A COMBINED CLASS OF SELF-SCALING AND MODIFIED QUASI-NEWTON METHODS *

MEHIDDIN AL-BAALI† AND HUMAID KHALFAN‡

Abstract. Techniques for obtaining safely positive definite Hessian approximations with self-scaling and modified quasi-Newton updates are combined to obtain 'better' curvature approximations in line search methods for unconstrained optimization. It is shown that this class of methods, like the BFGS method has global and superlinear convergence for convex functions. Numerical experiments with this class, using the well-known quasi-Newton BFGS, DFP and a modified SR1 updates, are presented to illustrate advantages of the new techniques. These experiments show that the performance of several combined methods are substantially better than that of the standard BFGS method. Similar improvements are also obtained if the simple sufficient function reduction condition on the steplength is used instead of the strong Wolfe conditions.

Key words. Unconstrained optimization, modified quasi-Newton updates, self-scaling technique, line-search framework.

AMS subject classifications. 90C30, 65K49

1. Introduction. This paper is concerned with some combined self-scaling and modified quasi-Newton methods for solving the unconstrained optimization problem

$$\min_{x \in R^n} f(x), \tag{1.1}$$

where $f : R^n \to R$ is a twice continuously differentiable function. The methods we consider have the following basic iteration. Given the current approximation x_k to a solution of (1.1), a new approximation is calculated by

$$x_{k+1} = x_k - \alpha_k B_k^{-1} g_k, \tag{1.2}$$

where α_k is a steplength, B_k is a positive definite matrix that approximates the Hessian $G_k = \nabla^2 f(x_k)$, and $g_k = \nabla f(x_k)$.

Here B_k is updated to a new Hessian approximation B_{k+1}, given by a combined Broyden family update of the form

$$B_{k+1} = \tau_k \left(B_k - \frac{B_k s_k s_k^T B_k}{s_k^T B_k s_k} + \theta_k \widehat{w}_k \widehat{w}_k^T \right) + \frac{\widehat{y}_k \widehat{y}_k^T}{\widehat{y}_k^T s_k}, \tag{1.3}$$

where τ_k and θ_k are parameters, $s_k = x_{k+1} - x_k$,

$$\widehat{w}_k = (s_k^T B_k s_k)^{1/2} \left(\frac{\widehat{y}_k}{\widehat{y}_k^T s_k} - \frac{B_k s_k}{s_k^T B_k s_k} \right), \tag{1.4}$$

and $\widehat{y}_k$ is some modification of the difference in gradients

$$y_k = g_{k+1} - g_k. \tag{1.5}$$

*Presented at the conference NAO2008 on "Numerical Analysis and Optimization," Muscat, 6-8 April, 2008.

†Department of Mathematics and Statistics, Sultan Qaboos University , P.O. Box 36, Muscat 123, Oman. (albaali@squ.edu.om)

‡Department of Mathematics and Computer Science, UAE University, Al-Ain 17551, United Arab Emirates. (humaidf@uaeu.ac.ae)

Thus, iteration (1.2) combines self-scaling methods with methods that modify the gradient difference which we discuss below.

Notice that the 'unmodified' choice $\widehat{y}_k = y_k$ reduces $\widehat{w}_k$ to w_k and formula (1.3) to the Broyden family of self-scaling updates. If, in addition, the self-scaling parameter $\tau_k = 1$, this family reduces to the 'unscaled' Broyden family of updates. It includes the well-known BFGS, DFP and SR1 updates, using the updating parameter $\theta_k = 0$; $\theta_k = 1$; and $\theta_k = y_k^T s_k/(y_k^T s_k - s_k^T B_k s_k)$, respectively (see for example Dennis and Schnabel, 1996, and Fletcher, 1987).

If the objective function f is convex, $\theta_k \in (\xi_k, 1)$, where ξ_k is a certain negative value, and the steplength α_k, with $\alpha_k = 1$ tried first, satisfies the Wolfe conditions

$$f_k - f_{k+1} \geq -\sigma_0 s_k^T g_k \tag{1.6}$$

and

$$y_k^T s_k \geq -(1-\sigma_1) s_k^T g_k, \tag{1.7}$$

where $\sigma_0 \in (0, 1/2)$ and $\sigma_1 \in (\sigma_0, 1)$, then iteration (1.2) with B_k defined by a Broyden family update converges globally and q-superlinearly (see Byrd, Liu and Nocedal, 1992).

Al-Baali (1998) extended this result to self-scaling methods under the restriction that $\tau_k \leq 1$ is sufficiently large. Al-Baali and Khalfan (2005) considered a wide interval for θ_k and found that the self-scaling technique not only accelerated the convergence of the unscaled methods, but also succeeded in solving many problems that certain unscaled methods failed to solve, especially when $\theta_k \geq 1$. In particular, they employed scaling only when $\theta_k \geq 0$ by

$$\tau_k = \frac{\min(1, \rho_k)}{\max\left([1 + \theta_k(b_k h_k - 1)]^{1/(n-1)}, \theta_k\right)}, \tag{1.8}$$

where

$$\rho_k = \frac{y_k^T s_k}{s_k^T B_k s_k}, \quad b_k = \frac{s_k^T B_k s_k}{y_k^T s_k}, \quad h_k = \frac{y_k^T B_k^{-1} y_k}{y_k^T s_k}. \tag{1.9}$$

Assuming ρ_k is bounded away from zero, the corresponding subclass of self-scaling methods converges globally for convex functions, and q-superlinearly for $\theta_k \in [0, 1]$ if

$$\sum \ln \min(1, \rho_k) > -\infty. \tag{1.10}$$

Since it is not known whether this condition holds, we will replace $\min(1, \rho_k)$ by 1 in the above expressions if $\rho_k < 0.5$ so that it has a better chance to be satisfied.

Another approach to improving the performance of the BFGS method focused on modifing the gradient difference vector y_k. Based on the modification of Powell (1978) for constrained optimization, Al-Baali (2004) modified y_k to $\widehat{y}_k$ in quasi-Newton methods for unconstrained optimization, to ensure that the modified curvature $\widehat{y}_k^T s_k$ is sufficiently positive, and reported significant improvement in the performance of the limited memory L-BFGS method on a set of standard test problems. Other modifications of the form $\widehat{y}_k = y_k + O(\|s_k\|)$, where $\|.\|$ denotes the Euclidean norm, were proposed recently by several authors (see for example Yuan, 1991, Zhang, Deng, and Chen, 1999, Xu and Zhang, 2001, Li and Fukushima, 2001, Wei et al., 2004, Yabe, Ogasawara and Yoshino, 2007, Li, Qi and Roshchina, 2008, Al-Baali and Grandinetti, 2009, and the references therein).

In this paper we consider combining the techniques of self-scaling with modifications of gradient difference in order to improve the overall performance of the reulting algorithm. In Section 2 we describe some of the methods that employ gradient difference modifications, which we found were efficient in practice. In section 3, we combine these methods with self-scaling and extend the global and superlinear convergence result of Al-Baali (1998) for convex functions to the resulting combined methods. Section 4 states some details for implementing the algorithms under consideration and Section 5 describes some results of a large number of numerical tests for some combined methods. It is shown that the combined technique improves the performance of several unmodified methods (including the well known BFGS, DFP and SR1 methods) substantially. Section 6 gives conclusion and future work.

2. Gradient Difference Modifications. In this section we discuss some y-modification techniques which we want to combine with self-scaling methods.

If B_k is positive definite and the curvature condition $y_k^T s_k > 0$ is satisfied, then the updated matrix B_{k+1} defined by (1.3) with $\widehat{y}_k = y_k$ is positive definite for any $\tau_k > 0$ and $\theta_k > \bar{\theta}_k$, where $\bar{\theta}_k = 1/\left(1 - b_k h_k\right)$. Since $\bar{\theta}_k < 0$ (by Cauchy's inequality), it follows that any update with $\theta_k \geqslant 0$ (such as the BFGS and DFP updates or their self-scaling updates) preserves positive definiteness if the curvature condition holds. The SR1 update preserves positive definiteness only if either $b_k < 1$ or $h_k < 1$, which may not hold even for exact line searches and quadratic functions (see for example Fletcher, 1987). Moreover although the second Wolfe condition (1.7) guarantees the curvature condition, too small values of $y_k^T s_k$ compared to $s_k^T B_k s_k$ may cause difficulty for correcting B_k safely (see for example Powell, 1986, Byrd, Nocedal and Yuan, 1987, and Byrd, Liu and Nocedal, 1992, and Al-Baali and Khalfan, 2005).

Powell (1978) suggested modifying y_k to ensure safely positive definite updates, for the BFGS method in an SQP algorithm for constrained optimization (see also Fletcher, 1987, and Nocedal and Wright, 1999, for instance). In this method y_k is replaced by

$$\widehat{y}_k = \varphi_k y_k + (1 - \varphi_k) B_k s_k, \tag{2.1}$$

where $\varphi_k \in (0, 1]$ is chosen as close as possible to 1 and such that $\widehat{y}_k^T s_k$ is safely positive. In practical implementation, Powell (1978) updates y_k to $\widehat{y}_k = y_k + \frac{0.2-\rho_k}{1-\rho_k}(B_k s_k - y_k)$ only when $\rho_k < 0.2$ (see also Gill and Leonard, 2003, for numerical experiments).

Al-Baali (2004) used modification (2.1) instead of y_k, in the limited memory L-BFGS method of Liu and Nocedal (1989) for large-scale unconstrained optimization, with φ_k chosen such that the conditions

$$(1 - \sigma_2) s_k^T B_k s_k \leq \widehat{y}_k^T s_k \leq (1 + \sigma_3) s_k^T B_k s_k, \tag{2.2}$$

where $\sigma_2 \in (0, 1)$ and $\sigma_3 > 0$, hold. Thus y_k is modified not only when ρ_k is too small, but also when it is too large. One modification of using formula (2.1) with least change in y_k subject to condition (2.2) is given by

$$y_k^1 = \begin{cases} y_k + (1 - \varphi_k^-)(B_k s_k - y_k), & \rho_k < 1 - \sigma_2 \\ y_k + (1 - \varphi_k^+)(B_k s_k - y_k), & \rho_k > 1 + \sigma_3 \\ y_k, & \text{otherwise,} \end{cases} \tag{2.3}$$

where

$$\varphi_k^- = \frac{\sigma_2}{1-\rho_k}, \quad \varphi_k^+ = \frac{\sigma_3}{\rho_k - 1}. \tag{2.4}$$

These parameters belong to the intervals $(\sigma_2, 1)$ and (0,1), respectively, and the latter one becomes $(\sigma_3, 1)$ if $\sigma_3 < \rho_k - 1 \leq 1$. Note that formula (2.3) reduces to the choice of Powell (1978) if $\sigma_2 = 0.8$ and $\sigma_3 = \infty$. A case worth noting is that when $\alpha_k = 1$ satisfies the strong Wolfe conditions and the choices $\sigma_3 = \sigma_2 = \sigma_1$ are used, then the curvature condition $y_k^{1T} s_k = y_k^T s_k > 0$ holds for all values of φ_k. On the other hand if a choice of $\sigma_2 < \sigma_1$ and $\rho_k < 1 - \sigma_2$ which may indicate that $y_k^T s_k$ is too small compared to $s_k^T B_k s_k$ (or that $y_k^T s_k \leq 0$ if the Wolfe condition (1.7) is not enforced, in particular when only condition (1.6) is used), then formula (2.3) enforces that $y_k^{1T} s_k = (1-\sigma_2) s_k^T B_k s_k$. Similarly, if $\sigma_3 < \sigma_1$ and $\rho_k > 1 + \sigma_3$, this formula also yields that $y_k^{1T} s_k = (1+\sigma_3) s_k^T B_k s_k$. Thus formula (2.3) modifies y_k only if ρ_k is sufficiently far away from 1 so that $y_k^{1T} s_k$ is sufficiently close to $s_k^T B_k s_k$.

Another modification of y_k was suggested by Zhang, Deng, and Chen (1999). Letting

$$t_k = 3[2(f_k - f_{k+1}) + (g_{k+1} + g_k)^T s_k], \tag{2.5}$$

the authors replaced y_k in the BFGS formula by the vector

$$y_k^2 = y_k + \frac{t_k}{||s_k||^2} s_k, \tag{2.6}$$

only when $y_k^{2T} s_k \geq 10^{-18} ||s_k||^2$ (which usually holds on most iterations). They showed that $t_k = 0$ if f is quadratic and for a general sufficiently smooth function f and small $||s_k||$, that $t_k = O(||s_k||^3)$ and

$$y_k^T s_k - s_k^T \nabla^2 f(x_{k+1}) s_k = O\left(||s_k||^3\right), \quad y_k^T s_k + t_k - s_k^T \nabla^2 f(x_{k+1}) s_k = O\left(||s_k||^4\right).$$

Thus $y_k^{2T} s_k$ approximates $s_k^T \nabla^2 f(x_{k+1}) s_k$ better than $y_k^T s_k$. The resulting modified BFGS method with the Wolfe conditions retains the global and q-superlinear convergence for convex functions, and performs slightly better than the standard BFGS method on some test problems.

Zhang and Xu (2001) extended choice (2.6) to the class of modified vectors

$$\widehat{y}_k = y_k + \frac{t_k}{u_k^T s_k} u_k, \tag{2.7}$$

where u_k is any vector such that $u_k^T s_k \neq 0$. Assuming $|u_k^T s_k| \geq \epsilon_1 \|s_k\| \|u_k\|$ and replacing t_k by $\widehat{t}_k = \max(t_k, (\epsilon_2 - 1) y_k^T s_k)$, where $\epsilon_1, \epsilon_2 > 0$, Xu and Zhang (2001) extended the above convergence result to class (2.7).

The authors also showed that t_k is invariant under linear transformation and quasi-Newton formulae remain invariant if u_k is chosen invariant. They considered a few choices for u_k and recommended $u_k = y_k$ to obtain the modified choice

$$y_k^3 = \left(1 + \frac{t_k}{y_k^T s_k}\right) y_k, \tag{2.8}$$

where t_k is defined by (2.5) and replaced by $(\epsilon_2 - 1) y_k^T s_k$ if $t_k < (\epsilon_2 - 1) y_k^T s_k$. Although, in practice, this case rarely happened for a very small value of ϵ_2, it might yield a nearly zero value of the modified curvature $\epsilon_2 y_k^T s_k$. To avoid this drawback, we replaced t_k by zero if the latter inequality holds so that the useful property of either y_k or y_k^3 is maintained (see also Al-Baali and Grandinetti, 2009). We observed that this modification improved the performance of the standard BFGS method substantially particularly when combined with self-scaling techniques as shown in Section 5.

Since choice (2.8) works better than other proposed modifications (considered in Al-Baali and Grandinetit, 2009, and Al-Baali and Khalfan, 2008), we will focus on combined methods of self-scaling technique with y-modification given by either (2.1) (with particular choice (2.3)) or (2.8) (with any of the above replacement whenever necessary).

3. Combining Methods. In the following algorithm we combine the self-scaling with y-modification techniques, discussed in the previous sections.

Algorithm 3.1

Step 0. Given a starting point x_1 and an initial symmetric and positive definite matrix B_1, choose values of σ_0 and σ_1, and set $k := 1$.
Step 1. Terminate if a convergence test holds.
Step 2. Calculate the search direction $d_k = -B_k^{-1} g_k$.
Step 3. Select a steplength α_k such that the new point (1.2) satisfies the Wolfe conditions (1.6) and (1.7).
Step 4. Compute the differences $s_k = x_{k+1} - x_k$ and $y_k = g_{k+1} - g_k$.
Step 5. Choose values for $\widehat{y}_k$, θ_k, and τ_k.
Step 6. Update B_k by (1.3) to obtain a new B_{k+1}.
Step 7. Set $k := k + 1$ and go to Step 1.

In order to obtain globally convergent methods, we assume that the updating and scaling parameters are chosen, as in Al-Baali (1998), such that

$$(1 - \nu_1)\bar{\theta}_k \le \theta_k \le \nu_2, \quad \theta_k \tau_k \le 1 - \nu_3, \quad \nu_4 \le \tau_k \le 1, \tag{3.1}$$

where $\nu_1, \ldots, \nu_4$ are positive constants. If the equation $b_k h_k = 1$ holds (which can happen near the solution), the author assumes that the first and middle of these conditions are not required on θ_k, because this equation yields $w_k = 0$ so that the Broyden family of updates becomes independent of θ_k. The modified vector $\widehat{y}_k$ is selected such that

$$\widehat{y}_k^T s_k \ge \nu_5 y_k^T s_k, \tag{3.2}$$

where $\nu_5 > 0$. If this condition does not hold for some $\widehat{y}_k$, we set $\widehat{y}_k = y_k$.

Here, we focus on choosing $\widehat{y}_k$ by either (2.1) or (2.8) which satisfy condition (3.2) with $\nu_5 = \varphi_k$ and $\nu_5 = \epsilon_2$, respectively. These choices maintain quasi-Newton methods invariant under linear transformation. For the former choice, Al-Baali (2004) shows that $\widehat{w}_k = \mu_k w_k$, where w_k is given by (1.4) with $\widehat{y}_k$ replaced by y_k and

$$\mu_k = \frac{\rho_k \varphi_k}{\rho_k \varphi_k + 1 - \varphi_k} \tag{3.3}$$

which belongs to (0,1]. Therefore, the modified self-scaling formula (1.3) can be written as

$$B_{k+1} = \tau_k \left(B_k - \frac{B_k s_k s_k^T B_k}{s_k^T B_k s_k} \right) + \phi_k w_k w_k^T + \frac{\widehat{y}_k \widehat{y}_k^T}{\widehat{y}_k^T s_k}, \tag{3.4}$$

where $\phi_k = \theta_k \tau_k \mu_k^2$. For the other choice (2.8), we also note that formulae (1.3) and (3.4) are equivalent if $\mu_k = 1$. Therefore, we use formula (3.4) to obtain the following result on the determinant and trace of the new Hessian approximation B_{k+1}.

LEMMA 3.1. *Assume that the curvature condition $y_k^T s_k > 0$ holds and the current matrix B_k is positive definite, and suppose that the updating and scaling parameters θ_k and τ_k are chosen such that condition (3.1) holds. Let y_k be modified to either (2.1) or (2.8) (with condition (3.2) holds). Then the determinant and trace of update (3.4) satisfy, respectively, the following inequalities*

$$\det(B_{k+1}) \geq \frac{\det(B_k)}{b_k}\nu_6, \tag{3.5}$$

where b_k is defined in (1.9) and ν_6 is a positive constant, and

$$\begin{aligned} trace(B_{k+1}) \leq trace(B_k) + \widetilde{\mu}_k \frac{\|y_k\|^2}{y_k^T s_k} + \phi_k \frac{\|y_k\|^2}{y_k^T s_k}\frac{s_k^T B_k s_k}{y_k^T s_k} \\ - (\mu_k - \phi_k)\frac{\|B_k s_k\|^2}{s_k^T B_k s_k} - 2\phi_k \frac{y_k^T B_k s_k}{y_k^T s_k}, \end{aligned} \tag{3.6}$$

where $\widetilde{\mu}_k$ is equal to either μ_k or $(1 + \frac{\max(t_k,0)}{y_k^T s_k})$ if $\widehat{y}_k$ is given by either (2.1) or (2.8), respectively.

Proof. Since the modified self-scaling formula (3.4) is obtained by replacing B_k by $\tau_k B_k$ in the unscaled modified Broyden family formula, it follows from Al-Baali (1998, 2004) that

$$\begin{aligned} \det(B_{k+1}) &= \frac{\det(B_k + \theta_k \mu_k^2 w_k w_k^T)}{\widehat{b}_k}\tau_k^{n-1} \\ &= \frac{\det(B_k)}{\widehat{b}_k}(1 + \theta_k \mu_k^2 (b_k h_k - 1))\tau_k^{n-1}, \end{aligned} \tag{3.7}$$

where $\widehat{b}_k$ is equal to b_k with y_k replaced by $\widehat{y}_k$. Noting that $\widehat{b}_k \leq b_k/\nu_5$ (by (3.2)), $b_k h_k \geq 1$ (by Cauchy's inequality) and $\mu_k^2 \leq 1$ and using condition (3.1), we obtain inequality (3.5) with $\nu_6 = \nu_1 \nu_4^{n-1} \nu_5$.

Now consider finding the other inequality (3.6). As in Al-Baali (1998), noting that the resulting matrix inside the brackets of (3.4) is positive semi-definite and using $\tau_k \leq 1$ (by (3.1)), it follows from (3.4) that

$$trace(B_{k+1}) \leq trace(B_k) - \frac{\|B_k s_k\|^2}{s_k^T B_k s_k} + \phi_k \|w_k\|^2 + \frac{\|\widehat{y}_k\|^2}{\widehat{y}_k^T s_k}. \tag{3.8}$$

For choice (2.1), we use the result of Al-Baali (2004) that

$$\frac{\|\widehat{y}_k\|^2}{\widehat{y}_k^T s_k} \leq (1 - \mu_k)\frac{\|B_k s_k\|^2}{s_k^T B_k s_k} + \mu_k \frac{\|y_k\|^2}{y_k^T s_k},$$

while for choice (2.8), we note that

$$\frac{\|\widehat{y}_k\|^2}{\widehat{y}_k^T s_k} = (1 + \frac{t_k}{y_k^T s_k})\frac{\|y_k\|^2}{y_k^T s_k}$$

if $t_k \geq (\epsilon_2 - 1)y_k^T s_k$ or, otherwise, t_k is replaced by either 0 or $(\epsilon_2 - 1)y_k^T s_k < 0$. Hence, on substituting these expressions and that of w_k (given by (1.4) with $\widehat{y}_k$ replaced y_k) into (3.8), we obtain (3.6). ▯

Note that if $\widetilde{\mu}_k = 1$ and $\mu_k = 1$, then inequality (3.6) is reduced to equation (3.2) of Byrd, Nocedal and Yuan (1987). Thus, we will use inequalities (3.5) and (3.6) to extend the convergence analysis of that paper to Algorithm 3.1, based on the analysis of Al-Baali (1998, 2004). We will combine the convergence results of both Al-Baali (1998) for self-scaling technique (which is an extension of those of Byrd, Liu and Nocedal, 1992, Zhang and Tewarson, 1988, Byrd, Nocedal and Yuan, 1987, and Powell, 1976) and Al-Baali (2004) for $y-$modification technique (which is an extension of the analyses of Powell, 1978, and Xu and Zhang, 2001). We first establish the global convergence result, using the following standard assumptions on the objective function.

Assumption 3.2.
1. *The objective function f is twice continuously differentiable.*
2. *The level set $\Omega = \{x : f(x) \leq f_1\}$ is convex, and there exist positive constants m and M such that*

$$m\|z\|^2 \leq z^T G(x) z \leq M\|z\|^2 \tag{3.9}$$

for all $z \in R^n$ and all $x \in \Omega$.

3. *The Hessian matrix G satisfies a Lipschitz condition*

$$\|G(x) - G(x_*)\| \leq L\|x - x_*\|, \tag{3.10}$$

where L is a positive constant, for all x in a neighborhood of x_*.

We note that condition (3.9) implies that

$$m\|s_k\|^2 \leq y_k^T s_k \leq M\|s_k\|^2, \quad \|y_k\| \leq M\|s_k\|, \tag{3.11}$$

since $y_k = \bar{G}_k s_k$, where $\bar{G}_k$ is the average Hessian along s_k (see for example Byrd, Nocedal and Yuan, 1987).

Theorem 3.3. *Let x_1 be any starting point for which Assumption 3.2 holds. Suppose that y_k is modified to either (2.1) or (2.8) (with condition (3.2) holds), and that the updating and scaling parameters θ_k and τ_k are chosen such that condition (3.1) holds. Then Algorithm 3.1 generates a sequence of points $\{x_k\}$ which converges R-linearly to the solution x_* such that $\sum_{k=1}^{\infty} \|x_k - x_*\| < \infty$.*

Proof. We note that the terms in expressions (3.5) and (3.6) are independent of τ_k, except the parameter $\phi_k (= \theta_k \tau_k \mu_k^2)$ which is strictly less than 1. Hence the proof simply follows from the analysis of Al-Baali (2004), who extended the convergence result of Byrd, Liu and Nocedal (1992) for a restricted Broyden family of methods to its modification with choice (2.1), in the following way.

For this choice we note that $\widetilde{\mu}_k = \mu_k \leq 1$. For choice (2.8) we calculate the Taylor series expansion of t_k (given by (2.5)) about x_k and use conditions (3.9) and (3.11) to obtain a bound on $\widetilde{\mu}_k$. Thus, for both choices, there exists a positive constant c such that $\widetilde{\mu}_k \leq c$ (see also Xu and Zhang, 2001, for a bound on choice (2.8)).

We notice that the right hand side of inequality (3.6) and that of equation (3.2) of Byrd, Nocedal and Yuan (1987) differ only in the coefficients $\widetilde{\mu}_k$ and $-(\mu_k - \phi_k)$. Since the former coefficient is bounded and the latter one is strictly negative, the analysis which is based on (3.2) of that paper (in particular inequality (3.7)) is still going through. Since, in addition, the determinant inequality (3.5) is the same as that given by Byrd, Liu and Nocedal (1992), the rest of the proof follows from Theorem 3.1 of that paper which is based on the analysis of Byrd, Nocedal and Yuan (1987). □

We note that this result is still valid if the globally convergence condition (3.1) is extended to

$$(1-\nu_1)\bar{\theta}_k \le \theta_k \mu_k^2 \le \nu_2, \quad \theta_k \mu_k^2 \tau_k \le 1-\nu_3, \quad \nu_4 \le \tau_k \le 1. \tag{3.12}$$

These conditions allow an interval for θ_k wider than that permitted by condition (3.1), for $\mu_k^2 < 1$. Thus to obtain the superlinear convergence result, we use the other conditions of Al-Baali (1998) with θ_k multiplied by μ_k^2. Therefore, we assume that

$$\sum_{\theta_k \le 0} \ln \tau_k^{n-1} + \sum_{\theta_k > 0} \ln \left[(1 + \theta_k \mu_k^2 (b_k h_k - 1)) \tau_k^{n-1} \right] > -\infty \tag{3.13}$$

and bound θ_k from below by a certain negative value ξ_k (given by (5.3) of Al-Baali, 1998) which depends on the Hessian matrix. We now state the superlinear convergence result of Algorithm 3.1.

THEOREM 3.4. *Let x_1 be any starting point for which Assumption 3.2 holds. Suppose that y_k is modified to either (2.1) or (2.8) (with condition (3.2) holds). Suppose also that the parameters θ_k and τ_k are chosen such that conditions (3.12), (3.13) and $\theta_k \mu_k^2 \ge \xi_k$ hold. Assume that the line search scheme for finding α_k starts with testing $\alpha_k = 1$. Then the sequence $\{x_k\}$ generated by Algorithm 3.1 converges to x_* q-superlinearly, the sequences $\{\|B_k\|\}$ and $\{\|B_k^{-1}\|\}$ are bounded, and*

$$\lim_{k\to\infty} b_k = \lim_{k\to\infty} h_k = 1. \tag{3.14}$$

Proof. Using expressions (3.5) and (3.6), the result follows from the above theorem, its proof, and Theorems 4.2 and 5.2 of Al-Baali (1998) with θ_k replaced by $\theta_k \mu_k^2$, based on Theorem 3.5 of Byrd, Liu and Nocedal (1992). □

This result shows that a combined class of methods, which converges superlinearly for $\theta_k \in [0,1]$ and globally for $\theta_k > 1$, can be implemented in practice by choosing $\tau_k = 1/\max\left([1+\theta_k\mu_k^2(b_kh_k-1)]^{1/(n-1)}, \theta_k\mu_k^2\right)$. This choice also yields superlinear convergence for $\theta_k > 1$ if it satisfies condition (3.13). In practice, we observed that this scaling technique improves substantially the performance of several unscaled methods defined for $\theta_k > 0$ (particularly as θ_k increases). Since $\theta_k = 0$ yields the unscaled value $\tau_k = 1$ and the scaled choice $\tau_k = \min(1, \rho_k)$ improves over the unscaled BFGS method (see for example Al-Baali and Khalfan, 2005), we consider the smaller scaling value

$$\tau_k = \frac{\min(1,\rho_k)}{\max\left([1+\theta_k\mu_k^2(b_kh_k-1)]^{1/(n-1)}, \theta_k\mu_k^2\right)}. \tag{3.15}$$

Hence for $\theta_k \in [0,1]$ and sufficiently small value of ν_3, condition (3.13) is reduced to (1.10). Because this condition is not guaranteed, we replace the numerator of (3.15) by the greater than or equal value

$$\widehat{\rho}_k = \begin{cases} \rho_k, & \nu_7 < \rho_k < 1 \\ 1, & \text{otherwise,} \end{cases} \tag{3.16}$$

where $\nu_7 \geq 0$. For a sufficiently large value of ν_7, small values of ρ_k are avoided and, hence, condition (3.1) on τ_k is easily satisfied and condition (1.10) has a better chance to be hold. Here, we choose $\nu_7 \geq 1 - \sigma_2$ so that combining self-scaling with y-modification choice (2.3) yields either $\widehat{\rho}_k = 1$ or $\mu_k = 1$. Since the latter equality is also always satisfied for choice (2.8), we suggest

$$\tau_k = \frac{\widehat{\rho}_k}{\max\left([1 + \theta_k(b_k h_k - 1)]^{1/(n-1)}, \theta_k\right)} \tag{3.17}$$

which reduces to (1.8) when $\widehat{\rho}_k = \rho_k$. The self-scaling parameter (3.17) works well in practice in the combined class of methods for both y-modifications (2.3) and (2.8) (see Section 5 for detail).

4. Implementation. We implemented Algorithm 3.1 as follows. We set the initial Hessian approximation $B_1 = I$, the identity matrix, and terminate the algorithm in Step 1 if either $\|g_k\|^2 \leq \epsilon \max(1, |f_k|)$, where $\epsilon = 2^{-52} \approx 2.22 \times 10^{-16}$ (the machine epsilon), $f_k \geq f_{k-1}$ for $k > 1$, or k exceeded 5000. In Step 3, we use the line search scheme of Fletecher (1987) for finding a step-length α_k such that the strong Wolfe conditions

$$f_{k+1} \leq f_k + \sigma_0 \alpha_k d_k^T g_k, \quad |d_k^T g_{k+1}| \leq -\sigma_1 d_k^T g_k, \tag{4.1}$$

with $\sigma_0 = 10^{-4}$ and $\sigma_1 = 0.9$, are satisfied. In the limit, this scheme tries $\alpha_k = 1$ first.

Various choices of the modified difference gradients and the updating and scaling parameters are defined in Step 5. For given θ_k, $\widehat{y}_k = y_k$ and $\tau_k = 1$, Algorithm 3.1 defines a Broyden family method. In particular, we use these values and $\theta_k = 0$ (which yields the standard BFGS method), unless otherwise stated. For all choices of $\widehat{y}_k$, condition (3.2) was tested with $\nu_5 = 10^{-16}$. If it does not hold (which rarely happened), we use $\widehat{y}_k = y_k$. However, for the choice $\widehat{y}_k = y_k^1$ given by (2.3), we enforce the Wolfe-like condition of Al-Baali (2003) (see also Al-Baali and Grandinetti, 2009), using the values

$$\sigma_2 = \max(0.9, 1 - \frac{1}{\alpha_k}), \quad \sigma_3 = \max(9, \frac{1}{\alpha_k} - 1). \tag{4.2}$$

Thus (by (2.3)) y_k is unmodified when $\rho_k \in [0.1, 10]$ (sufficiently close to 1, say). In practice y_k^1 works better than y_k. We choose the updating and scaling parameters such that condition (3.1) holds with $\nu_1 = 0.05$, $\nu_2 = 10^{16}$, $\nu_3 = 0$ and $\nu_4 = 10^{-4}$.

When self-scaling is considered, we always scale the initial Hessian approximation B_1 before updating by

$$\tau_1 = \frac{h_1}{1 + \theta_1 (b_1 h_1 - 1)} \tag{4.3}$$

which gives the least value of the condition number of the matrix $[(\tau_1 B_1)^{-1} B_2]$ (Oren and Spedicato, 1976). For $k > 1$, we let the scaling parameter τ_k be defined by (1.8). To ensure bounds on τ_k as in condition (3.1), we replace τ_k by $\max(\tau_k, \nu_4)$ (so that for $\nu_4 = 10^{-4}$, $\tau_k = \nu_4$ was rarely used in our experiments). Hence Algorithm 3.1 with $\widehat{y}_k = y_k$ in Step 5 yields the restricted self-scaling class of Al-Baali (1998) (which we refer to as SS1).

To reduce the total number of scaling in SS1, we redefine τ_k by

$$\tau_k = \begin{cases} h_1/\widetilde{\theta}_1, & k = 1 \\ \rho_k/\max(\widetilde{\theta}_k^{1/(n-1)}, \theta_k, 1), & k > 1 \text{ and } \nu_7 < \rho_k < 1 \\ 1/\max(\widetilde{\theta}_k^{1/(n-1)}, \theta_k, 1), & \text{otherwise,} \end{cases} \tag{4.4}$$

where $\widetilde{\theta}_k = 1 + \theta_k(b_k h_k - 1) > 0$ and $\nu_7 \geq 0$ (we used $\nu_7 = 0.5$). Because this value is greater than $1 - \sigma_2$ ($= 0.1$, here), we note that parameter (4.4) reduces to (3.17) when $\theta_k \geq 0$ and $k > 1$. (The resulting self-scaling class is referred to as SS2.)

Letting $\widehat{y}_k$ be a modification of y_k, Algorithm 3.1 yields classes of modified SS1 and SS2 methods. These combined classes (referred to as CSS1 and CSS2, respectively) clearly combine self-scaling technique with that of gradient difference modifications. Here we let $\widehat{y}_k$ be either y_k^1, y_k^2 or y_k^3, defined by (2.3), (2.6) and (2.8), respectively. Note that, vice versa, the choice $\widehat{y}_k = y_k$ reduces CSS1 and CSS2 to SS1 and SS2, respectively.

5. Numerical Experience. In this section we report the results of numerical experience with a large number of methods, resulting from combining the slef-scaling updates and the technique of gradient difference modifications that we outlined in the previous section. Step 5 of Algorithm 3.1 defines various type of algorithms. We use the notation Clji, to denote a combined algorithm, where

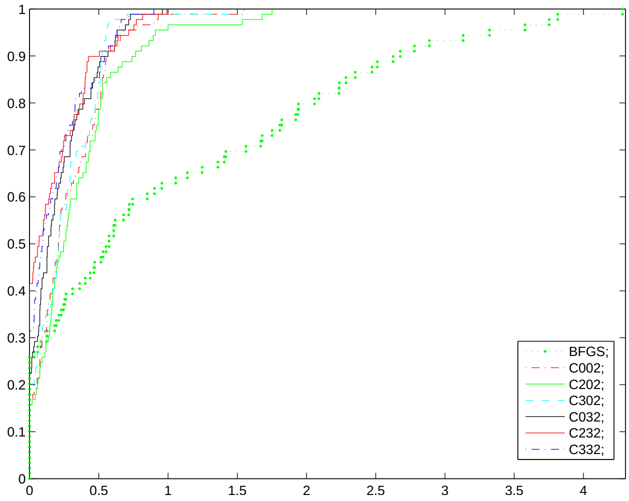
- $l = 0, 1, 2, 3$ denote respectively $\theta_k = 0$, $\theta_k = 1$, $\theta_k = 1/(1-b_k)$ if $h_k < 1$ else $\theta_k = 0$, and $\theta_k = \max\left[\theta_k^-, \min(0, 1 - b_k)\right]$, where θ_k^- is a certain negative value. The latter two choices for θ_k define, respectively, the switching BFGS/SR1 update of Al-Baali (1993) (see also Lukšan and Spedicato, 2000, for further experience), and a preconvex update of Al-Baali and Khalfan (2005).
- $j = 0, 1, 2, 3$ denote $\widehat{y}_k = y_k^j$, where $y_k^0 = y_k$.
- $i = 0, 1, 2$ denote respectively no scaling and the SS1 and SS2 self-scaling techniques.

Note that if $l \geq 2$, the choice of j should be made before defining l and i.

This results in 48 algorithms which we tested on a set of 89 standard test problems. The names and dimensions of each test is given in Table 6.1 in the Appendix. The dimensions of the tests ranged from 2 to 400. Two of these tests are from Fletcher and Powell (1963) and Grandinetti (1984) and the others are from Moré, Garbow and Hillstrom (1981) and Conn, Gould and Toint (1988).

We used the performance profiles tool of Dolan and Moré (2002) on the number of function evaluations and the number of gradient evaluations, denoted below by nfe and nge, respectively. Using this measure of performance, the results of all tests indicate that almost all modified methods outperform C000, the standard BFGS method. The most effective methods we found are C$lj2$ for all j and $l = 0, 2, 3$. Since, for these values of l, we observed (as should be expected) that the performance of class C$l3i$ is better than that of class C$l2i$, and the performance of the unmodified self-scaling C$l02$ class is similar to that of the combined C$l12$ class, we consider only C$lj2$ for $j = 0, 3$ in the following comparison of six methods to C000. The corresponding performance profile for nfe is plotted in Figure 5.1 which clearly shows that these methods are substantially better than C000 (a similar comparison's figure was obtained for nge). In terms of the average number of line searches, nfe and nge, these methods performed better than C000 by 30% approximately, where these averages are defined as in Al-Baali and Khalfan (2005), for instance. In fact, on many problems, the improvement was more than 60%.

FIG. 5.1. *nfe Comparison*



We also observed that the combined C032, C232 and C332 methods seem to be a little better than the unmodified self-scaling C002, C202 and C302 methods. A comparison of the three methods is shown in Figures 5.2 and 5.3 in terms of nfe and nge, respectively. These figures indicate that these methods have similar performance. Note that C232 combines the best features of the BFGS, SR1, self-scaling and y-modification methods. We also observed that C012 is also efficient with $\sigma_3 = \infty$ (as in Powell, 1978).

It is worth mentioning that C010 performed substantially better than C030, and that the self-scaling technique improved C010 slightly and C030 significantly (from 7%/7% to 28%/29% in terms of nfe/nge) which indicates the advantage of combining the self-scaling and y-modification techniques. (For further details see Al-Baali and Khalfan, 2008.)

We observed that the combined technique also improved the performance of less efficient methods such as the DFP method. For example, the combined C102, C122 and C132 methods which use the DFP updating formula succeeded in solving all the problems while C100 (the standard DFP method) failed on 45 problems.

Motivated by these results, we tested the above combined methods using a simpler standard backtracking line search framework which accepts the largest value of $2^{-i}\bar{\alpha}$ for $i = 0, 1, \ldots$, and $\bar{\alpha} = 1$ such that the function reduction condition (1.6) holds (see for example Nocedal and Wright, 1999). Although the curvature condition $y_k^T s_k > 0$ may not hold for this line search, the combined $Cl1i$ class maintains Hessian approximations positive definite. In the BFGS method, we skip the update if the latter condition does not hold. We observed that the average improvement of this class over BFGS is about 20% in terms of nge. When we repeated the run, however, starting the line search framework with $\bar{\alpha}$ as recommended by Fletcher (1987), we noticed that the average improvement increased from 2% to 16% but remained 20% in terms of nfe and nge, respectively. Similar improvement were observed for class $Clji$ with $j \neq 1$ which replaced y_k^j by $\widehat{y}_k^j$ if $y_k^{jT} s_k \leq 0$, where $\widehat{y}_k^j$ is given by the right hand side of (2.3) with y_k replaced by y_k^j so that Hessian approximations maintained positive definite.

FIG. 5.2. *nfe Comparison*

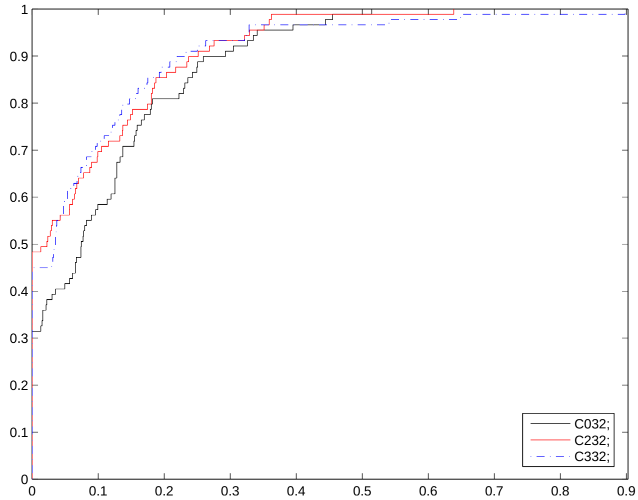
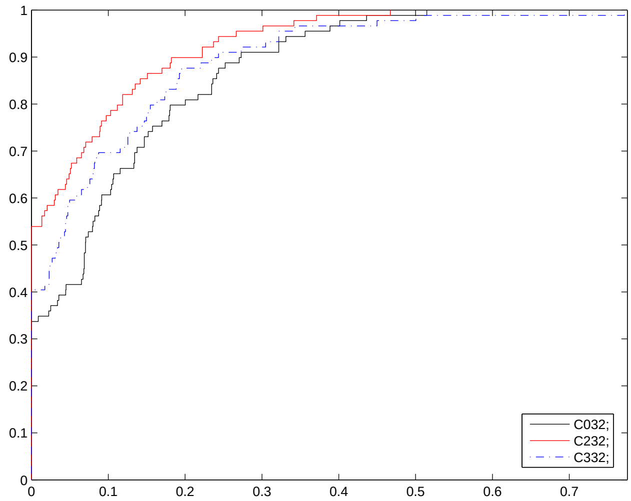


FIG. 5.3. *nge Comparison*



6. Conclusion. In this paper we presented some efficient methods that combine self-scaling updates and the technique of gradient difference modifications. We extended the known global and superlinear convergence property that the BFGS method has for convex functions to these methods, for a wide interval of the updating parameter θ_k. This interval includes values from not only the so-called convex class [0,1] of updates, but also from the preconvex and postconvex intervals.

We showed that practical implementations of some globally convergent combined methods improved substantially the performance of robust unscaled and self-scaling methods, such as BFGS, and significantly inefficient methods such as DFP. Specifically, we showed that the scaling parameter (3.17) works well for several choices of θ_k. It was shown that combing this scaling technique with y-modification technique

(2.8) gave the best features of both techniques.

It would be interesting to prove that condition (1.10) holds for a suiatble ρ_k (as that given in (1.9)) and investigate the combined methods in the trust region framework for constrained and unconstrained optimization.

REFERENCES

[1] Al-Baali, M. 1993. Variational Quasi-Newton Methods for Unconstrained Optimization. *JOTA*, **77**: 127–143.

[2] Al-Baali, M. 1998. Global and Superliner Convergence of a Restricted Class of Self-Scaling Methods with Inexact Line Searches for Convex Functions. *COAP*, **9**: 191–203.

[3] Al-Baali, M. 2003. Quasi-Wolfe Conditions for Newton-Like Methods. *Presented at 18th International Symposium on Mathematical Programming,* Copenhagen, August 18–22.

[4] Al-Baali, M. 2004. Quasi-Wolfe Conditions for Quasi-Newton Methods for Large-Scale Optimization. *Presented at 40th Workshop on Large Scale Nonlinear Optimization,* Erice, Italy, June 22 - July 1.

[5] Al-Baali, M. and Grandinetti, L. 2009. On Practical Modifications of the Quasi-Newton BFGS Method. *AMO - Advanced Modeling and Optimization*, **11**: 63–76.

[6] Al-Baali, M. and Khalfan, H. 2005. A Wide Interval for Efficient Self-Scaling Quasi-Newton Algorithms. *OMS*, **20**: 679–691.

[7] Al-Baali, M. and Khalfan, H. 2008. On Modified Slef-Scaling Quasi-Newton Methods, Research Report DOMAS 08/1, Sultan Qaboos University, Oman.

[8] Gill, P.E., Leonard, M.W. 2003. Limited-Memory Reduced-Hessian Methods for Large-Scale Unconstrained Optimization. *SIAM J. Optim.*, **14:** 380–401.

[9] Grandinetti, L. 1984. Some Investigations in a New Algorithm for Nonlinear Optimization Based on Conic Models of the Objective Function. *JOTA*, **43:** 1–21.

[10] Li, D. and Fukushima, M. 2001. A Modified BFGS Method and its Global Convergence in Nonconvex Minimiztion. *J. Compt. Appl. Math.*, **129**: 15–35.

[11] Li, D., Qi, L. and Roshchina, V. 2008. A New Class of Quasi-Newton Updating Formulas. *OMS*, **23**: 237–249.

[12] Liu, D.C. and Nocedal, J. 1989. On the Limited Memory BFGS Method for Large Scale Optimization. *Math. Programming*, **45**: 503–528.

[13] Lukšan, L. and Spedicato, E. 2000. Variable Metric Methods for Unconstrained Optimization and Nonlinear Least Squares. *J. Compt. Appl. Math.*, **124**: 61–95.

[14] Moré J.J., Garbow B.S. and Hillstrom K.E, 1981. Testing Unconstrained Optimization Software, *ACM transactions on mathematical software*, **7**: 17–41.

[15] Nocedal, J. and Wright, S.J. 1999. *Numerical Optimization*, Springer, London.

[16] Oren, S.S. and Spedicato, E. 1976. Optimal Conditioning of Self-Scaling Variable Metric Algorithms. *Math. Programming*, **10**: 70–90.

[17] Powell, M.J.D. 1976. Some Global Convergence Properties of a Variable Metric Algorithm for Minimization without Exact Line Searches. In R.W. Cottle and C.E. Lemke, editors, Nonlinear Programming. SIAM-AMS Proceedings, Vol. IX, SIAM Publications.

[18] Powell, M.J.D. 1978. Algorithms for Nonlinear Constraints that Use Lagrange Functions. *Math. Programming*, **14**: 224–248.

[19] Powell, M.J.D. 1986. How Bad are the BFGS and DFP Methods when the Objective Function is Quadratic?. *Math. Programming*, **34**: 34—47

[20] Wei, Z., Yu, G., Yuan, G. and Lian, Z. 2004. The Superlinear Convergence of a Modified BFGS-Type Method for Unconstrained Optimization. *COAP*, **29**: 315–332.

[21] Xu, C. and Zhang, J. 2001. A Survey of Quasi-Newton Equations and Quasi-Newton Methods for Optimization. *Annals of Operations research*, **103**: 213–234.

[22] Yabe, H., Ogasawara, H. and Yoshino, M. 2007. Local and Superlinear Convergence of Quasi-Newton Methods Based on Modified Secant Conditions. *Journal of Computational and Applied Mathematics*, **205**: 617–632.

[23] Yuan, Y. 1991. A Modified BFGS Algorithm for Unconstrained Optimization. *IMA J. of Numerical Analysis*, **11**: 325–332.

[24] Zhang, J.Z., Deng, N.Y. and Chen, L.H. 1999. Quasi-Newton Equation and Related Methods for Unconstrained Optimization. *JOTA*, **102**: 147–167.

[25] Zhang, J.Z. and Xu, C.X. 2001. Properties and Numerical Performance of Quasi-Newton Methods with Modified Quasi-Newton Equations. *J. Comput. Appl. Math.*, **137**: 269–278.

[26] Zhang, Y. and Tewarson, R.P. 1988. Quasi-Newton Algorithms with Updates from the Precon-

TABLE 6.1
Test Functions

Test Code	n	Function's name
MGH3	2	Powell badly scaled
MGH4	2	Brown badly scaled
MGH5	2	Beale
MGH7	3†	Helical valley
MGH9	3	Gaussian
MGH11	3	Gulf research and development
MGH12	3	Box three-dimensional
MGH14	4†	Wood
MGH16	4†	Brown and Dennis
MGH18	6	Biggs Exp 6
MGH20	6,9,12,20	Watson
MGH21	2†,10†,20†, ‡	Extended Rosenbrock
MGH22	4†,12†,20†, ‡	Extended Powell singular
MGH23	10,20, ‡	Penalty I
MGH25	10†,20†, ‡	Variably dimensioned
MGH26	10,20, ‡	Trigonometric of Spedicato
MGH35	8,9,10,20, ‡	Chebyquad
TRIGFP	10,20, ‡	Trigonometric of Fletcher and Powell
CH-ROS	10†,20†, ‡	Chained Rosenbrock
CGT1	8	Generalized Rosenbrock
CGT2	25	Another chained Rosenbrock
CGT4	20	Generalized Powell singular
CGT5	20	Another generalized Powell singular
CGT10	30, ‡	Toint's seven-diagonal generalization of Broyden tridiagonal
CGT11	30, ‡	Generalized Broyden tridiagonal
CGT12	30, ‡	Generalized Broyden banded
CGT13	30, ‡	Another generalized Broyden banded
CGT14	30, ‡	Another Toint's seven-diagonal generalization of Broyden tridiagonal
CGT15	10	Nazareth
CGT16	30, ‡	Trigonometric
CGT17	8, ‡	Generalized Cragg and Levy

†: Two initial points are used; one of them is the standard.
‡: $n = 40, 100, 200, 400$ are used to define large dimensional tests.
MGH: Problems from Moré, Garbow and Hillstrom (1981).
CGT: Problems from Conn, Gould and Toint (1988).
TRIGFP: Problem from Fletcher and Powell (1963).
CH-ROS: Problem from Grandinetti (1984).

vex Part of Broyden's Family. *IMA J. Numer. Anal.*, **8**: 487–509.