New Class of Limited-Memory Variationally-Derived Variable Metric Methods

Vlček, Jan
2006

Institute of Computer Science
Academy of Sciences of the Czech Republic

New class of limited-memory variationally-derived variable metric methods

J. Vlček, L. Lukšan

Technical report No. V 973

December 2006

Pod Vodárenskou věží 2, 182 07 Prague 8 phone: +420 2 688 42 44, fax: +420 2 858 57 89,
e-mail:luksan@cs.cas.cz, vlcek@cs.cas.cz

Institute of Computer Science
Academy of Sciences of the Czech Republic

New class of limited-memory variationally-derived variable metric methods

J. Vlček, L. Lukšan[1]

Technical report No. V 973

December 2006

Abstract:

A new family of limited-memory variationally-derived variable metric or quasi-Newton methods for unconstrained minimization is given. The methods have quadratic termination property and use updates, invariant under linear transformations. Some encouraging numerical experience is reported.

Keywords:
Unconstrained minimization, variable metric methods, limited-memory methods, quadratic termination property, invariance property, numerical results

[1]This work was supported by the Grant Agency of the Czech Academy of Sciences, project No. IAA1030405 and the Institutional research plan No. AV0Z10300504, L. Lukšan is also from Technical University of Liberec, Hálkova 6, 461 17 Liberec

1 Introduction

In this report we present a new family of limited-memory variationally-derived variable metric (VM) line search methods for unconstrained minimization. VM line search methods (see [6], [3]) are iterative. Starting with an initial point $x_0 \in \mathcal{R}^N$, they 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 the direction vectors $d_k \in \mathcal{R}^N$ are required to be descent, i.e. $g_k^T d_k < 0$, $k \ge 0$, and the stepsizes t_k are chosen in such a way that $t_k > 0$ and

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

$k \ge 0$, with $0 < \varepsilon_1 < 1/2$ and $\varepsilon_1 < \varepsilon_2 < 1$, where $f_k = f(x_k)$, $g_k = \nabla f(x_k)$. We denote $y_k = g_{k+1} - g_k$, $k \ge 0$ and by $\|.\|_F$ the Frobenius matrix norm.

We describe a new family of limited-memory methods with some minimum change properties in Section 2 and prove their quadratic termination property. In Section 3 we give a correction formula, which significantly improves efficiency of all methods from the new family. Numerical results are presented in Section 4.

2 A new family of limited-memory methods

We proceed from the shifted VM methods, see [10]-[12], which appeared to be a very efficient tool. Unfortunately, their efficiency is not so good for ill-conditioned problems in comparison with e.g. the Nocedal method based on the Strang formula, see [9] or with the matrix variant of this method after [2]. The cause of this drawback probably consists in the fact that shifted VM updates are not invariant under linear transformations (significance of the invariance property of methods for solution of ill-conditioned problems is discussed in [3]).

Our new methods are based on approximations $\bar{H}_k = U_k U_k^T$, $k > 0$, $\bar{H}_0 = 0$, of the inverse Hessian matrix, which are invariant under linear transformations, where U_k are $N \times \min(k, m)$ rectangular matrices, $1 \le m \ll N$, obtained by limited-memory updates with scaling parameters $\gamma_k > 0$ (see [6]) that satisfy the quasi-Newton condition (in the generalized form)

$$\bar{H}_{k+1} y_k = \varrho_k s_k, \tag{2.1}$$

where $\varrho_k > 0$ is a nonquadratic correction parameter (see [6]). Although we use the unit values of γ_k and ϱ_k in almost all cases, we will consider also non-unit values in the subsequent analysis as it is usual in case of VM methods (see [6]). We present this basic update in Section 2.1.

To have matrices $\bar{H}_k$ invariant, we use updates (related to the standard Broyden class updates, see [3]), which can be expressed in the sketch form $\bar{H}_{k+1} = \gamma_k \bar{H}_k + [\, d_k, U_k \hat{u}_k, U_k \hat{v}_k] M_k$, $k \ge 0$, where M_k is $3 \times N$ matrix and $\hat{u}_k, \hat{v}_k \in \mathcal{R}^m$. Unfortunately, having matrices $\bar{H}_k$ obtained by means of such updates, vectors $-\bar{H}_k g_k$ cannot be directly used as the direction vectors d_k, since they lie in range(U_k) and thus also $\bar{H}_{k+1} g_{k+1} \in$ range(U_k), $k \ge 1$, and method degenerates.

Therefore we use nonsingular corrected matrices H_k instead of $\bar{H}_k$, $k \ge 0$, $H_0 = I$, to calculate direction vectors $d_k = -H_k g_k$. Since the mere adding of matrix $\zeta_k I$ to

$\bar{H}_{k+1}$, $\zeta_k > 0$, $k \geq 0$, violates the quasi-Newton condition, we derive a class of simple corrections in Section 2.2 (note that another correction will be described in Section 3). In Section 2.3 we discuss some special choices of the vector parameter for this correction class. In Section 2.4 we show that methods from the family, obtained in this way, have quadratic termination property.

For given $r_k \in \mathcal{R}^N$, $r_k^T y_k \neq 0$, we denote by V_{r_k} the projection matrix $I - r_k y_k^T / r_k^T y_k$. To simplify the notation we frequently omit index k and replace index $k+1$ by symbol $+$ and index $k-1$ by symbol $-$. In the subsequent analysis we use the following notation

$$B = H^{-1}, \quad b = s^T y, \quad \bar{a} = y^T \bar{H} y, \quad \bar{b} = s^T B \bar{H} y, \quad \bar{c} = s^T B \bar{H} B s, \quad \bar{\delta} = \bar{a}\bar{c} - \bar{b}^2.$$

Note that $b > 0$ by (1.1) and that the Schwarz inequality implies $\bar{\delta} \geq 0$.

2.1 Variationally-derived invariant limited-memory method

Standard VM methods can be obtained by solving a certain variational problem - we find an update with the minimum change of VM matrix in the sense of some norm (see [6]). Using the product form of the update similarly as in [11], we can extend this approach to limited-memory methods to derive a very efficient class of methods. First we give the following general theorem, where the quasi-Newton condition $U_+ U_+^T y = \bar{H}_+ y = \varrho s$ is equivalently replaced by

$$U_+^T y = \sqrt{\gamma} z, \qquad U_+(\sqrt{\gamma} z) = \varrho s, \qquad z^T z = (\varrho/\gamma) b \tag{2.2}$$

(the first two conditions imply the third one).

Theorem 2.1. *Let T be a symmetric positive definite matrix, $\varrho > 0$, $\gamma > 0$, $z \in \mathcal{R}^m$, $1 \leq m \leq N$, and denote $\mathcal{U}$ the set of $N \times m$ matrices. Then the unique solution to*

$$\min\{\varphi(U_+) : U_+ \in \mathcal{U}\} \text{ s.t. } (2.2), \quad \varphi(U_+) = y^T T y \, \|T^{-1/2}(U_+ - \sqrt{\gamma} U)\|_F^2, \tag{2.3}$$

is

$$\frac{1}{\sqrt{\gamma}} U_+ = \frac{s z^T}{b} + \left(I - \frac{T y y^T}{y^T T y}\right) U \left(I - \frac{z z^T}{z^T z}\right) \tag{2.4}$$

and for this solution the value of $\varphi(U_+)/\gamma$ is

$$\frac{1}{\gamma}\varphi(U_+) = |U^T y - z|^2 + \frac{y^T T y}{z^T z} v^T T^{-1} v, \quad v = \left(I - \frac{T y y^T}{y^T T y}\right)\left(\frac{\varrho}{\gamma} s - U z\right). \tag{2.5}$$

Proof. We can proceed quite analogically as in the proof of Theorem 2.3 in [11] and then use (2.2). □

Denoting $p = Ty$, (2.4) yields the following projection form of limited-memory update, which shows the meaning of parameters z, Ty

$$\frac{1}{\gamma} \bar{H}_+ = \frac{\varrho}{\gamma} \frac{s s^T}{b} + V_p U \left(I - \frac{z z^T}{z^T z}\right) U^T V_p^T \tag{2.6}$$

by $\bar{H}_+ = U_+ U_+^T$, $z^T(I - z z^T / z^T z) = 0$ and $(I - z z^T / z^T z)^2 = I - z z^T / z^T z$.

For vector p lying in the subspace generated by vectors s, $\bar{H}y$ and Uz we can show that updates (2.4) and (2.6) are invariant under linear transformations, i.e. they preserve the same transformation property of $\bar{H} = UU^T$ as inverse Hessian.

Theorem 2.2. *Consider a change of variables $\tilde{x} = Rx + r$, where R is $N \times N$ nonsingular matrix, $r \in \mathcal{R}^N$. Let vector p lie in the subspace generated by vectors s, $\bar{H}y$ and Uz and suppose that z, γ and coefficients in the linear combination of vectors s, $\bar{H}y$ and Uz forming p are invariant under the transformation $x \to \tilde{x}$, i.e. they are not influenced by this transformation. Then for $\tilde{U} = RU$ matrix U_+ given by (2.4) also transforms to $\tilde{U}_+ = RU_+$.*

Proof. Since steps transform like points and the chain rule gives that gradients g, g_+ and true Hessian G transform to $\tilde{g} = R^{-T}g$, $\tilde{g}_+ = R^{-T}g_+$ and $\tilde{G} = R^{-T}GR^{-1}$, we get $\tilde{s} = Rs$, $\tilde{y} = R^{-T}y$ and $\tilde{b} = \tilde{s}^T\tilde{y} = s^Ty = b$.

Suppose that $\tilde{U} = RU$. Then $\bar{H}y$ and Uz transform to $\tilde{U}\tilde{U}^T\tilde{y} = RUU^Ty = R\bar{H}y$ and $\tilde{U}\tilde{z} = RUz$ by $\tilde{z} = z$, thus we have $\tilde{p} = Rp$, $\tilde{p}^T\tilde{y} = p^Ty$ and $RV_p = R - Rpy^T/p^Ty = R - \tilde{p}\tilde{y}^TR/\tilde{p}^T\tilde{y} = \left(I - \tilde{p}\tilde{y}^T/\tilde{p}^T\tilde{y}\right)R \triangleq \tilde{V}_{\tilde{p}}R$.

Substituting for these quantities to (2.4) in the transformed space, we obtain

$$\sqrt{\frac{1}{\tilde{\gamma}}}\,\tilde{U}_+ = \frac{\tilde{s}\tilde{z}^T}{\tilde{b}} + \tilde{V}_{\tilde{p}}\tilde{U}\left(I - \frac{\tilde{z}\tilde{z}^T}{\tilde{z}^T\tilde{z}}\right) = R\left[\frac{sz^T}{b} + V_pU\left(I - \frac{zz^T}{z^Tz}\right)\right],$$

therefore $\tilde{U}_+ = RU_+$ by (2.4) and $\tilde{\gamma} = \gamma$. □

In the special case

$$p = \frac{\lambda}{b}s + \frac{1-\lambda}{\bar{a}}\bar{H}y, \quad \bar{a} \neq 0, \qquad p = \frac{1}{b}s \ \text{ otherwise} \tag{2.7}$$

(in view of $\bar{a} = |U^Ty|^2$ this choice satisfies the assumptions of Theorem 2.2, since $\tilde{b} = b$ and $\tilde{U}^T\tilde{y} = U^Ty$, see the proof of Theorem 2.2) we can easily compare (2.6) with the scaled Broyden class update with parameter $\eta = \lambda^2$, whose usual form for any symmetric matrix A is (see [6])

$$\frac{1}{\gamma}A_+^{BC} = A + \frac{\varrho}{\gamma}\frac{ss^T}{b} - \frac{Ayy^TA}{a} + \frac{\lambda^2}{a}\left(\frac{a}{b}s - Ay\right)\left(\frac{a}{b}s - Ay\right)^T, \tag{2.8}$$

where $a = y^TAy \neq 0$ (if $a = 0$ we can choose $\lambda = 1$, i.e. the BFGS update in the form $(1/\gamma)A_+^{BFGS} = (\varrho/\gamma)ss^T/b + V_sAV_s^T$, see [6]), which can be readily rewritten, using straightforward arrangements and comparing corresponding terms, in the following quasi-product form

$$\frac{1}{\gamma}A_+^{BC} = \frac{\varrho}{\gamma}\frac{ss^T}{b} + \left(I - \left(\frac{\lambda}{b}s + \frac{1-\lambda}{a}Ay\right)y^T\right)A\left(I - y\left(\frac{\lambda}{b}s + \frac{1-\lambda}{a}Ay\right)^T\right). \tag{2.9}$$

Observing that $U(I - zz^T/z^Tz)\,U^T = \bar{H} - Uzz^TU^T/z^Tz$ and $p^Ty = 1$ by (2.7), we can use (2.6), (2.7) and (2.9) with $A = UU^T$ and $a = \bar{a}$ to obtain

$$\frac{1}{\gamma}\bar{H}_+ = \frac{1}{\gamma}\bar{H}_+^{BC} - \frac{V_pUz(V_pUz)^T}{z^Tz}. \tag{2.10}$$

Update (2.9) can be advantageously used for starting iterations. Setting $U_+ = \left[\sqrt{\varrho/b}\, s\right]$ in the first iteration, every update (2.9) modifies U and adds one column $\sqrt{\varrho/b}\, s$ to U_+. With the exception of the starting iterations we will assume that matrix U has $m \geq 1$ columns in all iterations.

In view of (2.2) we can write (2.4) in the form

$$\frac{1}{\sqrt{\gamma}} U_+ = U - \frac{Ty}{y^T Ty} y^T U + \left[s - \frac{\gamma}{\varrho} \left(Uz - \frac{y^T Uz}{y^T Ty} Ty \right) \right] \frac{z^T}{b}, \tag{2.11}$$

which is more suitable for calculation.

To choose parameter z, we utilize analogy with standard VM methods. Setting $H = SS^T$ and replacing U by $N \times N$ matrix S, we can use Theorem 2.1 for the standard scaled Broyden class update (see [6]) of matrix $H = B^{-1}$. Then (2.4) will be replaced by

$$\frac{1}{\sqrt{\gamma}} S_+ = \frac{sz^T}{b} + \left(I - \frac{Tyy^T}{y^T Ty} \right) S \left(I - \frac{zz^T}{z^T z} \right), \tag{2.12}$$

where $z^T z = (\varrho/\gamma) b$ by (2.2) and the following assertion holds. Note that scaling of Ty has no influence on vector $Ty/y^T Ty$.

Lemma 2.1. *Every update (2.12) with $z = \alpha_1 S^T y + \alpha_2 S^T Bs$, $Ty = \beta_1 s + \beta_2 Hy$, satisfying $z^T z = (\varrho/\gamma) b$ and $b\beta_1 + a\beta_2 > 0$ (i.e. $y^T Ty > 0$), belongs to the scaled Broyden class with*

$$\eta = b \frac{b\beta_1^2 - a(\gamma/\varrho)(\alpha_1\beta_1 - \alpha_2\beta_2)^2}{(b\beta_1 + a\beta_2)^2}. \tag{2.13}$$

Proof. See Lemma 2.2 in [11]. □

Thus we concentrate here on the choice $z = \alpha_1 U^T y + \alpha_2 U^T Bs$, $\alpha_2 \neq 0$, which can be written in the form $z = \alpha_1 U^T y - \alpha_2 t\, U^T g$ by $s = -tHg$, where t is the stepsize. Since z must satisfy the condition $z^T z = (\varrho/\gamma) b$, we have

$$z = \pm \sqrt{\frac{\varrho}{\gamma} \frac{b}{\bar{a}\theta^2 + 2\bar{b}\theta + \bar{c}}} (U^T Bs + \theta\, U^T y), \tag{2.14}$$

where $\theta = \alpha_1/\alpha_2$. The following lemma gives simple conditions for z to be invariant under linear transformations. Note that the standard unit values of ϱ, γ, used in our numerical experiments, satisfy this conditions.

Lemma 2.2. *Let numbers ϱ, γ and ratio θ/t are invariant under transformation of variables $\tilde{x} = Rx + r$, where R is $N \times N$ nonsingular matrix and $r \in \mathcal{R}^N$, and suppose that $\tilde{U} = RU$. Then vector z given by (2.14) is invariant under this transformation.*

Proof. In the proof of Theorem 2.2 we proved that $\tilde{b} = b$, $\tilde{y} = R^{-T} y$ and $\tilde{g} = R^{-T} g$, which yields invariance of vectors $U^T y$, $U^T g$ and therefore also $(U^T Bs + \theta\, U^T y)/t = -U^T g + (\theta/t) U^T y$. Since $\bar{a} = |U^T y|^2$, $\bar{b} = (U^T Bs)^T U^T y = -t(U^T g)^T U^T y$, $\bar{c} = |U^T Bs|^2 = t^2 |U^T g|^2$, we deduce that the term $\bar{a}\theta^2 + 2\bar{b}\theta + \bar{c}$, divided by t^2, is also invariant, which completes the proof. □

In our numerical experiments we use the choice $\theta = -\bar{b}/\bar{a}$ for $\bar{a} \neq 0$ (if $\bar{a} = 0$, we do not update), which gives good results. Then θ/t is invariant, see the proof of Lemma 2.2, and (2.14) gives

$$z = \pm\sqrt{\frac{\varrho}{\gamma}\frac{b}{\bar{a}\bar{\delta}}}(\bar{a}\, U^T B s - \bar{b}\, U^T y). \tag{2.15}$$

Moreover, in this case we have $y^T U z = 0$ and $V_p U z = U z$, thus relations (2.10), (2.11) can be simplified.

2.2 Variationally-derived simple correction

Similarly as in shifted VM methods, see [12], [10], we add a multiple of the unit matrix to $U_+ U_+^T$, which is singular, to obtain the direction vector. However, here this modification of VM matrix violates the quasi-Newton condition (2.1). We will find the minimum correction (in the sense of Frobenius matrix norm) of matrix $\bar{H}_+ + \zeta I$, $\zeta > 0$, in order that the resultant matrix H_+ may satisfy the quasi-Newton condition $H_+ y = \varrho s$. First we give the projection variant of the well-known Greenstadt's theorem, see [4].

Theorem 2.3. *Let M, W be symmetric matrices, W positive definite, $\varrho > 0$, $q = Wy$ and denote $\mathcal{M}$ the set of $N \times N$ symmetric matrices. Then the unique solution to*

$$\min\{\|W^{-1/2}(M_+ - M)W^{-1/2}\|_F : \, M_+ \in \mathcal{M}\} \quad \text{s.t.} \quad M_+ y = \varrho s \tag{2.16}$$

is determined by the relation $V_q\,(M_+ - M)\,V_q^T = 0$ and can be written in the form

$$M_+ = E + V_q\,(M - E)\,V_q^T, \tag{2.17}$$

where E is any symmetric matrix satisfying $Ey = \varrho s$, e.g. $E = (\varrho/b)ss^T$.

Proof. Denoting $w = (M_+ - M)y = \varrho s - My$, the unique solution to (2.16) is (see [4])

$$M_+ = M + \frac{wq^T + qw^T}{q^T y} - \frac{w^T y}{(q^T y)^2}\, qq^T. \tag{2.18}$$

Using $w = -(M - E)y$, $w^T y = -y^T(M - E)y$ and identity

$$V_q(M - E)V_q^T = M - E - \frac{(M - E)yq^T + qy^T(M - E)}{q^T y} + \frac{y^T(M - E)y}{(q^T y)^2}\, qq^T,$$

we immediately obtain (2.17) from (2.18); for $E = M_+$ we get $V_q\,(M_+ - M)\,V_q^T = 0$. □

In the case $M = \bar{H}_+ + \zeta I$, relation (2.17) can be simplified. The resulting correction (2.19) together with update (2.4) give the new family of limited-memory VM methods.

Theorem 2.4. *Let W be a symmetric positive definite matrix, $\zeta > 0$, $\varrho > 0$, $q = Wy$ and denote $\mathcal{M}$ the set of $N \times N$ symmetric matrices. Suppose that matrix $\bar{H}_+$ satisfies the quasi-Newton condition (2.1). Then the unique solution to*

$$\min\{\|W^{-1/2}(H_+ - \bar{H}_+ - \zeta I)W^{-1/2}\|_F : H_+ \in \mathcal{M}\} \quad \text{s.t.} \quad H_+ y = \varrho s$$

is

$$H_+ = \bar{H}_+ + \zeta V_q V_q^T. \tag{2.19}$$

Proof. Using Theorem 2.3 with $M = \bar{H}_+ + \zeta I$, $M_+ = H_+$, we get

$$H_+ = E + V_q \left(\bar{H}_+ + \zeta I - E\right) V_q^T, \tag{2.20}$$

where E is symmetric matrix and $Ey = \varrho s = \bar{H}_+ y$ by (2.1). Thus $(\bar{H}_+ - E)y = 0$, which yields $V_q(\bar{H}_+ - E) = \bar{H}_+ - E$, and we immediately obtain (2.19) from (2.20). $\square$

To choose parameter ζ, the good choice is $\zeta = \varrho b / y^T y$, which minimizes $|(\bar{H}_+ - \zeta I)y|$ and which is widely used for the scaling in the first iteration of VM methods, see [6]. We can obtain slightly better results, when we respect the current approximation $\bar{H}$ of the inverse Hessian, e.g. by the choice

$$\zeta = \frac{\varrho\, b}{y^T y + \omega\, \bar{a}} \tag{2.21}$$

with suitable $\omega > 0$; we obtained good results with $\omega \in [2, 20]$, e.g. $\omega = 4$.

As regards parameter q, we can utilize comparison with the scaled Broyden class (see [6]). First we show that for vector q lying in the subspace generated by the vectors s and My, update (2.17) belongs to the Broyden class update (see also a similar result in [5] or [6] for the inverse matrix updating).

Lemma 2.3. *Let A be a symmetric matrix, $\gamma > 0$, $\varrho > 0$ and denote $a = y^T A y$. Then every update (2.17) with $M = \gamma A$, $M_+ = A_+$, $q = s - \alpha A y$, $a \neq 0$ and $\alpha\, a \neq b$ represents the scaled Broyden class update with*

$$\eta = \frac{b^2}{(b - \alpha a)^2} \left(1 - \alpha^2 \frac{\varrho}{\gamma} \frac{a}{b}\right). \tag{2.22}$$

Proof. With $M = \gamma A$, $M_+ = A_+$ and $E = (\varrho / b) s s^T$ we can write update (2.17) in the form

$$\frac{1}{\gamma} A_+ = \frac{\varrho}{\gamma} \frac{s s^T}{b} + V_q A V_q^T - \frac{\varrho}{\gamma} \frac{V_q s s^T V_q^T}{b}. \tag{2.23}$$

Setting $\lambda = b/(b - \alpha a)$ we have $\alpha = -(1-\lambda) b / (\lambda a)$ and $(\lambda / b) q = (\lambda / b) s + ((1-\lambda)/a) A y$. Using (2.9), we can thus express (2.23) without the last term equivalently as (2.8). Since $q^T y = b / \lambda$ and $(1 - \lambda) b / a = -\lambda \alpha$, we get

$$V_q s = s - \lambda q = (1 - \lambda)\left(s - \frac{b}{a} A y\right) = (1 - \lambda) \frac{b}{a} \left(\frac{a}{b} s - A y\right) = -\lambda \alpha\, v,$$

where $v = (a/b)s - Ay$. Therefore the last term in (2.23) is $-(\delta/a)vv^T$, where $\delta = \lambda^2\alpha^2(\varrho/\gamma)a/b$. Comparing it with (2.8), we see that (2.23) represents the scaled Broyden class update with parameter $\eta = \lambda^2 - \delta$, which implies (2.22). $\square$

The following lemma enables us to determine vector q in such a way that correction (2.19) represents the Broyden class update of $\bar{H}_+ + \zeta I$ with parameter η.

Lemma 2.4. *Let $\varrho > 0$, $\zeta > 0$, $\kappa = \zeta\, y^T y/b$, $\eta > -\varrho/(\varrho+\kappa)$ and let matrix $\bar{H}_+$ satisfy the quasi-Newton condition (2.1). Then correction (2.19) with $q = s - \sigma y$, where*

$$\sigma = \frac{b}{y^T y}\left(1 \pm \sqrt{\frac{\varrho+\kappa}{\varrho+\eta\kappa}}\,\right) \tag{2.24}$$

represents the non-scaled Broyden class update of matrix $\bar{H}_+ + \zeta I$ with parameter η and nonquadratic correction ϱ.

Proof. It follows from $\eta > -\varrho/(\varrho+\kappa)$ that $\varrho+\eta\kappa > \varrho - \varrho\kappa/(\varrho+\kappa) = \varrho^2/(\varrho+\kappa)$, thus the right-hand side in (2.24) is well defined and $\varrho\sqrt{(\varrho+\kappa)/(\varrho+\eta\kappa)} < \varrho+\kappa$, which yields $\zeta + \varrho\,\sigma = (b/y^T y)\left[\varrho+\kappa \pm \varrho\sqrt{(\varrho+\kappa)/(\varrho+\eta\kappa)}\,\right] > 0$ by (2.24) and $\zeta = \kappa\, b/y^T y$. Vector q is proportional to $\bar{q} = s - \alpha(\bar{H}_+ + \zeta I)y$, where $\alpha = \sigma/(\zeta+\varrho\,\sigma)$, since

$$\bar{q} = (1-\varrho\alpha)s - \alpha\zeta y = \frac{\zeta}{\zeta+\varrho\,\sigma}s - \frac{\zeta\sigma}{\zeta+\varrho\,\sigma}y = \frac{\zeta}{\zeta+\varrho\,\sigma}\,q$$

by (2.1), therefore $V_q = V_{\bar{q}}$. It follows from Theorem 2.4 and Theorem 2.3 that correction (2.19) is a special case of update (2.17) for $M = \bar{H}_+ + \zeta I$.

In order to can use Lemma 2.3 for $A = \bar{H}_+ + \zeta I$, we show that $y^T A y \neq 0$ and $\alpha\, y^T A y \neq b$. By (2.1) we have $y^T A y = b(\varrho+\kappa) > 0$ and $\alpha\, y^T A y/b = (\kappa\sigma+\varrho\sigma)/(\zeta+\varrho\,\sigma)$, which cannot be equal to unit, since σ cannot be equal to $b/y^T y = \zeta/\kappa$ by (2.24). Using Lemma 2.3 with $\gamma = 1$, $a = b(\varrho+\kappa)$ and $\alpha = \sigma/(\zeta+\varrho\,\sigma)$, we obtain

$$\eta = \frac{1-\alpha^2\varrho(\varrho+\kappa)}{(1-\alpha(\varrho+\kappa))^2} = \frac{(\zeta+\varrho\,\sigma)^2 - \sigma^2\varrho(\varrho+\kappa)}{(\zeta+\varrho\,\sigma-\sigma(\varrho+\kappa))^2} = \frac{\zeta^2 + 2\,\zeta\sigma\varrho - \sigma^2\kappa\varrho}{\zeta^2 - 2\,\zeta\sigma\kappa + \sigma^2\kappa^2}$$

and consequently the quadratic equation $\sigma^2\kappa(\varrho+\eta\kappa) - 2\sigma\zeta(\varrho+\eta\kappa) + \zeta^2(\eta-1) = 0$ with the solution

$$\sigma = \frac{\zeta}{\kappa} \pm \frac{\zeta}{\kappa}\sqrt{1 + \frac{\kappa(1-\eta)}{\varrho+\eta\kappa}},$$

which gives (2.24) by $\kappa = \zeta\, y^T y/b$. $\square$

If we choose $q = s$, i.e. $\eta = 1$, we get the BFGS update. Better results were obtained with the special formula, which is based on analogy with the shifted VM methods (see [12]) and on the following lemma.

Lemma 2.5. *Let $\varrho > 0$, $\zeta > 0$, $\kappa = \zeta\, y^T y/b$, $\check{s} = s - (b/y^T y)y$, $\eta > -\varrho/(\varrho+\kappa)$ and suppose that $q = s - \sigma y$, where σ is given by (2.24). Then*

$$\zeta V_q V_q^T = \zeta V_s V_s^T + \frac{(\eta-1)\kappa^2}{(\varrho+\kappa)b}\check{s}\check{s}^T. \tag{2.25}$$

Proof. Denoting $\hat{a} = y^T y$, we get $q^T y = b - \sigma\hat{a} \neq 0$ by (2.24). Therefore we can write

$$V_q V_q^T = I - \frac{q y^T + y q^T}{q^T y} + \frac{\hat{a}}{(q^T y)^2}\, q q^T = I + \frac{\hat{a}}{(q^T y)^2}\Big(q - \frac{q^T y}{\hat{a}} y\Big)\Big(q - \frac{q^T y}{\hat{a}} y\Big)^T - \frac{y y^T}{\hat{a}}$$

and similarly $V_s V_s^T = I + (\hat{a}/b^2)\check{s}\check{s}^T - y y^T/\hat{a}$. Since $q - (q^T y/\hat{a})y = s - \sigma y - (b/\hat{a} - \sigma)y = \check{s}$, we obtain

$$V_q V_q^T = V_s V_s^T + \Big(\frac{\hat{a}}{(b-\sigma\hat{a})^2} - \frac{\hat{a}}{b^2}\Big)\check{s}\check{s}^T.$$

Using (2.24) and $\zeta = \kappa b/\hat{a}$, we get

$$\zeta\Big(\frac{\hat{a}}{(b-\sigma\hat{a})^2} - \frac{\hat{a}}{b^2}\Big) = \frac{\kappa}{b}\Big(\frac{1}{(1-\sigma\hat{a}/b)^2} - 1\Big) = \frac{\kappa}{b}\Big(\frac{\varrho + \eta\kappa}{\varrho + \kappa} - 1\Big) = \frac{\eta - 1}{b}\frac{\kappa^2}{\varrho + \kappa},$$

which gives (2.25). □

Assuming, in virtue of analogy with the shifted VM methods, that the matrices ss^T and $\check{s}\check{s}^T$ have a similar character, we see from (2.6), that the adding of the correction matrix $V_q V_q^T$ to $\bar{H}_+$ in (2.19) corresponds to the adding of the number $(\eta-1)\kappa^2/(\varrho+\kappa)$ to the nonquadratic correction parameter ϱ. Denoting the total by $\bar{\varrho}$, we have $\eta = 1 + (\bar{\varrho} - \varrho)(\varrho + \kappa)/\kappa^2$. Our numerical experiments indicate that we should choose $\eta \in [0, 1]$ (note that for any $\eta \geq 0$ matrix H_+ in (2.19) is positive definite in view of the Broyden class updates properties, see e.g. [3]). To have $\eta \geq 0$, we need

$$\bar{\varrho} \geq \varrho - \kappa^2/(\varrho + \kappa) = (\varrho^2 + \varrho\kappa - \kappa^2)/(\varrho + \kappa) \geq \varrho^2/(\varrho + \kappa) \geq \varrho/2$$

in view of $\kappa \leq \varrho$ by (2.21). Since the suitable value of $\bar{\varrho}/\varrho$ for the shifted VM updates is e.g. $\zeta_-/(\zeta_- + \zeta)$ (see [12]), which is less than 1/2 for $\zeta > \zeta_-$, we scale this value to have $\eta \geq 0$ more often. This leads to the formula

$$\eta = \min\left[1, \max\left[0\,, 1 + \varrho\frac{\varrho + \kappa}{\kappa^2}\Big(\frac{1.2\,\zeta_-}{\zeta_- + \zeta} - 1\Big)\right]\right]. \tag{2.26}$$

2.3 Relationship between updates with minimum change property

In this section we describe properties of variationally-derived update (2.17) for some other interesting choices of vector q. We do not concern with the correction term ζI, since from (2.17) we can see that the adding ζI to matrix M causes the adding of the term $\zeta V_q V_q^T$ to matrix M_+.

In case that $A = \bar{H} = UU^T$, we can use Theorem 2.3 to find such vector q that the solution to problem (2.16) also represents the solution to problem (2.3) with $Ty = q$.

Theorem 2.5. *Let W be a symmetric positive definite matrix, $\bar{H} = UU^T$, $\varrho > 0$, $\gamma > 0$, $q = Wy$ and $z \in \mathcal{R}^m$ any vector satisfying $z^T z = (\varrho/\gamma)b$. Then for $q = (\varrho/\gamma)s \pm Uz$ the Frobenius norm $\|W^{-1/2}(\bar{H}_+ - \gamma\bar{H})W^{-1/2}\|_F$ reaches its minimum on the set of symmetric matrices $\bar{H}_+$ satisfying $\bar{H}_+ y = \varrho s$, if and only if $\bar{H}_+ = U_+ U_+^T$, where U_+ is given by (2.4) with $Ty = q$, which can be for $q = (\varrho/\gamma)s - Uz$ written in the form*

$$\frac{1}{\sqrt{\gamma}}U_+ = U + \frac{q(z - U^T y)^T}{q^T y} = U + \frac{q(z - U^T y)^T}{(z - U^T y)^T z}. \tag{2.27}$$

Proof. Using Theorem 2.3 with $M = \gamma \bar{H}$, $M_+ = \bar{H}_+$ and $E = (\varrho/b) ss^T$ we can see that the only minimizing matrix $\bar{H}_+$ satisfies

$$\frac{1}{\gamma}\bar{H}_+ = \frac{\varrho}{\gamma}\frac{ss^T}{b} + V_q\left(\bar{H} - \frac{\varrho}{\gamma}\frac{ss^T}{b}\right)V_q^T.$$

By $V_q q = 0$ we have $V_q s = \mp(\gamma/\varrho) V_q U z$. Using $z^T z = (\varrho/\gamma) b$, it gives

$$\begin{aligned}\frac{1}{\gamma}\bar{H}_+ &= \frac{\varrho}{\gamma}\frac{ss^T}{b} + V_q\left(\bar{H} - \frac{Uzz^TU^T}{z^Tz}\right)V_q^T \\ &= \left[\frac{sz^T}{b} + V_q U\left(I - \frac{zz^T}{z^Tz}\right)\right]\left[\frac{sz^T}{b} + V_q U\left(I - \frac{zz^T}{z^Tz}\right)\right]^T\end{aligned}$$

by $z^T(I - zz^T/z^Tz) = 0$ and $(I - zz^T/z^Tz)^2 = I - zz^T/z^Tz$, which gives (2.4) with $Ty = q$.

If $q = (\varrho/\gamma)s - Uz$, we have $(\gamma/\varrho)V_q U z = V_q s$ by $V_q q = 0$ and for U_+ defined this way we obtain from (2.4) by $z^T z = (\varrho/\gamma) b$

$$\frac{1}{\sqrt{\gamma}}U_+ = V_q U + \frac{sz^T}{b} - \frac{V_q U zz^T}{z^T z} = V_q U + \frac{(s - V_q s)z^T}{b} = U - \frac{qy^T U}{q^T y} + \frac{qz^T}{q^T y},$$

which yields (2.27). □

We can obtain similar result for any symmetric matrix A and find such vector q that the solution to problem (2.16) can be expressed in the product form.

Theorem 2.6. *Let A, W be symmetric matrices, W positive definite, $\varrho > 0$, $\gamma > 0$, $q = Wy$ and $r \in \mathcal{R}^N$ any vector satisfying $r^T A r = (\varrho/\gamma) b$. Then for $q = (\varrho/\gamma)s \pm Ar$ the Frobenius norm $\|W^{-1/2}(A_+ - \gamma A)W^{-1/2}\|_F$ reaches its minimum on the set of symmetric matrices A_+ satisfying $A_+ y = \varrho s$, if and only if $(1/\gamma)A_+ = CAC^T$, where*

$$C = \frac{sr^T}{b} + V_q\left(I - \frac{Arr^T}{r^TAr}\right). \tag{2.28}$$

If $q = (\varrho/\gamma)s - Ar$, we can write (2.28) in the form

$$C = I + \frac{q(r-y)^T}{q^Ty} = I + \frac{q(r-y)^T}{(r-y)^TAr}. \tag{2.29}$$

Proof. Using Theorem 2.3 with $M = \gamma A$, $M_+ = A_+$ and $E = (\varrho/b) ss^T$ we can see that the only minimizing matrix A_+ satisfies

$$\frac{1}{\gamma}A_+ = \frac{\varrho}{\gamma}\frac{ss^T}{b} + V_q\left(A - \frac{\varrho}{\gamma}\frac{ss^T}{b}\right)V_q^T.$$

By $V_q q = 0$ we have $V_q s = \mp(\gamma/\varrho) V_q A r$. Using $r^T A r = (\varrho/\gamma) b$, it gives

$$\begin{aligned}\frac{1}{\gamma}A_+ &= \frac{\varrho}{\gamma}\frac{ss^T}{b} + V_q\left(A - \frac{Arr^TA}{r^TAr}\right)V_q^T \\ &= \left[\frac{sr^T}{b} + V_q\left(I - \frac{Arr^T}{r^TAr}\right)\right]A\left[\frac{sr^T}{b} + V_q\left(I - \frac{Arr^T}{r^TAr}\right)\right]^T\end{aligned}$$

by $(I - Arr^T/r^TAr)Ar = 0$ and $(I - Arr^T/r^TAr)A(I - Arr^T/r^TAr)^T = A - Arr^TA/r^TAr$, which gives (2.28).

If $q = (\varrho/\gamma)s - Ar$, we have $V_qAr = (\varrho/\gamma)V_qs$ by $V_qq = 0$ and from (2.28) we obtain

$$C = V_q + \frac{sr^T}{b} - \frac{V_qArr^T}{r^TAr} = V_q + \frac{(s - V_qs)r^T}{b} = I - \frac{qy^T}{q^Ty} + \frac{qr^T}{q^Ty},$$

by $r^TAr = (\varrho/\gamma)b$, which yields (2.29). $\square$

Using this theorem we can obtain the product form for many variationally-derived VM updates, e.g. the choice $r = \pm\sqrt{(\varrho/\gamma)b/s^TBs}\, Bs$ with $A = H$ and $A_+ = H_+$ gives the product form of the BFGS update, see [6].

2.4 Quadratic termination property

In this section we give conditions for our family of limited-memory VM methods with exact line searches to terminate on a quadratic function in at most N iterations.

Theorem 2.7. *Let $m \in \mathcal{N}$ be given and let $Q : \mathcal{R}^N \to \mathcal{R}$ be a strictly convex quadratic function $Q(x) = \frac{1}{2}(x - x^*)^TG(x - x^*)$, where G is an $N \times N$ symmetric positive definite matrix. Suppose that $\zeta_k > 0$, $\varrho_k > 0$, $\gamma_k > 0$, $k \geq 0$, and that for $x_0 \in \mathcal{R}^N$ iterations x_{k+1} are generated by the method*

$$x_{k+1} = x_k + t_kd_k, \quad d_k = -H_kg_k, \quad g_k = \nabla Q(x_k) = G(x_k - x^*) \tag{2.30}$$

$k \geq 0$, with exact line searches, i.e. $g_{k+1}^Td_k = 0$, where

$$H_0 = I, \quad H_{k+1} = U_{k+1}U_{k+1}^T + \zeta_kV_{q_k}V_{q_k}^T,\ k \geq 0, \tag{2.31}$$

$N \times \min(k, m)$ matrices U_k, $k > 0$, satisfy

$$U_1 = \left(\sqrt{\frac{\varrho_0}{b_0}}s_0\right), \quad \frac{1}{\gamma_k}U_{k+1}U_{k+1}^T = \frac{\varrho_k}{\gamma_k}\frac{s_ks_k^T}{b_k} + V_{p_k}U_kU_k^TV_{p_k}^T,\ 0 < k < m, \tag{2.32}$$

$$\frac{1}{\gamma_k}U_{k+1}U_{k+1}^T = \frac{\varrho_k}{\gamma_k}\frac{s_ks_k^T}{b_k} + V_{p_k}U_k\left(I - \frac{z_kz_k^T}{z_k^Tz_k}\right)U_k^TV_{p_k}^T,\ k \geq m, \tag{2.33}$$

vectors $z_k \in \mathcal{R}^m$, $k \geq m$, satisfy $z_k^Tz_k = (\varrho_k/\gamma_k)b_k$, vectors p_k, $k > 0$, lie in $\mathrm{range}([U_k, s_k])$ *and satisfy $p_k^Ty_k \neq 0$, vectors q_k for $k > 0$ lie in* $\mathrm{span}\{s_k, U_kU_k^Ty_k\}$ *and satisfy $q_k^Ty_k \neq 0$ and vector $q_0 = s_0$. Then there exists a number $\bar{k} \leq N$ with $g_{\bar{k}} = 0$ and $x_{\bar{k}} = x^*$.*

Proof. We assume that $g_k \neq 0$, $k < N$ and show that then $g_N = 0$. First we prove by induction that for $k = 0, \ldots, N-1$ matrix H_k is well defined and the following hold

(α) $g_k^Td_i = 0,\ i < k,$ $\quad(\beta)$ $g_k^TU_i = 0,\ 1 \leq i \leq k,$ $\quad(\gamma)$ $g_k^Td_k < 0,\ t_k > 0,$
(δ) $d_k^TGd_i = 0,\ i < k,$ $\quad(\varepsilon)$ $g_i \in \mathrm{span}\{d_i, d_j\},\ i \leq k,$

where $j = \max(i-1, 0)$. For $k = 0$, (α), (β) and (δ) are vacuous, $H_0 = I$ by (2.31) and (ε) is true, since $d_0 = -g_0$ by (2.30). Thus we have $g_0^Td_0 = -g_0^Tg_0 < 0$, which yields $t_0 > 0$ by convexity of Q. Suppose that these relations hold for $k < N-1$.

(a) The exact line search gives $d_k^T g_{k+1} = 0$, thus $b_k = s_k^T y_k = -t_k \, d_k^T g_k > 0$ by (γ) and matrix H_{k+1} is well defined. Since $y_k = G s_k$ by (2.30), we get $g_{k+1}^T d_i = g_k^T d_i + y_k^T d_i = s_k^T G d_i = 0$ by (α) and (δ) for $i < k$, thus (α) also holds for $k+1$.

(b) Due to (a) and (2.32) we have $g_{k+1}^T U_1 = 0$. By induction, let $g_{k+1}^T U_i = 0$ for some $1 \le i \le k$. Since $g_{k+1}^T s_i = 0$ by (a) and $p_i \in \text{range}([U_i, s_i])$, we obtain $g_{k+1}^T p_i = 0$, which yields $V_{p_i}^T g_{k+1} = g_{k+1}$ and $U_i^T V_{p_i}^T g_{k+1} = 0$. Using (2.32) or (2.33) we get $|U_{i+1}^T g_{k+1}|^2 = 0$, which completes the induction and (β) also holds for $k+1$.

(c) It follows from (b) that $U_k^T g_{k+1} = U_k^T g_k = 0$, which yields $U_k^T y_k = 0$. In view of $q_0 = s_0$ and $q_i \in \text{span}\{s_i, U_i U_i^T y_i\}$, $i > 0$, we have $q_k = \alpha_k d_k$, $\alpha_k \in \mathcal{R}$, thus $g_{k+1}^T q_k = 0$ by (a) and $V_{q_k}^T g_{k+1} = g_{k+1}$. From (2.31) we get

$$-d_{k+1} = H_{k+1} g_{k+1} = \zeta_k V_{q_k} V_{q_k}^T g_{k+1} = \zeta_k V_{q_k} g_{k+1} = \zeta_k \left(g_{k+1} - \frac{g_{k+1}^T y_k}{q_k^T y_k} q_k \right) \quad (2.34)$$

by (b), thus $g_{k+1}^T d_{k+1} = -\zeta_k |g_{k+1}|^2 < 0$ and $t_{k+1} > 0$, i.e. (γ) also holds for $k+1$.

(d) From (2.34) we obtain $d_{k+1}^T y_k = 0$, thus $d_{k+1}^T G s_k = 0$. For $i < k$ it follows from $q_k = \alpha_k d_k$, $\alpha_k \in \mathcal{R}$, which we proved in (c), that $q_k^T G s_i = 0$ by (δ). It follows from (ε) that $y_i \in \text{span}\{d_0, \ldots, d_k\}$ and (2.34) gets $-d_{k+1}^T G s_i = \zeta_k g_{k+1}^T G s_i = \zeta_k g_{k+1}^T y_i = 0$ by (a), thus (δ) also holds for $k+1$.

(e) It follows directly from (2.34) and $q_k = \alpha_k d_k$ that (ε) also holds for $k+1$.

Now we establish $g_N = 0$. Proceeding as in (a) for $k = N-1$, we get $g_N^T d_i = 0$ for all $i < N$. Since vectors $d_0, \ldots, d_{N-1}$ are conjugate to the positive definite matrix G, they are independent, thus $g_N = 0$ and $x_N = x^*$ by (2.30) and positive definiteness of G. $\square$

3 Correction formula

Efficiency of all methods from our new family can be increased, if we use additional correction of matrix H_+ for the calculation of the direction vector d_+.

Corrections in Section 2.2 respect only the latest vectors s_k, y_k. Thus for $k > 0$ we can again correct (without scaling) the resulting matrices $\check{H}_{k+1} = \bar{H}_{k+1} + \zeta_k V_{q_k} V_{q_k}^T$, obtained from (2.19), using previous vectors s_i, y_i, $i = k-j, \ldots, k-1$, $j \le k$. Our experiments indicate that the choice $j = 1$ brings the maximum improvement. Note that the correcting of matrix $\bar{H}_{k+1} + \zeta_k I$ instead of $\check{H}_{k+1}$ does not give so good results.

Replacing q by s, the correction formula (2.17) has the simple form

$$M_+ = \frac{\varrho}{b} s s^T + V_s M V_s^T \quad (3.1)$$

by $V_s E V_s^T = E - \varrho \, s s^T / b$, which holds for any symmetric matrix E satisfying $Ey = \varrho s$, thus we confine in this section to this formula. To correct matrix $\check{H}_+$, we use (3.1) first with vectors s_-, y_- and then again with s, y. This leads to the formula

$$H_+ = \varrho \frac{s s^T}{b} + V_s \left[\varrho_- \frac{s_- s_-^T}{b_-} + V_s^- \left(\bar{H}_+ + \zeta V_q V_q^T \right) (V_s^-)^T \right] V_s^T, \quad (3.2)$$

where $V_s^- = I - s_- y_-^T / b_-$, which is less sensitive to the choice of ζ than (2.19).

To calculate the direction vector $d_+ = -H_+ g_+$, we can utilize the Strang formula, see [9], which can be for H_+ given by (3.2) written as the following algorithm:

(1) $\alpha_1 = -s^T g_+ / b$, $\quad u = -g_+ - \alpha_1 y$,
(2) $\alpha_2 = s_-^T u / b_-$, $\quad u := u - \alpha_2 y_-$,
(3) $u := \bar{H}_+ u + \zeta V_q V_q^T u$,
(4) $\beta_1 = y_-^T u / b_-$, $\quad u := u + (\varrho_- \alpha_2 - \beta_1) s_-$,
(5) $\beta_2 = y^T u / b$, $\quad d_+ = u + (\varrho\, \alpha_1 - \beta_2) s$.

4 Computational experiments

Our new limited-memory VM methods were tested, using the collection of sparse, usually ill-conditioned problems for large-scale nonlinear least squares from [7] (Test 15 without problem 18, which was very sensitive to the choice of the maximum stepsize in linesearch, i.e. 21 problems) with $N = 500$ and 1000, $m = 10$, $\varrho = \gamma = 1$, the final precision $\|g(x^\star)\|_\infty \le 10^{-5}$ and ζ given by (2.21) with $\omega = 4$.

η_p	$N = 500$				$N = 1000$			
	Corr-0	Corr-1	Corr-2	Corr-q	Corr-0	Corr-1	Corr-2	Corr-q
0.0	(2)76916	32504	22626	24016	(3)99957	(1)58904	44608	(1)47204
0.1	(3)99032	36058	21839	35756	(3)98270	(1)54494	42649	(1)47483
0.2	(2)97170	29488	23732	29310	(3)89898	(1)52368	36178	(1)44115
0.3	(1)79978	28232	18388	18913	(3)80087	47524	33076	38030
0.4	(1)70460	24686	18098	17673	(3)78498	44069	32403	34437
0.5	60947	22532	17440	17181	(3)88918	41558	32808	31874
0.6	56612	21240	17800	17164	(2)76264	38805	31854	30784
0.7	52465	20289	17421	17021	(2)72626	39860	32345	30802
0.8	51613	20623	17682	17076	(1)69807	37501	32292	32499
0.9	50877	20548	18102	17424	(2)69802	38641	32926	31385
1.0	49672	20500	18109	17913	(1)68603	38510	33539	32456
1.1	52395	20994	18694	18470	(1)65676	41284	35103	33053
1.2	51270	21444	19230	18372	(1)68711	41332	35649	34028
1.3	(1)50064	21899	19289	19890	(2)67976	41491	36155	34776
1.4	(1)52255	21900	19737	19695	(2)67340	43758	35793	35998
1.5	(1)51094	22808	20487	20060	(2)66220	42906	36775	36323
2.0	(1)50776	24318	21710	21639	(2)66594	46139	40279	39199
3.0	(1)54714	28641	24634	24675	(2)68680	(1)54531	45366	44785
BNS	18444				33131			

Table 1. Comparison of various correction methods.

The following procedure for computing of matrices U_{k+1}, $k \ge 0$, was used (details are described in Section 2.1):

(1) If $k = 0$, set $U_1 = \left[\sqrt{1/b_0}\, s_0\right]$.

(2) If $0 < k < m$, set $U_{k+1} = \left[V_{s_k} U_k, \sqrt{1/b_k}\, s_k\right]$.

(3) If $k \geq m$, set

$$U_{k+1} = U_k - \frac{p_k}{p_k^T y_k} y_k^T U_k + \frac{s_k - U_k z_k}{b_k} z_k^T$$

with the chosen parameter p_k and z_k given by (2.15).

Results of these experiments are given in three tables, where $\eta_p = \lambda^2$ is the value of parameter η of the Broyden class used to determine parameter p by (2.7) and η_q is the value of this parameter used in (2.24) to determine parameter $q = s - \sigma y$.

	η_p						
η_q	0.4	0.5	0.6	0.7	0.8	0.9	1.0
0.0	-343	-394	-967	-813	-538	32	141
0.1	211	-1154	-1028	-1100	-880	-585	-188
0.2	2424	1902	1759	2088	1869	2268	2746
0.3	-492	-1064	-1136	-992	-1036	-901	-939
0.4	-599	-1069	-718	-1160	-668	-934	-512
0.5	-493	-722	-727	-665	-487	-516	-399
0.6	-251	-648	-798	-965	-750	-176	-371
0.7	-342	-764	-441	-320	-474	-749	-284
0.8	-481	-706	-857	-579	-449	-497	-606
0.9	-872	-759	-370	-559	-820	275	-135
1.0	-346	-1004	-644	-1023	-762	-342	-335
1.1	1939	1265	2326	791	2444	1958	1910
1.2	1024	700	719	1452	967	1479	1982
1.3	-322	-410	-785	-872	-332	333	174
1.4	-600	-718	-839	-1324	-959	-811	222
1.5	-596	-436	-912	-937	-770	-285	307
1.6	-256	-474	-365	-370	-517	-86	203
1.7	-61	-430	-526	-158	-356	-211	85
1.8	-206	-102	-240	-618	-412	71	359
1.9	-293	-235	-169	-332	32	23	607
2.0	150	-396	85	259	336	222	684
2.5	467	357	863	701	890	1274	356
3.0	7698	5036	4903	4337	4218	3577	3541
(2.26)	-771	-1263	-1280	-1423	-1368	-1020	-531

Table 2. Comparison with BNS for N=500.

In Table 1 we compare the method after [2] (BNS) with our new family, using various values of η_p and the following correction methods: Corr-0 – the adding of matrix ζI to $\bar{H}_+$, Corr-1 – correction (2.19), Corr-2 – correction (3.2). We use $\eta_q = 1$ (i.e. $q = s$) in columns Corr-0, Corr-1 and Corr-2 and η_q given by (2.26) in columns

Corr-q together with correction (3.2). We present the total numbers of function and also gradient evaluations (over all problems), preceded by the number of problems (in parentheses, if any occurred) which were not solved successfully (usually if the number of evaluations reached its limit, which was here 19000 evaluations).

In Table 2 and Table 3 we give the differences $n_{p,q} - n_{BNS}$, where $n_{p,q}$ is the total number of function and also gradient evaluations (over all problems) for selected values of η_p and η_q with correction (3.2) and n_{BNS} is the number of evaluations for method BNS (negative values indicate that our method is better than BNS). In the last row we present this difference for η_q given by (2.26).

	η_p						
η_q	0.4	0.5	0.6	0.7	0.8	0.9	1.0
0.0	1916	-912	-681	-876	-119	-744	116
0.1	1052	-732	-974	-1647	-1043	-1215	320
0.2	903	-187	-1669	-1708	-1219	-28	-567
0.3	793	-363	-975	-1731	-289	360	-484
0.4	925	-1398	-1708	-1554	-1184	-498	-482
0.5	-757	-644	-965	-1729	-1380	-926	-207
0.6	1	-1396	-1291	-835	-1044	-767	190
0.7	-195	-901	-356	-1019	-1482	-398	-454
0.8	-770	-690	-1763	-886	-1009	-256	-977
0.9	8	-821	-939	-674	-696	-764	657
1.0	-728	-323	-1277	-786	-839	-205	408
1.1	-773	115	183	48	-411	-619	736
1.2	269	155	-670	295	-649	-113	647
1.3	51	150	-234	-527	-158	-323	1381
1.4	498	298	-522	246	-383	696	2533
1.5	377	-181	-29	908	1323	441	1310
1.6	1072	1135	766	-39	853	1307	2065
1.7	825	874	-199	79	607	1108	3370
1.8	1334	1147	667	1064	821	3854	2908
1.9	1470	486	1863	1047	1973	2609	3156
2.0	2164	767	994	2035	2577	2869	3036
2.5	2284	3821	3325	3337	3838	4929	5167
3.0	4570	4457	3423	4106	5172	4430	4818
(2.26)	1306	-1257	-2347	-2329	-632	-1746	-675

Table 3. Comparison with BNS for N=1000.

In these numerical experiments, limited-memory VM methods from our new family with suitable values of parameters η_p (e.g. $\eta_p = 0.7$) and η_q (e.g. η_q given by (2.26)) give better results than method BNS.

For a better comparison with method BNS, we performed additional tests with problems from the widely used CUTE collection [1] with various dimensions N and the final precision $\|g(x^\star)\|_\infty \le 10^{-6}$. The results are given in Table 4, where Corr-LMM is limited-memory VM methods from our new family with $\eta_p = \eta_q = 0.5$ and correction (3.2) (the other parameters are the same as above), NIT is the number of iterations, NFV the number of function and also gradient evaluations and Time the computer time in seconds.

CUTE		Corr-LMM			BNS		
Problem	N	NIT	NFV	Time	NIT	NFV	Time
ARWHEAD	5000	8	18	0.19	8	18	0.18
BDQRTIC	5000	216	301	1.49	145	220	1.04
BROWNAL	500	7	16	0.30	6	16	0.29
BROYDN7D	2000	2830	2858	10.28	2953	3021	10.03
BRYBND	5000	31	40	0.34	31	42	0.30
CHAINWOO	1000	414	467	0.36	429	469	0.36
COSINE	5000	21	30	0.19	14	19	0.14
CRAGGLVY	5000	88	101	0.77	84	101	0.69
CURLY10	1000	5428	5436	3.97	5827	5975	3.37
CURLY20	1000	5813	5818	5.05	6720	6907	5.06
CURLY30	1000	6537	6544	6.84	6831	7010	6.08
DIXMAANA	3000	10	14	0.06	9	13	0.06
DIXMAANB	3000	13	17	0.06	7	11	0.03
DIXMAANC	3000	12	16	0.06	9	13	0.06
DIXMAAND	3000	15	19	0.06	11	15	0.05
DIXMAANE	3000	392	396	1.08	237	249	0.55
DIXMAANF	3000	328	332	0.89	180	188	0.43
DIXMAANG	3000	345	349	0.80	178	187	0.44
DIXMAANH	3000	299	303	0.80	183	192	0.47
DIXMAANI	3000	2649	2653	6.88	855	877	1.97
DIXMAANJ	3000	776	780	1.97	340	351	0.84
DIXMAANK	3000	596	573	1.41	314	326	0.70
DIXMAANL	3000	541	545	1.42	221	230	0.52
DQRTIC	5000	966	907	2.86	235	236	0.52
EDENSCH	5000	26	28	0.25	25	29	0.23
EG2	1000	4	9	0.01	4	9	0.02
ENGVAL1	5000	23	40	0.24	26	35	0.20
EXTROSNB	5000	39	43	0.27	40	46	0.32
FLETCBV2	1000	1246	1248	1.33	1162	1182	1.14
FLETCHCR	1000	68	73	0.08	50	58	0.08
FMINSRF2	1024	405	408	2.33	332	340	1.73

Table 4a: Comparison with BNS for CUTE

CUTE		Corr-LMM			BNS		
Problem	N	NIT	NFV	Time	NIT	NFV	Time
FMINSURF	1024	513	517	2.97	462	477	2.50
FREUROTH	5000	22	47	0.31	24	32	0.27
GENHUMPS	1000	2424	2698	4.58	1802	2271	3.70
GENROSE	1000	2088	2199	1.63	2106	2374	1.58
LIARWHD	1000	21	29	0.16	23	28	0.19
MOREBV	5000	114	116	0.45	112	116	0.39
MSQRTALS	529	3136	3142	6.81	2880	2947	6.08
NCB20	510	783	845	4.38	505	561	2.81
NCB20B	1010	2087	2204	11.27	1584	1715	8.61
NONCVXU2	1000	2492	2493	2.45	3603	3685	3.06
NONCVXUN	1000	23993	23994	23.42	-	>50000	-
NONDIA	5000	14	19	0.19	25	30	0.27
NONDQUAR	5000	16080	16090	49.25	3210	3588	8.42
PENALTY1	1000	61	69	0.00	64	72	0.05
PENALTY3	100	61	91	0.63	56	92	0.66
POWELLSG	5000	45	57	0.09	37	46	0.14
POWER	1000	489	496	0.13	104	110	0.02
QUARTC	5000	966	967	2.70	235	236	0.52
SBRYBND	5000	-	-	-	-	-	-
SCHMVETT	5000	35	37	0.39	36	42	0.38
SCOSINE	5000	-	-	-	-	-	-
SINQUAD	5000	288	386	2.25	250	338	1.83
SPARSINE	1000	9396	9400	11.20	9347	9726	9.66
SPARSQUR	1000	35	41	0.06	37	43	0.05
SPMSRTLS	4999	201	204	1.24	213	223	1.14
SROSENBR	5000	12	19	0.08	18	23	0.11
TOINTGSS	5000	4	6	0.11	4	7	0.08
TQUARTIC	5000	19	25	0.17	21	30	0.20
VARDIM	1000	24	41	0.02	33	40	0.03
VAREIGVL	1000	143	146	0.14	164	171	0.16
WOODS	4000	34	41	0.14	28	33	0.11

Table 4b: Comparison with BNS for CUTE

Our limited numerical experiments indicate that methods from our new family can compete with the well-known BNS method.

References

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

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

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

[4] J. Greenstadt, *Variations on variable metric methods*, Math. Comput. 24 (1970) 1-22.

[5] J. Huschens, *On the use of product structure in secant methods for nonlinear least squares problems*, SIAM J. Optim. 4 (1994), 108-129.

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

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

[8] L. Lukšan, J. Vlček: *Test problems for unconstrained optimization*, Report V-897, Prague, ICS AS CR, 2003.

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

[10] J. Vlček, L. Lukšan: *New variable metric methods for unconstrained minimization covering the large-scale case*, Report V-876, Prague, ICS AS CR, 2002.

[11] J. Vlček, L. Lukšan: *Additional properties of shifted variable metric methods*, Report V-899, Prague, ICS AS CR, 2004.

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