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COMPUTATIONAL EXPERIENCE WITH IMPROVED VARIABLE METRIC METHODS FOR UNCONSTRAINED MINIMIZATION

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The paper describes three improved variable metric methods for unconstrained minimization and shows their efficiency on a broad class of test problems. These methods are based on the controlled scaling and on the pertinent combination of the rank-one method with other variable metric methods.

1. INTRODUCTION

Variable metric methods are the most frequently used optimization methods for problems of a moderate size or for problems with structured Hessian matrices. These methods are iterative and their iteration step has the form

$$x^+ = x + \alpha s \quad \text{where} \quad Bs = -g\,, \tag{1.1}$$

Here x and x^+ are old and new vector of variables respectively, s is a direction vector, α is a positive stepsize chosen so that

$$F^+ - F \leqq \varepsilon_1 \alpha s^T g \quad \text{and} \quad s^T g^+ \geqq \varepsilon_2 s^T g\,, \tag{1.2}$$

with $0 < \varepsilon_1 < \frac{1}{2}$ and $\varepsilon_1 < \varepsilon_2 < 1$, F and F^+ are old and new value of the objective function respectively, g and g^+ are old and new gradient of the objective function respectively, and B is a symmetric positive definite approximation of the Hessian matrix that is constructed iteratively by means of the formula

$$B^+ = \frac{1}{\gamma}\left(B + \frac{\gamma}{\varrho}\frac{1}{b} yy^T - \frac{1}{c} Bd(Bd)^T + \frac{\beta}{c}\left(\frac{c}{b} y - Bd\right)\left(\frac{c}{b} y - Bd\right)^T\right) \tag{1.3}$$

with three parameters $\varrho > 0$, $\gamma > 0$ and β. In (1.3) we use the notation

$$d = x^+ - x = \alpha s\,, \tag{1.4}$$

$$y = g^+ - g\,,$$

and
$$a = y^T B^{-1} y ,$$
$$b = y^T d , \tag{1.5}$$
$$c = d^T B d ,$$

From (1.2) and from the positive definiteness of the matrix B we get $a > 0$, $b > 0$, $c > 0$. If we denote

$$\lambda = \frac{b^2}{ac}, \tag{1.6}$$

the positive definiteness of the matrix B and (1.5) together with the Schwartz inequality give $0 < \lambda \leqq 1$.

The parameter $\varrho > 0$ (so called Biggs's parameter) has been introduced to improve the behavior of the variable metric methods in a strongly nonlinear case (see [1]). The parameter $\gamma > 0$ (so called Oren's parameter) is important especially for the first iteration and serves to the scaling to the variable metric methods (see [14]). The parameter β determines particular variable metric methods and it has to be chosen to keep the hereditary positive definiteness of the matrix B^+, i.e. to satisfy the inequality $\beta > \beta^*$ where

$$\beta^* = -\frac{\lambda}{1-\lambda} \tag{1.7}$$

is the degenerate value of the parameter β. The inequality $0 < \lambda \leqq 1$ implies $\beta^* < 0$.

If we set $H = B^{-1}$ and $H^+ = (B^+)^{-1}$ we can write (1.1) and (1.3) in the inverse form. Then

$$x^+ = x + \alpha s \quad \text{where} \quad s = -Hg \tag{1.8}$$

and

$$H^+ = \gamma\left(H + \frac{\varrho}{\gamma}\frac{1}{b} dd^T - \frac{1}{a} Hy(Hy)^T + \right.$$
$$\left. + \frac{\eta}{a}\left(\frac{a}{b} d - Hy\right)\left(\frac{a}{b} d - Hy\right)^T\right) \tag{1.9}$$

The parameter η in (1.9) is connected with the parameter β in (1.3) by means of the relation

$$\eta = \frac{(\beta - 1)\beta^*}{\beta - \beta^*} \quad \text{or} \quad \beta = \frac{(\eta - 1)\eta^*}{\eta - \eta^*} \tag{1.10}$$

where

$$\eta^* = -\frac{\lambda}{1-\lambda} \tag{1.11}$$

is again the degenerate value of the parameter η and the matrix H^* is positive definite for $\eta > \eta^*$.

The most frequently studied variable metric methods lie in the so-called convex

β-class which is defined by the inequality $0 \leqq \beta \leqq 1$ (or $0 \leqq \eta \leqq 1$ by (1.10)). It has been proved, under mild assumptions, that variable metric methods from the convex β-class are n-step quadratically convergent (see [20]) or superlinearly convergent (see [10]). In [5] and [12] it was shown that all variable metric methods with perfect line search i.e. with stepsize α chosen by the rule $s^T g^+ = 0$, are equivalent to each other. If we use a more economical imperfect line search (1.2), the efficiency of particular variable metric methods differs very much. Numerical comparisons show that the best variable metric method of the convex β-class is the BFGS method (see [2], [6], [9], [17]) which uses the value $\beta = 0$ (or $\eta = 1$ by (1.10)). Recently variable metric methods have been analyzed theoretically in [3] and it was pointed out that the BFGS method could be improved. This idea was confirmed experimentally in [21] and [22], where two new variable metric methods were introduced and their efficiency was demonstrated. These methods lie in the so called preconvex β-class which is defined by the inequality $\beta^* < \beta < 0$ (or $1 < \eta < \infty$ by (1.10)). Moreover, a scaled rank-one method was described in [16] and it was shown that this method is also better than the BFGS method.

The main purpose of this paper is to introduce three new variable metric methods which are better than the classical BFGS method. In Section 2 we propose the concept of controlled scaling, which improves the classical BFGS method. In Section 3 we introduce a simple safeguarded rank-one method. In Section 4 we describe a simple variable metric method which lies in the preconvex β-class. Numerical comparison of these methods is presented in Section 5. Test problems used are given in the Appendix.

2. THE CONTROLLED SCALING

Let G be a matrix that satisfies condition $Gd = y$ and let $R = G^{1/2}HG^{1/2}$ and $R^+ = G^{1/2}H^+G^{1/2}$. Then from (1.9) it follows that

$$R^+ = \gamma\left(R + \frac{\varrho}{\gamma}\frac{1}{b}\,zz^T - \frac{1}{a}\,Rz(Rz)^T + \frac{\eta}{a}\left(\frac{a}{b}\,z - Rz\right)\left(\frac{a}{b}\,z - Rz\right)^T\right) \tag{2.1}$$

where

$$z = G^{1/2}d = G^{-1/2}y \tag{2.2}$$

and

$$\begin{aligned} a &= z^T R z = y^T H y \\ b &= z^T z = y^T d\,, \\ c &= z^T R^{-1} z = \mathrm{d}^T H^{-1} d\,. \end{aligned} \tag{2.3}$$

The scaling of the variable metric methods was introduced in [14] to keep the condition number of the matrix R^+ as small as possible. Next result has been proved in[14].

Lemma 2.1. Suppose that (2.1)–(2.3) hold where R is a symmetric positive definite matrix. Let

$$0 \leqq \eta \leqq 1 \tag{2.4}$$

and

$$\frac{b}{c} \leqq \frac{\varrho}{\gamma} \leqq \frac{a}{b}. \tag{2.5}$$

Then $\varkappa(R^+) \leqq \varkappa(R)$ where $\varkappa(R)$ is the spectral condition number of the matrix R.

It is clear (see (2.4)) that this lemma is useful only for the convex β-class of variable metric methods. We prove a similar result for the preconvex β-class of variable metric methods.

Lemma 2.2. Suppose that (2.1)–(2.3) hold where R is a symmetric positive definite matrix. Let

$$1 < \eta < \infty \tag{2.6}$$

and

$$\frac{b}{c} \leqq \frac{\varrho}{\gamma} \leqq \eta \frac{a}{b}. \tag{2.7}$$

Then $\varkappa(R^+) \leqq \eta\, \varkappa(R)$ where $\varkappa(R)$ is the spectral condition number of the matrix R.

Proof. From (2.1) we have $R^+z = \varrho z$ so that ϱ is the eigenvalue of the matrix R^+ that corresponds to the eigenvector z. Let v is an arbitrary eigenvector of the matrix R^+ which satisfies $z^{\mathrm{T}}v = 0$. Then

$$v^{\mathrm{T}}R^+v = \gamma\left(v^{\mathrm{T}}Rv + \frac{\eta - 1}{z^{\mathrm{T}}Rz}(v^{\mathrm{T}}Rz)^2\right)$$

by (2.1), which together with (2.6) gives

$$\frac{v^{\mathrm{T}}R^+v}{v^{\mathrm{T}}v} = \gamma\left(\frac{v^{\mathrm{T}}Rv}{v^{\mathrm{T}}v} + (\eta - 1)\frac{(v^{\mathrm{T}}Rz)^2}{v^{\mathrm{T}}vz^{\mathrm{T}}R^2z}\frac{z^{\mathrm{T}}R^2z}{z^{\mathrm{T}}Rz}\right) \leqq$$

$$\leqq \gamma(1 + \eta - 1)\,\|R\| = \gamma\eta\|R\|$$

where $\|R\|$ is the spectral norm of the matrix R. Therefore

$$\|R^+\| \leqq \max(\varrho, \gamma\eta\|R\|)\,. \tag{2.8}$$

On the other hand, (2.3) and (2.7) imply

$$\frac{\varrho}{\gamma} \leqq \eta\frac{a}{b} = \eta\frac{z^{\mathrm{T}}Rz}{z^{\mathrm{T}}z} \leqq \eta\|R\|,$$

which together with (2.8) gives $\|R^+\| \leqq \eta\gamma\|R\|$. Since $\beta^* < \beta < 0$ for $1 < \eta < \infty$, we can continue as in the proof of Lemma 2.1 given in [14], so that we obtain $\|(R^+)^{-1}\| \leqq (1/\gamma)\,\|R^{-1}\|$ which together with $\|R^+\| \leqq \eta\gamma\|R\|$ gives $\varkappa(R^+) \leqq \eta\varkappa(R)$. □

Another approach to the scaling of the variable metric methods was proposed in [15]. It is based on the optimal conditioning of the matrix $\bar{R}^+ = R^{-1/2}R^+R^{-1/2}$. Since

$$\varkappa(\bar{R}^+) \leqq \varkappa(R)\,\varkappa(R^+) \leqq \varkappa^2(R)\,\varkappa(\bar{R}^+)\,, \tag{2.9}$$

the minimal value of $\varkappa(\bar{R}^+)$ could give nearly minimal value of $\varkappa(R^+)$. We summarize the results given in [15].

Lemma 2.3. Suppose that (2.1)–(2.3) hold where R is a symmetric positive definite matrix. Denote $\bar{R}^+ = R^{-1/2}R^+R^{-1/2}$. Then the matrix $\bar{R}^+$ has $n - 2$ unit eigenvalues and the remaining two eigenvalues $\xi_1 \leqq \xi_2$ satisfy the equation

$$\xi^2 - p\xi + q = 0\,,$$

where

$$p = 1 - \frac{\eta}{\eta^*} + \frac{\varrho}{\gamma}\frac{c}{b}$$

and

$$q = \frac{\varrho}{\gamma}\frac{c}{b}\lambda\left(1 - \frac{\eta}{\eta^*}\right).$$

If we denote $\tilde{\eta} = 1 - \eta/\eta^*$ and $\tilde{\omega} = (\varrho/\gamma)(c/b)$ then:

(i) The ratio ξ_2/ξ_1 can be expressed in the form

$$\frac{\xi_2}{\xi_1} = \frac{\left(\frac{\tilde{\eta}}{\tilde{\omega}} + 1\right) + \sqrt{\left(\left(\frac{\tilde{\eta}}{\tilde{\omega}} + 1\right)^2 - 4\lambda\frac{\tilde{\eta}}{\tilde{\omega}}\right)}}{\left(\frac{\tilde{\eta}}{\tilde{\omega}} + 1\right) - \sqrt{\left(\left(\frac{\tilde{\eta}}{\tilde{\omega}} + 1\right)^2 - 4\lambda\frac{\tilde{\eta}}{\tilde{\omega}}\right)}}.$$

(ii) The ratio ξ_2/ξ_1 reaches its minimum for $\tilde{\eta} = \tilde{\omega}$.

(iii) If $\tilde{\eta} = \tilde{\omega}$ then $\xi_1 \leqq 1 \leqq \xi_2$ if and only if $\eta^2 - 2\eta + \eta^* \leqq 0$.

Lemma 2.3 is a basis for the optimal scaling of the variable metric methods. For a given parameter $\varrho > 0$ and a parameter η which satisfies the condition $\eta^2 - 2\eta + \eta^* \leqq 0$ we can determine the optimal scaling factor γ from the equation

$$\frac{\varrho}{\gamma}\frac{c}{b} = 1 - \frac{\eta}{\eta^*}\,. \tag{2.10}$$

It can be easily proved that the optimal choice (2.10) satisfies the condition (2.5) for $0 \leqq \eta \leqq 1$ and the condition (2.7) for $1 < \eta < \infty$. Moreover, from Lemma 2.3 it follows that

$$\varkappa(\bar{R}^+) = \frac{1 + \sqrt{(1 - \lambda)}}{1 - \sqrt{(1 - \lambda)}} \tag{2.11}$$

for the optimal choice (2.10). However, (1.6) and (2.3) together with the Kantorovich inequality imply

$$\lambda = \frac{z^T z}{z^T R z z^T R^{-1} z} \geqq \frac{4\varkappa(R)}{(\varkappa(R) + 1)^2},$$

which after setting into the equation (2.11) gives

$$\varkappa(\bar{R}^+) \leqq \varkappa(R).$$

This result together with Lemma 2.2 and the inequality (2.9) imply

$$\varkappa(R^+) = \min(\eta, \varkappa(R))\, \varkappa(R). \tag{2.12}$$

This shows that, for the optimal choice (2.10), $\varkappa(R^+)$ is bounded from above even if the parameter η tends to infinity. Let us note that from $\eta^* < 0$ it follows

$$1 - \sqrt{(1 - \eta^*)} < 0 < 2 < 1 + \sqrt{(1 - \eta^*)}$$

so that the inequality $\eta^2 - 2\eta + \eta^* \leqq 0$ is satisfied for the convex β-class of variable metric methods and for a sufficiently broad part of the prevonvex β-class of variable metric methods.

After this theoretical introduction to the scaling of the variable metric methods we pass to practical questions. The main significance of the scaling consists in the requirement of the acceptance of the initial stepsize ((1.2) could be satisfied for $\alpha = 1$). This is the case when variable metric methods spare function evaluations. In [18] it was pointed out that the scaling in the first iteration only (so-called preliminary scaling) is often sufficient for this purpose. In Section 5 (Table 1) we show, for the case of the BFGS method, that the preliminary scaling reduces the number of function evaluations very much while scaling in each iteration can be unstable. But, in many cases, scaling in each iteration has a better performance than the preliminary scaling. This fact invites the proposition of a new scaling strategy. An easy one which we recommend (so-called controlled scaling) is based on the success in the first attempt with the stepsize α_1 (usually $\alpha = \alpha_1 = 1$).

Algorithm 2.4. Given F, F_1, F^+, g, g_1, g^+, s (usually $F_1 = F^+$, $g_1 = g^+$) and ε.

Step 1: In the first iteration (or after restart) determine γ from (2.10) and go to Step 5. Otherwise compute the ratio $\tau = s^T g_1 / s^T g$.

Step 2: If $|\tau| \leqq \varepsilon$ and $F \leqq F^+$ then set $\gamma = 1$ and go to Step 5. Otherwise determine γ for (2.10).

Step 3: If $\gamma > 1$ and ($F > F^+$ or $\tau < 0$) then set $\gamma = 1$ and go to Step 5. If $\gamma < 1$ and ($F \leqq F^+$ and $\tau > 0$) then set $\gamma = 1$ and go to Step 5.

Step 4: If $\gamma < \varepsilon$ or $\gamma > 1/\varepsilon$ then set $\gamma = 1$.

Step 5: Continue in the update (1.3) or (1.9) with the given value γ.

The choice of the parameter ε is very selective and our recommended value $\varepsilon = 0{\cdot}4$ gives a very good compromise between the preliminary scaling and scaling in each iteration. As we can see from Table 1, there is some reserve in the efficiency of the controlled scaling. It could stimulate further research in this field.

3. THE SAFEGUARDED RANK-ONE METHOD

The rank-one method is defined as that for which

$$\beta = \frac{\frac{\gamma}{\varrho} b}{\frac{\gamma}{\varrho} b - c} . \tag{3.1}$$

Then

$$B^{+} = \frac{1}{\gamma}\left(B + \frac{1}{\frac{\gamma}{\varrho} b - c}\left(\frac{\gamma}{\varrho} y - Bd\right)\left(\frac{\gamma}{\varrho} y - Bd\right)^{\mathrm{T}}\right) . \tag{3.2}$$

The rank-one method has two advantages. It is very simple and it has a quadratic termination property (it finds the minimum of a quadratic function within at most n steps) even if the line search is imperfect. Unfortunately, this method does not preserve the hereditary positive definitieness of the matrix B^{+} (for an arbitrary value of γ/ϱ) since the case $\beta < \beta^{*}$ can occur. Therefore it can be unstable and it has to be adapted. There are two possibilities how to safeguard the rank-one method. The first one is based on the suitable scaling and the second one is based on the pertinent combination of the rank-one method with other variable metric methods.

The scaling is a known and frequently studied mean for improving the rank-one method (see [1], [19]). The most accomplished algorithm of this type has been proposed recently in [16]. We summarize the main ideas contained in [16].

Using (1.10) we can transform (3.1) into

$$\eta = \frac{\frac{\varrho}{\gamma} b}{\frac{\varrho}{\gamma} b - a} . \tag{3.3}$$

If we substitute (2.10) into (3.3), we get

$$\eta^{2} - 2\eta + \eta^{*} = 0 \tag{3.4}$$

after some algebraic manipulations. The equation (3.4) has two real roots. We choose the root belonging to the preconvex β-class. Hence

$$\eta = 1 + \sqrt{(1 - \eta^{*})} \tag{3.5}$$

and according to (2.10) we obtain

$$\frac{\varrho}{\gamma} = \frac{a}{b}\left(1 + \sqrt{(1 - \lambda)}\right) . \tag{3.6}$$

Note that the inequality $\eta^{2} - 2\eta + \eta^{*} \leqq 0$ used in Lemma 2.3 is always satisfied (see (3.4)).

The basic strategy proposed in [16] is the following: if $\varrho b > a$ then set $\gamma = 1$ else compute γ from (3.6). This strategy is superior than the unscaled BFGS method, but it is inferior than the preliminary scaled BFGS method (in fact the basic strategy has been slightly modified in [16] to give better results). This fact is probably caused by too frequent scaling. Therefore we recommend a different strategy:

Algorithm 3.1. Given a, b, c and ϱ.

Step 1: Compute the value γ using either the preliminary scaling strategy or the controlled scaling strategy (Algorithm 2.4).

Step 2: If $(\varrho/\gamma)\, b > a$ then use rank-one method (3.2) else use the BFGS method (i.e. (1.3) with $\beta = 0$).

This algorithm is very effective as it is shown in Section 5.

4. A SIMPLE PRECONVEX METHOD

Recently most attention has been devoted to the preconvex β-class of variable metric methods. In [21] the new variable metric method has been derived by variational means as the least-change update to Cholesky factors subject to the nonlinear quasi-Newton condition. This method belongs to the preconvex β-class but is more complicated then other variable metric methods because a four-degree polynomial equation has to be solved.

Another variable metric method which lies in the preconvex β-class has been proposed in [22]. It is exactly the one which minimizes the angle between the new direction vector and the new negative gradient. This method gives better results than the BFGS method, namely in case of the preliminary scaling, but it is again more complicated then other variable metric methods.

In the rest of this paper we are going to show that there exists a simple preconvex variable metric method which is comparable with the methods described in [21] and [22]. This method is defined by the choice

$$\eta = \min\left(1 + \sqrt{(1 - \eta^*)}, \eta_{\max}\right), \tag{4.1}$$

where $\eta_{\max}$ is the value which serves for safeguard. If we use (1.10), we can write

$$\beta = \frac{\eta^*}{1 + \sqrt{(1 - \eta^*)}}, \quad |\eta^*| \leqq \eta^*_{\max} \quad \text{and} \quad \beta = \frac{(\eta_{\max} - 1)\,\eta^*}{\eta_{\max} - \eta^*}, \quad |\eta^*| > \eta^*_{\max}, \tag{4.2}$$

where $\eta^*_{\max} = (\eta_{\max} - 1)^2 - 1$ (we recommend the value $\eta_{\max} = 1000$ so that $\eta^*_{\max} \approx$ $\approx 1\,000\,000$). Moreover, from (2.10) and (1.11) we obtain

$$\frac{\varrho}{\gamma} = \frac{a}{b}\left(1 + \sqrt{1 - \lambda}\right), \quad |\eta^*| \leqq \eta^*_{\max}$$

and

$$\frac{\varrho}{\gamma} = \frac{a}{b}\left(1 - \frac{\eta_{\max}}{\eta^*}\right), \quad |\eta^*| > \eta^*_{\max}, \tag{4.3}$$

Let $|\eta^*| \leqq \eta^*_{\max}$ (the other case is very improbable). Then the choice (4.2) is the most negative one which can be optimally scaled by means of the theory explained in Section 2. Moreover, if (4.3) is used, the resulting method is exactly the optimally scaled rank-one method (see (3.5) and (3.6)). However, if (4.3) is not used, the method (4.2) differs from the rank-one method, but maintains the positive definiteness even if the rank-one methods generates indefinite matrices.

5. COMPUTATIONAL EXPERIMENTS

In this section we present numerical results of comparative experiments for three methods: the BFGS method, the safeguarded rank-one (SRO) method described in Section 3, and the simple preconvex (SPC) method described in Section 4. All these methods were implemented by the same algorithm which differs only in computation of the parameters $\varrho > 0$, $\gamma > 0$ and β. This algorithm is based on the Cholesky decomposition $B = LDL^T$. The matrices L, D are updated using the technique described in [8] and the direction vector s is obtained as a solution of the equation $LDL^T s = -g$. The condition

$$-s^T g \geqq \varepsilon_0 \|s\| \, \|g\| \tag{5.1}$$

with $\varepsilon_0 = 10^{-4}$ is tested and $L = I$, $D = I$ (as in the first iteration) is set whenever (5.1) does not hold. The line search procedure used in our experiments is in fact an implementation of the algorithm given in [7; p. 25]. As is the usual practice, we take $\varepsilon_1 = 10^{-4}$ and $\varepsilon_2 = 0{\cdot}9$ in the criterion (1.2). To improve stability of the variable metric methods within the bounds of precision in function evaluation the additional criterion

$$|F^+ - F| \leqq \varepsilon_3 |F| \quad \text{and} \quad |s^T g^+| \leqq \varepsilon_4 |s^T g| \tag{5.2}$$

with $\varepsilon_3 = 2 \, . \, 10^{-13}$ and $\varepsilon_4 = 5 \, . \, 10^{-1}$ was added to (1.2) which was active for problem 9. In our implementation we have used the initial stepsize

$$\alpha_1 = \min\left(1, 4(F_{\min} - F)/s^T g\right) \tag{5.3}$$

where $F_{\min} = -10^{50}$ for problems with negative minima (Problems 9, 15) and $F_{\min} = 0$ for other problems. Moreover, we have used the stepsize bound $\|x^+ - x\| = \alpha\|s\| \leqq \Delta$, where $\Delta = 1$ for some problems with exponential functions (Problems 9, 11) and $\Delta = 1000$ for other problems. The unified termination criterion $\|g\| \leqq 10^{-6}$ was used for all our experiments.

The comparative experiments for three variable metric methods was made with different scaling strategies and with different choices of the parameters $\varrho > 0$. We use the notation SCALING = 1 for unscaled case ($\gamma = 1$), SCALING = 2 for the preliminary scaling, SCALING = 3 for the controlled scaling (Algorithm 2.4), and SCALING = 4 for the scaling in each iteration. Furthermore, $\varrho = 1$ denotes the usual unit choice and $\varrho \neq 1$ denotes the choice proposed in [17]. The last one is defined by the following strategy: $\varrho = 1$ for $\varrho^* < 10^{-2}$, $\varrho = \varrho^*$ for $10^{-2} \leqq \varrho^* \leqq 10^{+2}$, and $\varrho = 1$ for $10^{+2} < \varrho^*$, where

$$\varrho^* = \frac{d^T y}{2(F - F^+ + d^T g^+)} . \tag{5.4}$$

The results of our experiments are summarized in four tables that contain two numbers IT and IF for each run. Here IT is the number of iteration and IF is both the number of function evaluations and the number of gradient evaluations (in our line search procedure the value and the gradient of the objective function are evaluated at the same time). The rows of these tables correspond to 15 test problems that are given in the Appendix. All test problems were solved for 20 variables ($n = 20$) and in all cases the required precision $\|g\| \leqq 10^{-6}$ was reached. The row denoted by $\sum$ contains total numbers over all test problems while the row denoted by % contains an average efficiency of particular methods related to the BFGS method with the preliminary scaling.

Table 1 contains the comparison of several scaling strategies applied to the BFGS method. This table shows that the BFGS method without scaling is not sufficiently efficient for more complicated or more extensive problems while the preliminary scaling improves considerably its behavior (this was also pointed out in [18]). The

Table 1. BFGS method.

	SCALING = 1		SCALING = 2		SCALING = 3		SCALING = 4	
	IT	IF	IT	IF	IT	IF	IT	IF
1	131	196	120	131	119	128	346	356
2	220	313	275	298	231	251	>400	>403
3	106	145	105	107	73	76	70	72
4	124	207	193	194	58	60	56	57
5	42	64	46	47	25	26	20	21
6	56	80	112	113	36	37	24	25
7	32	68	20	21	20	21	23	24
8	39	123	24	43	29	48	62	121
9	41	64	34	36	34	36	89	93
10	>400	>555	215	237	57	59	53	59
11	244	293	132	158	148	174	313	333
12	9	21	40	51	39	50	18	28
13	8	9	6	7	7	8	5	6
14	33	49	58	60	54	58	56	58
15	22	42	16	18	19	21	18	20
$\sum$	>1507	>2229	1396	1521	949	1053	>1553	>1676

Table 2. BFGS method.

	$\varrho = 1$				$\varrho \neq 1$			
	SCALING = 2		SCALING = 3		SCALING = 2		SCALING = 3	
	IT	IF	IT	IF	IT	IF	IT	IF
1	120	131	119	128	95	108	106	119
2	275	298	231	251	258	280	233	251
3	105	107	73	76	97	100	66	71
4	193	194	58	60	175	176	55	56
5	46	47	25	26	31	32	25	26
6	112	113	36	37	88	89	31	32
7	20	21	20	21	19	20	18	19
8	24	43	29	48	41	76	31	44
9	34	36	34	36	50	52	42	43
10	215	237	57	59	173	196	55	58
11	132	158	148	174	131	152	109	127
12	40	51	39	50	17	31	19	33
13	6	7	7	8	5	6	5	6
14	58	60	54	58	58	60	54	58
15	16	18	19	21	16	18	19	21
$\sum$	1396	1521	949	1053	1254	1396	868	964
%	100·0	100·0	68·0	69·2	89·8	91·8	62·2	63·4

scaling in each iteration can be inefficient in some cases (Problems 1, 2, 9, 11), but it can be the best one in some other cases (Problems 4, 5, 6, 13). The controlled scaling proposed in Section 2 is a suitable compromise between known scaling strategies and it is the best one for the BFGS method.

Tables 2, 3, 4 contain the comparison of three variable metric methods: the BFGS method, the SRO method, and the SPC method. All studied methods was tested with two different scaling strategies and with two different choices of the parameter $\varrho > 0$. We pointed out the following conclusions:

1) Both the SRO method and the SPC method perform much better then the BFGS method in the case of the preliminary scaling.
2) Controlled scaling improves the behavior of all studied methods and, at the same time, it suppresses differences among them.
3) Controlled scaling is very effective especially in combination with the choice $\varrho \neq 1$.

To confirm our results we have performed additional tests with problems given in [13]. We used first 30 problems from [13] except problems 3 and 10 which are impertent for variable metric methods. Problems 1–19 has the same dimensionality as in [13]. Problems 20–30 were considered with 20 variables. Summary results are given in Table 5.

Table 3. SRO method.

	$\varrho = 1$				$\varrho \neq 1$			
	SCALING = 2		SCALING = 3		SCALING = 2		SCALING = 3	
	IT	IF	IT	IF	IT	IF	IT	IF
1	122	141	123	142	99	117	99	117
2	164	188	222	278	229	268	157	181
3	65	67	81	86	61	62	56	60
4	106	124	73	76	93	100	61	63
5	41	44	37	39	31	32	25	26
6	71	73	60	63	58	60	48	49
7	19	21	19	21	19	20	22	23
8	25	39	24	40	23	66	23	66
9	36	40	40	42	46	50	47	50
10	106	139	55	63	92	126	57	68
11	84	105	86	106	96	118	99	120
12	16	30	16	30	17	32	19	34
13	6	7	7	8	5	6	5	6
14	32	38	32	38	32	38	32	38
15	16	21	16	21	16	21	16	21
$\sum$	909	1077	891	1053	917	1116	766	922
%	65·1	70·8	63·8	69·2	65·7	73·4	54·9	60·6

Table 4. SPC method.

	$\varrho = 1$				$\varrho \neq 1$			
	SCALING = 2		SCALING = 3		SCALING = 2		SCALING = 3	
	IT	IF	IT	IF	IT	IF	IT	IF
1	121	161	119	159	111	139	106	134
2	163	191	227	285	171	203	233	280
3	76	77	67	68	71	72	65	73
4	116	124	63	64	107	113	60	63
5	38	39	36	37	30	32	29	31
6	76	77	70	71	63	64	51	52
7	19	20	20	21	18	23	19	23
8	28	38	35	53	39	68	29	42
9	39	40	50	51	46	48	43	45
10	116	144	58	68	114	133	54	62
11	86	107	93	115	102	133	107	132
12	31	42	30	41	18	32	18	32
13	5	6	7	8	5	6	5	6
14	43	45	43	45	43	45	43	45
15	15	17	15	17	16	18	16	18
$\sum$	972	1128	933	1103	954	1129	878	1038
%	69·6	74·2	66·8	72·5	68·3	74·2	62·9	68·2

Table 5.

		Sum over 28		Consumption in %	
		IT	IF	IT	IF
BFGS	SCALING = 2, $\varrho = 1$	1555	1915	100·0	100·0
	SCALING = 3, $\varrho = 1$	1242	1538	79·8	80·3
	SCALING = 3, $\varrho \neq 1$	1143	1426	73·5	74·5
SRO	SCALING = 2, $\varrho = 1$	1155	1524	74·3	79·6
	SCALING = 3, $\varrho = 1$	1157	1535	74·4	80·2
	SCALING = 3, $\varrho \neq 1$	1045	1447	67·2	75·6
SPC	SCALING = 2, $\varrho = 1$	1161	1519	74·7	79·3
	SCALING = 3, $\varrho = 1$	1150	1592	74·0	83·1
	SCALING = 3, $\varrho \neq 1$	1154	1552	74·2	81·0

APPENDIX

Our test problems were taken from [4] but they were slightly modified. These 15 test problems consists in searching local minima of the objective function $F(x)$ from the starting point $\bar{x}$.

Problem 1.

$$F(x) = \sum_{i=2}^{n} [100(x_{i-1}^2 - x_i)^2 + (x_{i-1} - 1)^2]$$

$$\bar{x}_i = -1{\cdot}2\,, \quad i - \text{odd}$$

$$\bar{x}_i = 1{\cdot}0\,, \quad i - \text{even}$$

Problem 2.

$$F(x) = \sum_{\substack{i=2 \\ i-\text{even}}}^{n-2} [100(x_{i-1}^2 - x_i)^2 + (x_{i-1} - 1)^2 + 90(x_{i+1}^2 - x_{i+2})^2 +$$

$$+ (x_{i+1} - 1)^2 + 10(x_i + x_{i+2} - 2)^2 + (x_i - x_{i+2})^2/10]$$

$$\bar{x}_i = -3\,, \quad i - \text{odd}\,, \quad i \leqq 4$$

$$\bar{x}_i = -2\,, \quad i - \text{odd}\,, \quad i > 4$$

$$\bar{x}_i = -1\,, \quad i - \text{even}\,, \quad i \leqq 4$$

$$\bar{x}_i = 0\,, \quad i - \text{even}\,, \quad i > 4$$

Problem 3.

$$F(x) = \sum_{\substack{i=2 \\ i-\text{even}}}^{n-2} [(x_{i-1} + 10x_i)^2 + 5(x_{i+1} - x_{i+2})^2 +$$

$$+ (x_i - 2x_{i+1})^4 + 10(x_{i-1} - x_{i+2})^4]$$

$$\bar{x}_i = 3\,, \quad \mathrm{mod}\,(i, 4) = 1$$
$$\bar{x}_i = -1\,, \quad \mathrm{mod}\,(i, 4) = 2$$
$$\bar{x}_i = 0\,, \quad \mathrm{mod}\,(i, 4) = 3$$
$$\bar{x}_i = 1\,, \quad \mathrm{mod}\,(i, 4) = 0$$

Problem 4.

$$F(x) = \sum_{\substack{i=2 \\ i-\text{even}}}^{n-2} \left[(e^{x_{i-1}} - x_i)^4 + 100(x_i - x_{i+1})^6 + \right.$$
$$\left. + \tan^4(x_{i+1} - x_{i+2}) + x_{i-1}^8 + (x_{i+2} - 1)^2\right]$$
$$\bar{x}_i = 1\,, \quad i = 1$$
$$\bar{x}_i = 2\,, \quad i > 1$$

Problem 5.

$$F(x) = \sum_{i=1}^{n} \left|(3 - 2x_i)\, x_i - x_{i-1} - x_{i+1} + 1\right|^p$$
$$p = 7/3\,, \quad x_0 = x_{n+1} = 0$$
$$\bar{x}_i = -1\,, \quad \forall i$$

Problem 6.

$$F(x) = \sum_{i=1}^{n} \left|(2 + 5x_i^2)\, x_i + 1 + \sum_{j \in J_i} x_j(1 + x_j)\right|^p$$
$$p = 7/3\,, \quad J_i = (j\colon \max\,(1, i - 5) \leqq j \leqq \min\,(n, i + 1))$$
$$\bar{x}_i = -1\,, \quad \forall i$$

Problem 7.

$$F(x) = \sum_{i=1}^{n} \left|(3 - 2x_i)\, x_i - x_{i-1} - x_{i+1} + 1\right|^p + \sum_{i=1}^{n/2} \left|x_i + x_{i+n/2}\right|^p$$
$$p = 7/3\,, \quad x_0 = x_{n+1} = 0$$
$$\bar{x}_i = -1\,, \quad \forall i$$

Problem 8.

$$F(x) = \sum_{i=1}^{n} \left[n + i - \sum_{j=1}^{n} (a_{ij} \sin\,(x_j) + b_{ij} \cos\,(x_j))\right]^2$$
$$a_{ij} = 5[1 + \mathrm{mod}\,(i, 5) + \mathrm{mod}\,(j, 5)]$$
$$b_{ij} = (i + j)/10$$
$$\bar{x}_i = 1/n\,, \quad \forall i$$

Problem 9.

$$F(x) = \sum_{(i,j)\in J} \alpha_{ij} \sin(\beta_i x_i + \beta_j x_j + \gamma_{ij})$$

$$\alpha_{ij} = 5(1 + \text{mod}(i, 5) + \text{mod}(j, 5))$$

$$\beta_i = 1 + i/10, \quad \beta_j = 1 + j/10$$

$$\gamma_{ij} = (i + j)/10$$

$$J = \{(i, j): \text{mod}(|i - j|, 4) = 0\}$$

$$\bar{x}_i = 1, \quad \forall i$$

Problem 10.

$$F(x) = \sum_{i=1}^{n} |x_i| + 1000\left(1 - \sum_{i=1}^{n} \frac{1}{x_i}\right)^2 + 1000\left(1 - \sum_{i=1}^{n} \frac{i}{x_i}\right)^2$$

$$\bar{x}_i = 1, \quad \forall i$$

Problem 11.

$$F(x) = \sum_{i\in J} [\exp(\prod_{j=1}^{5} x_{i+1-j}) + 10((\sum_{j=1}^{5} x_{i+1-j}^2 - 10 - \lambda_1)^2 +$$

$$+ (x_{i-3}x_{i-2} - 5x_{i-1}x_i - \lambda_2)^2 + (x_{i-4}^3 + x_{i-3}^3 + 1 - \lambda_3)^2)]$$

$$\lambda_1 = -0{\cdot}002008, \quad \lambda_2 = -0{\cdot}001900, \quad \lambda_3 = -0{\cdot}000261$$

$$J = \{i, \text{mod}(i, 5) = 0\}$$

$$\bar{x}_i = -2, \quad \text{mod}(i, 5) = 1, \quad i \leqq 2$$

$$\bar{x}_i = -1, \quad \text{mod}(i, 5) = 1, \quad i > 2$$

$$\bar{x}_i = 2, \quad \text{mod}(i, 5) = 2, \quad i \leqq 2$$

$$\bar{x}_i = -1, \quad \text{mod}(i, 5) = 2, \quad i > 2$$

$$\bar{x}_i = 2, \quad \text{mod}(i, 5) = 3$$

$$\bar{x}_i = -1, \quad \text{mod}(i, 5) = 4$$

$$\bar{x}_i = -1, \quad \text{mod}(i, 5) = 0$$

Problem 12.

$$F(x) = (\sum_{\substack{i=2 \\ i-\text{even}}}^{n} (x_{i-1} - 3))^2 +$$

$$+ \sum_{\substack{i=2 \\ i-\text{even}}}^{n} [(x_{i-1} - 3)^2/1000 + (x_{i-1} - x_i) + \exp(20(x_{i-1} - x_i))]$$

$$\bar{x}_i = 0, \quad i - \text{odd}$$

$$\bar{x}_i = -1, \quad i - \text{even}$$

Problem 13.

$$F(x) = \sum_{\substack{i=2 \\ i-\text{even}}}^{n} \left[(x_{i-1}^2)^{(x_i^2+1)} + (x_i^2)^{(x_{i-1}^2+1)}\right]$$

$$\bar{x}_i = -1\,, \quad i - \text{odd}$$

$$\bar{x}_i = \ \ 1\,, \quad i - \text{even}$$

Problem 14.

$$F(x) = \sum_{i=1}^{n} \left[2x_i - x_{i-1} - x_{i+1} + h^2(x_i + ih + 1)^3/2\right]^2$$

$$h = 1/(n+1)\,, \quad x_0 = x_{n+1} = 0$$

$$\bar{x}_i = ih(ih - 1)\,, \quad \forall i$$

Problem 15.

$$F(x) = 2\sum_{i=1}^{n} (x_i(x_i - x_{i+1}))/h - 6{\cdot}8h \sum_{i=0}^{n} (e^{x_{i+1}} - e^{x_i})/(x_{i+1} - x_i)$$

$$h = 1/(n+1)\,, \quad x_0 = x_{n+1} = 0$$

$$\bar{x}_i = i(n + 1 - i)\, h/10$$

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