Lemma 2.2 and it suffices to use Theorem 2.2 with $\mathcal{I}_k = \{k - \tilde{m}, \dots, k\} \supset \mathcal{I}_{k+1}$, $k \ge 0$. □

Comparing these results with those given by Theorem 3.2 in [16] for unit stepsizes, we see that they are similar - all stored corrected vectors $\tilde{s}_k$ ($\bar{s}_k$ in [16]) are conjugate and $\tilde{m}$ previous QN conditions are preserved, although only one correction vector is used for difference vectors in [16]. The following theorem gives an interesting explanation - if we generate all matrices $\tilde{H}$ in accordance with Theorem 3.2 and $t = 1$, then vector s_+ is conjugate with columns of $\underline{\tilde{S}}$, thus only correction vectors $\tilde{s}, \tilde{y}$ are useful to correct s_+, y_+, while columns of $\underline{\tilde{S}}, \underline{\tilde{Y}}$ as additional correction vectors have no influence on $\tilde{s}_+, \tilde{y}_+$:

Theorem 3.3. *Let* $\tilde{H}, \tilde{H}_+$ *be symmetric positive definite matrices satisfying* $\tilde{H}\tilde{Y}_- = \tilde{S}_-$*,* $\tilde{H}_+ \underline{\tilde{Y}} = \underline{\tilde{S}}$*,* $d = -\tilde{H}g$ *and* $d_+ = -\tilde{H}_+ g_+$*,* f *be a quadratic function* $f(x) = \frac{1}{2}(x - \bar{x})^T G(x - \bar{x})$*,* $\bar{x} \in \mathcal{R}^N$*, with a symmetric positive definite matrix* G *and suppose that* $t = 1$*, i.e.* $s = d$*. Then* $\underline{\tilde{S}}^T y_+ = \underline{\tilde{Y}}^T s_+ = 0$*, i.e. columns of* $\underline{\tilde{S}}$ *are conjugate with non-corrected vector* s_+*.*

Proof. Since assumption $\tilde{H}\tilde{Y}_- = \tilde{S}_-$ implies $\tilde{H}\underline{\tilde{Y}} = \underline{\tilde{S}}$, we can use other assumptions and $\underline{\tilde{S}}^T y = \underline{\tilde{S}}^T G s = \underline{\tilde{Y}}^T s$ to obtain

$$-\underline{\tilde{Y}}^T d_+ = -\underline{\tilde{S}}^T \tilde{B}_+ d_+ = \underline{\tilde{S}}^T g_+ = \underline{\tilde{S}}^T (y + g) = \underline{\tilde{Y}}^T s + \underline{\tilde{S}}^T g = \underline{\tilde{Y}}^T (s + \tilde{H}g) = 0,$$

which immediately gives $\underline{\tilde{Y}}^T s_+ = \underline{\tilde{S}}^T G s_+ = \underline{\tilde{S}}^T y_+ = 0$. □

4 Implementation

From theory in Section 3 we could deduce that to improve convergence properties of the BNS method, we should use the corrected difference vectors whenever an objective function is close to a quadratic function (e.g. near to a local minimum), see below. On the other hand, Theorem 3.3 indicate that a influence of more correction vectors than one can be negligible in such situation, corrections can deteriorate stability and the computation of vectors $\tilde{s}, \tilde{y}$ according to (2.1) requires additional arithmetic operations in comparison with the non-corrected BNS method, proportionally to the number of currently used correction vectors. Thus we should not correct if a benefit of corrections is negligible.

It follows from the proof of Theorem 2.1 that $\|\ddot{G}^{1/2} \ddot{H}_+ \ddot{G}^{1/2} - I\|_F^2 = \varphi(\xi) \ge \varphi(1)$, $\xi = b^*/\tilde{b} \in (0, 1]$, where convex function φ, nonincreasing on $[0, 1]$, is given by quadratic function (2.13), with all coefficients independent of $(\hat{\sigma}, \hat{\eta}) \in \mathcal{S}(\underline{\hat{S}}, \underline{\hat{Y}})$ by Lemma 2.4. Numerical experiments indicate that the ratio $b/\tilde{b}$ and the decrease of φ on $[\tilde{b}/b, 1]$ are good indicators of the benefit of corrections, in spite of the fact that $(0, 0) \notin \mathcal{S}(\underline{\hat{S}}, \underline{\hat{Y}})$ for non-quadratic functions generally. Although we cannot calculate either $\varphi(\xi)$ or $\varphi'(\xi)$, we can utilize value $\varphi''/2 = (1 - \ddot{a}/\tilde{b})^2$ and the length of interval $[\tilde{b}/b, 1]$, see below.

As a measure of the deviation from a quadratic function in points $x_{k-\tilde{m}}, \dots, x_k$, $k > 0$, e.g. values (zero for quadratic functions) $\Delta_i^k = (s_i^T y_k - s_k^T y_i)^2 / (b_k b_i)$, $i \in \{k - \tilde{m}, \dots, k - 1\}$, could serve. We use values $\tilde{\Delta}_i^k = (\tilde{s}_i^T y_k - s_k^T \tilde{y}_i)^2/(b_k \tilde{b}_i)$, see (2.16), which utilize stored corrected difference vectors and give a damage of the QN condition for non-corrected vectors s, y caused by these corrections, see (2.16). Principally, we do not use vectors $\tilde{s}_i, \tilde{y}_i$, $i \in \{k-\tilde{m}, \dots, k-1\}$, for correction process (i.e. we decide that $i \notin \underline{\mathcal{I}}_k$) if $\tilde{b} < \delta_1 b$, $\delta_1 < 1$, if $\tilde{\Delta}_i^k > \delta_2$, $\delta_2 < 1$, or if $i \notin \mathcal{I}_{k-1}$, in view of our strategy described in Section 2.2.

For $i \in \underline{\mathcal{I}}_{k-1}$, we also take into consideration if the benefit of corrections is great enough, see above. We do not correct if $\tilde{\Delta}_i^k > \delta_3$, $\delta_3 < \delta_2$ together with $(b/\tilde{b})\sqrt{\varphi''/2}(1-\tilde{b}/b) = |1 - \ddot{a}/\tilde{b}|(b/\tilde{b} - 1) < 1$, or if $\tilde{\Delta}_i^k > \min[\delta_2, \delta_3 + (1 - \tilde{b}/b)^4/2]$, $k > 0$ (these formulas were found empirically). Besides, we do not use $\tilde{s}_i, \tilde{y}_i$ as correction vectors if the influence of these vectors is too small, i.e. if $[(\tilde{s}_i^T y_k)^2 + (s_k^T \tilde{y}_i)^2]/(b_k \tilde{b}_i) < \delta_4$, $\delta_4 < 1$, $k > 0$, to increase the efficiency of our method (see the beginning of this section).

To calculate number $\ddot{a} = \tilde{y}^T \ddot{H} \tilde{y}$ for $\ddot{H} = \tilde{H}_k^{k+1}$, $k > 0$, we can use formula (2.19), where value $y^T \ddot{H} y$ can be efficiently calculated by

$$y^T \ddot{H} y = \zeta |y|^2 + y^T \underline{\tilde{S}}\, \underline{\tilde{U}}^{-T} \Big[\underline{\tilde{D}} + \zeta \underline{\tilde{Y}}^T \underline{\tilde{Y}} \Big] \underline{\tilde{U}}^{-1} \underline{\tilde{S}}^T y - 2\,\zeta y^T \underline{\tilde{S}}\, \underline{\tilde{U}}^{-T} \underline{\tilde{Y}}^T y, \tag{4.1}$$

where $\tilde{D} = \mathrm{diag}[\underline{\tilde{D}}_k, \tilde{b}_k]$, $(\underline{\tilde{U}})_{i,j} = (\underline{\tilde{S}}^T \underline{\tilde{Y}})_{i,j}$ for $i \le j$, $(\underline{\tilde{U}})_{i,j} = 0$ otherwise, which can be derived from the following analogy of (1.5) for corrected matrix $\ddot{H} = \tilde{H}_k^{k+1}$, $k > 0$,

$$\ddot{H} = \underline{\tilde{S}}\, \underline{\tilde{U}}^{-T} \underline{\tilde{D}}\, \underline{\tilde{U}}^{-1} \underline{\tilde{S}}^T + \zeta (I - \underline{\tilde{S}}\, \underline{\tilde{U}}^{-T} \underline{\tilde{Y}}^T)(I - \underline{\tilde{Y}}\, \underline{\tilde{U}}^{-1} \underline{\tilde{S}}^T)\,. \tag{4.2}$$

To increase stability, we also do not use $\tilde{s}_i, \tilde{y}_i$, $i \in \{k-\tilde{m}, \dots, k-1\}$, $k > 0$, for corrections, if numbers $\ddot{a}$ or $\tilde{s}^T \tilde{B} \tilde{s}$, see (2.20), are too small with respect to b, i.e. $\ddot{a} < \delta_5 b$ or $\tilde{s}^T \tilde{B} \tilde{s} < \delta_6 b$, and moreover, in order to prove global convergence, if $|\tilde{s}_i| > \Delta |s_i|$ or $|\tilde{y}_i| > \Delta |y_i|$, $\Delta > 1$. Note that in our numerical experiments with $N = 5000$, values $|\tilde{y}|/|y|, |\tilde{s}|/|s|$ were rarely greater than 50.

First we give a procedure for updating of basic low-order matrices $\tilde{S}^T \tilde{Y}$, $\tilde{Y}^T \tilde{Y}$, similar to the algorithm given in [2] for updating of matrices D, U, $Y^T Y$ in (1.6). We present the whole procedure for completeness, although parts of steps (ii), (iii) are contained in Step 1 of Algorithm 4.2. Note that number of arithmetic operations is approximately the same as for the corresponding algorithm in [2], although we use additional vector $\underline{\tilde{Y}}^T s = -t \underline{\tilde{Y}}^T \tilde{H} g$, see Algorithm 4.2.

Procedure 4.1 *(Matrix Updating)*

Given: $t > 0$, matrices $\underline{\tilde{S}}$, $\underline{\tilde{Y}}$, $\underline{\tilde{S}}^T \underline{\tilde{Y}}$, $\underline{\tilde{Y}}^T \underline{\tilde{Y}}$ and vectors $s, y, g_+, \tilde{s}, \tilde{y}$, $\underline{\tilde{S}}^T g$, $\underline{\tilde{Y}}^T g$, $\underline{\tilde{Y}}^T \tilde{H} g$, $\tilde{\sigma}, \tilde{\eta}$.

(i): Set $\tilde{S} = [\underline{\tilde{S}}, \tilde{s}]$, $\tilde{Y} = [\underline{\tilde{Y}}, \tilde{y}]$.

(ii): Compute $\tilde{S}^T g_+ = [\underline{\tilde{S}}^T g_+, \tilde{s}^T g_+]$, $\tilde{Y}^T g_+ = [\underline{\tilde{Y}}^T g_+, \tilde{y}^T g_+]$, $\underline{\tilde{Y}}^T s = -t \underline{\tilde{Y}}^T \tilde{H} g$.

(iii): Compute $\underline{\tilde{S}}^T y = \underline{\tilde{S}}^T g_+ - \underline{\tilde{S}}^T g$, $\underline{\tilde{Y}}^T y = \underline{\tilde{Y}}^T g_+ - \underline{\tilde{Y}}^T g$, $\tilde{y}^T \tilde{y} = y^T y + 2\tilde{\eta}^T \underline{\tilde{Y}}^T y + \tilde{\eta}^T (\underline{\tilde{Y}}^T \underline{\tilde{Y}}) \tilde{\eta}$.

(iv): Compute $\underline{\tilde{S}}^T \tilde{y} = \underline{\tilde{S}}^T y + (\underline{\tilde{S}}^T \underline{\tilde{Y}}) \tilde{\eta}$, $\underline{\tilde{Y}}^T \tilde{s} = \underline{\tilde{Y}}^T s + (\underline{\tilde{Y}}^T \underline{\tilde{S}}) \tilde{\sigma}$, $\underline{\tilde{Y}}^T \tilde{y} = \underline{\tilde{Y}}^T y + (\underline{\tilde{Y}}^T \underline{\tilde{Y}}) \tilde{\eta}$.

(v): Set $\tilde{S}^T \tilde{Y} = \begin{bmatrix} \underline{\tilde{S}}^T \underline{\tilde{Y}} & \underline{\tilde{S}}^T \tilde{y} \\ \tilde{s}^T \underline{\tilde{Y}} & \tilde{s}^T \tilde{y} \end{bmatrix}$, $\tilde{Y}^T \tilde{Y} = \begin{bmatrix} \underline{\tilde{Y}}^T \underline{\tilde{Y}} & \underline{\tilde{Y}}^T \tilde{y} \\ \tilde{y}^T \underline{\tilde{Y}} & \tilde{y}^T \tilde{y} \end{bmatrix}$ and return.

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

Algorithm 4.2

Data: A number $m > 1$ of VM updates per iteration, line search parameters ε_1, ε_2, $0 < \varepsilon_1 < 1/2$, $\varepsilon_1 < \varepsilon_2 < 1$, correction parameters $\delta_1, \delta_2, \delta_3, \delta_4, \delta_5, \delta_6, \Delta$, $0 < \delta_i < 1 < \Delta$, $i \in \{1, ..., 6\}$, $\delta_2 < \delta_3$, and a maximum number of correction vectors $n \in [0, m-1]$.

Step 0: Initiation. Choose starting point $x_0 \in \mathcal{R}^N$, define starting matrix $\tilde{H}_0 = I$ and direction vector $d_0 = -g_0$ and initiate iteration counter k to zero.

Step 1: Line search. Compute $x_{k+1} = x_k + t_k d_k$, where t_k satisfies (1.1), $g_{k+1} = \nabla f(x_{k+1})$, $s_k = t_k d_k$, $y_k = g_{k+1} - g_k$, $b_k = s_k^T y_k$, $\zeta_k = b_k / y_k^T y_k$ and set $\tilde{m} = \min(k, m\text{–}1)$. If $k = 0$ set $\tilde{s}_k = s_k$, $\tilde{y}_k = y_k$, $\tilde{b}_k = \tilde{s}_k^T \tilde{y}_k$, $\mathcal{I}_k = \{0\}$, $\tilde{S}_k = [\tilde{s}_k]$, $\tilde{Y}_k = [\tilde{y}_k]$, $\tilde{S}_k^T \tilde{Y}_k = [\tilde{s}_k^T \tilde{y}_k]$, $\tilde{Y}_k^T \tilde{Y}_k = [\tilde{y}_k^T \tilde{y}_k]$, compute $\tilde{S}_k^T g_{k+1}$, $\tilde{Y}_k^T g_{k+1}$ and go to Step 9, otherwise compute $\underline{\tilde{S}}_k^T g_{k+1}$, $\underline{\tilde{Y}}_k^T g_{k+1}$, $\underline{\tilde{Y}}_k^T s_k = -t_k \underline{\tilde{Y}}_k^T \tilde{H}_k g_k$, $\underline{\tilde{S}}_k^T y_k = \underline{\tilde{S}}_k^T g_{k+1} - \underline{\tilde{S}}_k^T g_k$, $\underline{\tilde{Y}}_k^T y_k = \underline{\tilde{Y}}_k^T g_{k+1} - \underline{\tilde{Y}}_k^T g_k$.

Step 2: Preparation. Set $\underline{\mathcal{I}}_k = \{i \in \mathcal{I}_{k-1} : i \geq k-n\}$. If $\underline{\mathcal{I}}_k = \emptyset$ go to Step 7, otherwise set $i = k-1$, $\tilde{b}_i^k = b_k$ and compute $\ddot{a}_i^k = y_k^T \tilde{H}_k y_k$ by (4.1) and $\tilde{c}_i^k = -t_k\, s_k^T g_k$.

Step 3: General elimination of indices. If $i \notin \underline{\mathcal{I}}_k$ go to Step 6. Compute $\tilde{\Delta}_i^k = (\tilde{s}_i^T y_k - s_k^T \tilde{y}_i)^2 / (b_k \tilde{b}_i)$. If $\tilde{b}_i^k - \tilde{s}_i^T y_k\, s_k^T \tilde{y}_i / \tilde{b}_i < \delta_1 b$ or $\ddot{a}_i^k - (\tilde{s}_i^T y_k)^2 / \tilde{b}_i < \delta_5 b_k$ or $\tilde{c}_i^k - (s_k^T \tilde{y}_i)^2 / \tilde{b}_i < \delta_6 b_k$ or $|\tilde{s}_i| > \Delta |s_i|$ or $|\tilde{y}_i| > \Delta |y_i|$ or $\tilde{\Delta}_i^k > \delta_2$ set $\underline{\mathcal{I}}_k := \underline{\mathcal{I}}_k \setminus \{i\}$. If $i = k-1$ go to Step 5.

Step 4: Additional elimination of indices. If $\tilde{\Delta}_i^k > \delta_3$ and $|1 - \ddot{a}_i^k / \tilde{b}_i^k|(b_k / \tilde{b}_i^k - 1) < 1$ then set $\underline{\mathcal{I}}_k := \underline{\mathcal{I}}_k \setminus \{i\}$. If $\tilde{\Delta}_i^k > \min[\delta_2, \delta_3 + (1 - \tilde{b}_i^k / b_k)^4 / 2]$ set $\underline{\mathcal{I}}_k := \underline{\mathcal{I}}_k \setminus \{i\}$.

Step 5: Update of auxiliary quantities. If $i \in \underline{\mathcal{I}}_k$ set $\tilde{b}_i^k := \tilde{b}_i^k - \tilde{s}_i^T y_k\, s_k^T \tilde{y}_i / \tilde{b}_i$, $\ddot{a}_i^k := \ddot{a}_i^k - (\tilde{s}_i^T y_k)^2 / \tilde{b}_i$ and $\tilde{c}_i^k := \tilde{c}_i^k - (s_k^T \tilde{y}_i)^2 / \tilde{b}_i$.

Step 6: Loop. Set $i := i - 1$. If $i \geq k - \tilde{m}$ go to Step 3.

Step 7: Correction. Compute $(\tilde{\sigma}_k)_i = -s_k^T \tilde{y}_i / \tilde{b}_i$, $(\tilde{\eta}_k)_i = -\tilde{s}_i^T y_k / \tilde{b}_i$ for $i \in \underline{\mathcal{I}}_k$, $(\tilde{\sigma}_k)_i = 0$, $(\tilde{\eta}_k)_i = 0$ for $i \notin \underline{\mathcal{I}}_k$, $\tilde{s}_k, \tilde{y}_k$ by (2.1) and $\tilde{b}_k = \tilde{s}_k^T \tilde{y}_k$. If $\tilde{b}_k < \tilde{b}_i^k / 2$ set $\tilde{b}_k = \tilde{b}_i^k$. Set $\mathcal{I}_k = \underline{\mathcal{I}}_k \cup \{k\}$.

Step 8: Matrix updating. Using Procedure 4.1, form matrices $\tilde{S}_k$, $\tilde{Y}_k$, $\tilde{S}_k^T \tilde{Y}_k$, $\tilde{Y}_k^T \tilde{Y}_k$.

Step 9: Direction vector. Set $\tilde{D}_k = \mathrm{diag}[\tilde{b}_{k-\tilde{m}}, \ldots, \tilde{b}_k]$ and $(\tilde{U}_k)_{i,j} = (\tilde{S}_k^T \tilde{Y}_k)_{i,j}$ for $i \leq j$, $(\tilde{U}_k)_{i,j} = 0$ otherwise. Compute $d_{k+1} = -\tilde{H}_{k+1} g_{k+1}$ by (1.10) and an auxiliary vector $\tilde{Y}_k \tilde{H}_{k+1} g_{k+1}$ by (1.11), where matrix $\tilde{H}_{k+1}$ is defined by the analogy of (1.5) with corrected quantities. Set $k := k + 1$. If $k \geq m$ delete the first column of $\tilde{S}_{k-1}$, $\tilde{Y}_{k-1}$ and the first row and column of $\tilde{S}_{k-1}^T \tilde{Y}_{k-1}$, $\tilde{Y}_{k-1}^T \tilde{Y}_{k-1}$, to form matrices $\underline{\tilde{S}}_k$, $\underline{\tilde{Y}}_k$, $\underline{\tilde{S}}_k^T \underline{\tilde{Y}}_k$, $\underline{\tilde{Y}}_k^T \underline{\tilde{Y}}_k$. Go to Step 1.

5 Global convergence

In this section, we establish global convergence of Algorithm 4.2. The following assumption and lemma are presented in [16].

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* $G(x)$*)*.

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

Theorem 5.1. *Let objective function* f *satisfy Assumption 5.1. 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. All updates in (1.9) are the standard BFGS updates with vectors $\tilde{s}_i$, $\tilde{y}_i$ instead of s_i, y_i, therefore we have (see [15])

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

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

$k - \tilde{m} \le i \le k$, where $\tilde{B}^{k+1}_j = (\tilde{H}^{k+1}_j)^{-1}$, $\tilde{c}^{k+1}_j = \tilde{s}^T_j\tilde{B}^{k+1}_j\tilde{s}_j$, $j = k - \tilde{m}, \dots, k+1$, $k \ge 0$.

(i) Since $\tilde{B}^{k+1}_{k-\tilde{m}} = (|y_k|^2/b_k)I$ by (1.8), Lemma 5.1 gives

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

(ii) The safeguarding technique in Step 3 of Algorithm 4.2 guarantees

$$\tilde{b}_k \ge \delta_1 b_k, \qquad |\tilde{s}_i| \le \Delta|s_i|, \ |\tilde{y}_i| \le \Delta|y_i|, \quad i \in \underline{\mathcal{I}}_k, \tag{5.4}$$

therefore for $\underline{\mathcal{I}}_k \ne \emptyset$ and $k > 0$ from (2.18) we get

$$|\tilde{s}_k| \le \left\| \prod_{i\in\underline{\mathcal{I}}_k}\left(I - \frac{\tilde{s}_i\,\tilde{y}^T_i}{\tilde{b}_i}\right)\right\| |s_k| \le |s_k| \prod_{i\in\underline{\mathcal{I}}_k}\frac{|\tilde{s}_i|\,|\tilde{y}_i|}{\tilde{b}_i} \le \frac{\Delta^{2\tilde{m}}}{\delta^{\tilde{m}}_1}\,\frac{|s_i|\,|y_i|}{b_i}|s_k| \le C_0|s_k|, \tag{5.5}$$

with $C_0 = (\Delta^2/\delta_1)^{\tilde{m}}\sqrt{\overline{G}/\underline{G}}$ by Lemma 5.1. Similarly we obtain $|\tilde{y}_k| \le C_0|y_k|$ for $\underline{\mathcal{I}}_k \ne \emptyset$ and $k > 0$, which together with (5.5) gives

$$|\tilde{s}_k|^2/\tilde{b}_k \le (C^2_0/\delta_1)|s_k|^2/b_k \le (C^2_0/\delta_1)/\underline{G} \triangleq C_1, \tag{5.6}$$

$$|\tilde{y}_k|^2/\tilde{b}_k \le (C^2_0/\delta_1)|y_k|^2/b_k \le (C^2_0/\delta_1)\overline{G} \triangleq C_2 \tag{5.7}$$

for all $k \ge 0$ by Lemma 5.1 and $C^2_0/\delta_1 > 1$.

(iii) From (5.1), (5.3) and (5.7) we have

$$\mathrm{Tr}(\tilde{B}^{k+1}_{i+1}) \le N\overline{G} + mC_2 \triangleq C_3, \quad k - \tilde{m} - 1 \le i \le k, \quad k > 0, \tag{5.8}$$

which yields

$$\mathrm{Tr}(\tilde{B}_{k+1}) = \mathrm{Tr}(\tilde{B}^{k+1}_{k+1}) \le C_3, \quad k > 0. \tag{5.9}$$

(iv) Using (5.2), (5.6) and (5.8), we obtain

$$\det(\tilde{B}^{k+1}_{i+1})/\det(\tilde{B}^{k+1}_i) = (\tilde{b}_i/|\tilde{s}_i|^2)(|\tilde{s}_i|^2/\tilde{s}^T_i\tilde{B}^{k+1}_i\tilde{s}_i) \ge 1/(C_1C_3),$$

$k - \tilde{m} \le i \le k$. From this and (5.3) we get

$$\det(\tilde{B}_{k+1}) = \det(\tilde{B}^{k+1}_{k+1}) \ge \underline{G}^N/(C_1C_3)^m \triangleq C_4, \quad k > 0. \tag{5.10}$$

(v) The lowest eigenvalue $\underline{\lambda}(\tilde{B}_k)$ of matrix $\tilde{B}_k$ satisfies $\underline{\lambda}(\tilde{B}_k) \ge \det(\tilde{B}_k)/\mathrm{Tr}(\tilde{B}_k)^{N-1}$, $k \ge 0$. Setting $q_k = \tilde{B}^{1/2}_k s_k$, from (5.9) and (5.10) we conclude

$$\frac{(s^T_k\tilde{B}_ks_k)^2}{|s_k|^2|\tilde{B}_ks_k|^2} = \frac{s^T_k\tilde{B}_ks_k}{s^T_ks_k}\,\frac{q^T_kq_k}{q^T_k\tilde{B}_kq_k} \ge \frac{\det(\tilde{B}_k)}{\mathrm{Tr}(\tilde{B}_k)^{N-1}}\,\frac{1}{\mathrm{Tr}(\tilde{B}_k)} \ge \frac{C_4}{C^N_3}, \quad k > 1,$$

which implies $\lim_{k\to\infty}|g_k| = 0$, see Theorem 3.2 and relations (3.17)-(3.18) in [15]. □

6 Numerical experiments

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

- Test 11 from [9] (55 chosen problems, computed repeatedly ten times for better comparison), which are modified problems from CUTE collection [3]; used N are given in Table 1, where problems, modified in some way, are marked with '*',
- test from [1], termed Test 12 here, 73 problems, $N = 10000$,
- Test 25 from [8] (68 chosen problems), $N = 10000$.

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 6.1: Dimensions for Test 11 – modified CUTE collection.

For comparison, Table 2 contains the total number of function and also gradient evaluations (NFV) and the total computational time (Time) for the following limited-memory methods: L-BFGS – the Nocedal method based on the Strang formula, see [14], method from [16] (Algorithm 4.1), see Section 1, and new Algorithm 4.2 for $n = 2, 4$. All methods are implemented in the optimization software system UFO, described in [11] and introduced in `www.cs.cas.cz/luksan/ufo.html`. We have used $m = 5$, $\delta_1 = 10^{-4}$, $\delta_2 = 10^{-2}$, $\delta_3 = \delta_5 = 10^{-5}$, $\delta_4 = 10^{-10}$, $\delta_6 = 10^{-3}$, $\Delta = 1000$, $\varepsilon_1 = 10^{-4}$, $\varepsilon_2 = 0.8$ and the final precision $\|g(x^\star)\|_\infty \le 10^{-6}$.

Method	Test 11		Test 12		Test 25	
	NFV	Time	NFV	Time	NFV	Time
L-BFGS	80539	10.361	119338	50.88	502966	429.01
Alg. 4.1 in [16]	64395	9.614	67619	32.61	325441	318.71
Alg. 4.2, $n=2$	62770	8.795	67372	31.06	302908	302.62
Alg. 4.2, $n=4$	64127	8.977	66403	30.77	308847	298.05

Table 6.2: Comparison of the selected methods.

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

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

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

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

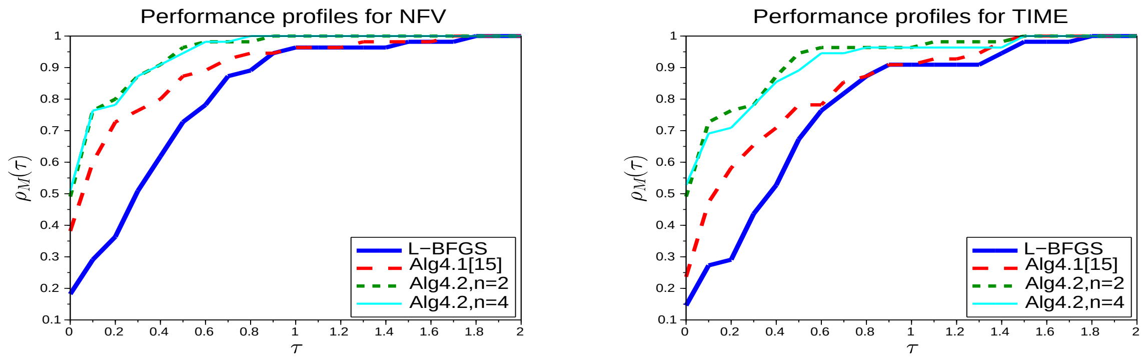

Figure 6.1: Comparison of $\rho_M(\tau)$ for Test 11 and various methods.

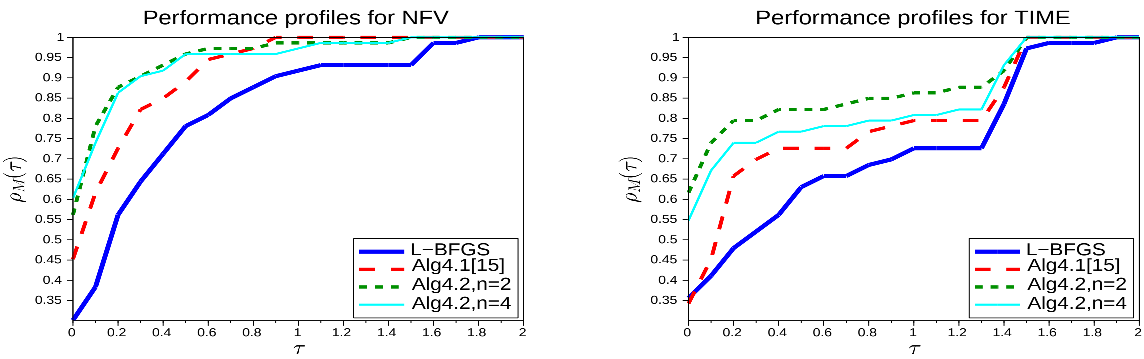

Figure 6.2: Comparison of $\rho_M(\tau)$ for Test 12 and various methods.

7 Conclusions

In this contribution, we propose some modifications of the BNS method based on the idea of conjugate directions consisting in such corrections of difference vectors which provide

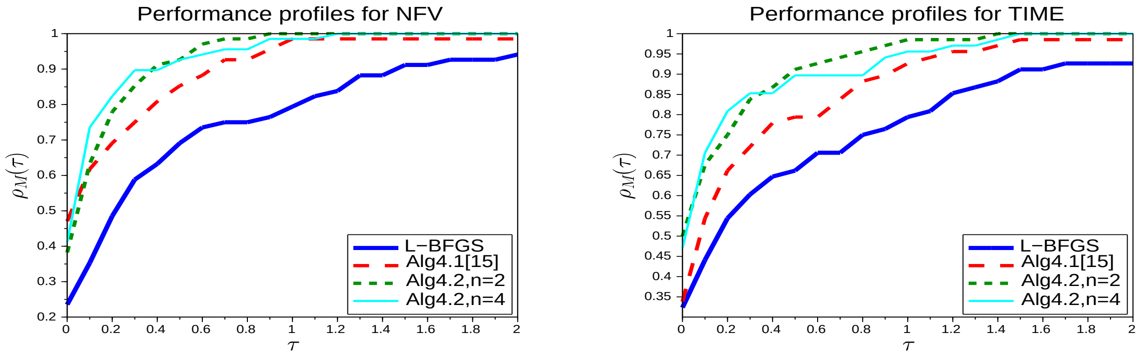

Figure 6.3: Comparison of $\rho_M(\tau)$ for Test 25 and various methods.

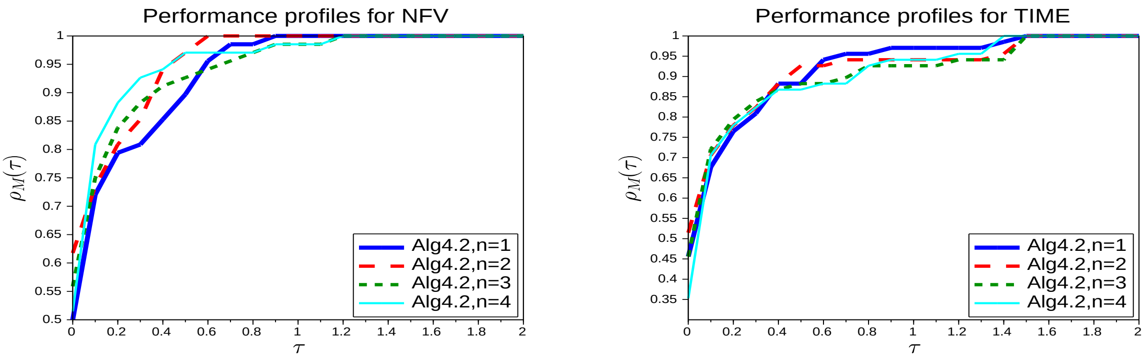

Figure 6.4: Comparison of $\rho_M(\tau)$ for Test 25 and various n.

conjugacy of all stored corrected vectors for quadratic objective functions. In comparison with [16], where a similar approach is used, more correction vectors can be applied here.

We show that the update VM matrices constructed by means of these vectors have some positive properties and that this approach can improve unconstrained large-scale minimization results significantly compared with the frequently used L-BFGS method (the BNS and the L-BFGS methods give very similar results) and the method from [16].

Our limited experiments also indicate that numerical results for 1, 2, 3 or 4 correction vectors are not too different and that two correction vectors can mostly be recommended.

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