# A New Variable -Metric Conjugate Gradient Algorithm 

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#### Abstract

Motivated by the success of Shanno's memoryless Conjugate Gradient (CG) methods [28,29], this paper derives three new scaled quasi-Newton like CG algorithm that utilize an update formula that is invariant to a scaling of the objective function. The computation of the search directions, at each iteration, is done in two steps. The aim of developing such self scaling Variable Metric CG methods is to improve the quality of the generated search direction vectors. The computations involved are rather cheap as they merely involve a number of inner products and require just extra $\mathrm{O}(\mathrm{n})$ storage requirements. The extra requirements are shown to pay off when the algorithm is numerically compared to that developed by Shanno.


Keywords— Unconstrained Optimization, Conjugate Gradient Methods, Variable Metric methods, Inexact Line Search

## 1 Introduction

Conjugate Gradient (CG) methods were initially developed by Fletcher and Reeves [12] and were used to solve general unconstrained minimization problems. Those methods are still favored to the more rapidly convergent Quasi-Newton methods (QN) for big problems due to their low storage requirements $(\mathrm{O}(\mathrm{n}))$, instead of $\mathrm{O}\left(\mathrm{n}^{2}\right)$, as is the case with QN methods. This constitutes enough justification for constantly attempting to improve these methods. In this work the focus is rather on methods which combine the merits of both the CG and QN methods, as was done earlier by Perry [23] and Shanno [28,29]. Our derivation exploits the success of the multi-step QN methods $[18,19]$ to derive a CG algorithm that utilizes data available from recent iterations so that convergence is numerically accelerated further. Section 2 of this paper briefly introduces the CG methods and variants. Section 3 presents the idea of memoryless self scaling Variable-Metric CG methods. Section 4 focuses on the derivation of the new algorithms. Then, the numerical results are discussed in Section 4.

## 2 Memoryless Self-Scaling Variable-Metric Conjugate Gradient Methods

For a symmetric positive definite matrix $A$, the finite set of non-null linearly independent vectors $d_{1}, d_{2}, d_{3}, \ldots d_{k}$ is said to be conjugate if

$$
\begin{equation*}
d_{i}^{T} A d_{j}=0, \forall i \neq j . \tag{1}
\end{equation*}
$$

CG- methods are iterative and generate a sequence of approximations to the minimum $x^{*}$ of a scalar function $f(x)$ in order to solve

$$
\text { minmize } f(x), x \in R^{n} \text {, where } f: R^{n} \rightarrow R
$$

The sequence $x_{i}$ is defined by the following recurrence

$$
d_{i}= \begin{cases}-g_{i}, & \text { for } i=0,  \tag{2}\\ -g_{i}+\beta_{i-1} d_{i-1}, & \text { for } i \geq 1,\end{cases}
$$

where $g_{i}$ is the gradient of $f\left(x_{i}\right), \beta_{i}$ is a positive scalar chosen to minimize $f(x)$ along the search direction $d_{i}$, and the standard definition of $\beta_{i}$ is given by

$$
\beta_{i}=\begin{gather*}
y_{i}^{T} g_{i+1}  \tag{3}\\
d_{i}^{T} y_{i}
\end{gather*},
$$

for

$$
\begin{equation*}
y_{i}=g_{i+1}-g_{i} . \tag{4}
\end{equation*}
$$

The definition of $\beta_{i}$ in (3) is the one given in Hestenes and Stiefel [17] and is a modification to the original CG method derived by Polak and Ribiére [24] and Polyak [25].

This choice for the scalar $\beta_{i}$ is such that to make the search vectors $d_{k}$ and $d_{k+1}$ conjugate when the line searches are exact (ELS). However, since in practice line searches are not exact, Perry [23] rewrote (2) under the assumption of inexact line searches (ILS) as follows

$$
\begin{align*}
d_{i+1}=-[I- & y_{i}^{s_{i} y_{i}^{T}}{ }_{y_{i}^{T} s_{i}}^{s_{i} s_{i}^{T}}+y_{i}^{T} s_{i}  \tag{5}\\
= & Q_{i+1} g_{i+1}  \tag{6}\\
& s_{i}=x_{i+1}-x_{i} . \tag{7}
\end{align*}
$$

for

The matrix $\mathrm{Q}_{\mathrm{i}+1}$ satisfies a relation similar to the Secant relation, namely

$$
\begin{equation*}
Q_{i+1}{ }^{T} y_{i}=s_{i} \tag{8}
\end{equation*}
$$

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Perry's method [23] performance is only slightly better than the standard CG-method. Besides, the matrix $Q_{i+1}$ is not necessarily symmetric or positive definite so that the direction vector in (7) may not be a descent direction.
Shanno [28] derived a similar algorithm that satisfies the Secant relation

$$
\begin{equation*}
H_{i+1}{ }^{T} y_{i}=s_{i}, \tag{9}
\end{equation*}
$$

where $H_{i+1}$ is an approximation to the inverse Hessian. Shanno proposed

$$
\begin{equation*}
Q_{i+1}=I-\frac{s_{i} y_{i}^{T}+y_{i} T_{i}^{T}}{y_{i}^{T} s_{i}}+\left[1+\frac{y_{i}^{T} y_{i}}{y_{i}^{T} s_{i}}\right] \frac{s_{i} S_{i}^{T}}{y_{i}^{T} s_{i}} . \tag{10}
\end{equation*}
$$

Update formula (10) is actually the BFGS update formula with the update applied to the identity matrix at each iteration.

In fact, a similar dual relationship to (9)-(10) can be exhibited for any member of Broyden's $\theta$-class update [5,8,20].

The CG-method for which the search direction is computed using

$$
\begin{equation*}
d_{i+1}=-Q_{i+1}{ }^{T} g_{i+1} \tag{11}
\end{equation*}
$$

is referred to as a memoryless BFGS method.

The idea of self-scaling was originally developed by Oren [21] and Oren \& Spedicato [22]. Oren modified in [21] the Broyden $\vartheta$-class of updates as follows

$$
H_{i+1}=\left[H_{i}-\frac{H_{i} y_{i} y_{i}^{T} H_{i}}{y_{i}^{T} H_{i} y_{i}}+\vartheta_{i} r_{i} r_{i}^{T}\right] \mu_{i}+\frac{s_{i} s_{i}^{T}}{y_{i}^{T} s_{i}},
$$

where

$$
r_{i}=\sqrt{y_{i}^{T} H_{i} y_{i}}\left(\frac{s_{i}}{y_{i}^{T} s_{i}}-\frac{H_{i} y_{i}}{y_{i}^{T} H_{i} y_{i}}\right)
$$

and the specific value chosen for $\vartheta_{i}$ results in different update formula that belong to the Broyden family. For example, the BFGS update corresponds to $\vartheta_{i}=1$. The scaler $\mu_{i}$ is defined by (see [21])

$$
\mu_{i}=\frac{y_{i}^{T} s_{i}}{y_{i}^{T} H_{i} y_{i}} .
$$

Shanno [28] used this formula for $H_{i+1}$ to derive a modified CG-method with $H_{i}$ replaced by the identity matrix to eliminate the need for storing any matrices. This resulted in the following memoryless search direction formula

$$
d_{i+1}=-\left[\frac{y_{i}^{T} s_{i}}{y_{i}^{T} y_{i}} g_{i+1}+\left(\frac{2 g_{i+1}^{T} s_{i}}{s_{i}^{T} s_{i}}-\frac{g_{i+1}^{T} y_{i}}{y_{i}^{T} y_{i}}\right) s_{i}-\frac{g_{i+1}^{T} s_{i}}{y_{i}^{T} y_{i}} y_{i}\right] .
$$

This choice is equivalent to scaling the memoryless BFGS by by $\mu_{i}$.

The results given by this modified CG-method in [27] were rather disappointing.

Another memoryless Variable Metric (VM) method can be obtained by scaling, at each iteration, the update

$$
H_{i+1}=\left[H_{i}-\frac{H_{i} y_{i} y_{i}^{T} H_{i}}{y_{i}^{T} H_{i} y_{i}}+\vartheta_{i} r_{i} r_{i}^{T}\right] \mu_{i}+\frac{s_{i} s_{i}^{T}}{y_{i}^{T} s_{i}},
$$

by a positive scalar $\sigma_{\mathrm{k}}$ given by [27]

$$
\sigma_{i}=\frac{1}{\mu_{i}}
$$

The parameter $\sigma_{i}$ has the advantage of making the sequence of iterates invariant under multiplication of the objective function by a constant scalar. This results in the following memoryless VM search direction

$$
\begin{equation*}
d_{i+1}=-g_{i+1}-\left[\left(\frac{2 y_{i}^{T} y_{i} g_{i+1}^{T} s_{i}}{\left(y_{i}^{T} s_{i}\right)^{2}}-\frac{g_{i+1}^{T} y_{i}}{y_{i}^{T} s_{i}}\right) s_{i}+\frac{g_{i+1}^{T} s_{i}}{y_{i}^{T} s_{i}}\right] y_{i} \tag{12}
\end{equation*}
$$

For exact line search, we have $g_{i+1}^{T} s_{i}=0$ and hence $d_{i+1}$ becomes

$$
d_{i+1}=-g_{i+1}+\frac{g_{i+1}^{T} y_{i}}{y_{i}^{T} s_{i}} d_{i}
$$

which is the standard Hestenes \& Stiefel CG-method [17] and therefore has $n$-step convergence to the minimum of a quadratic function. Thus the CG-method is defined precisely by this new VM update (12), where the approximation to the inverse Hessian is reset to the identity matrix at every step.

The CG-algorithm defined by (2)-(4) exhibit a linear rate of convergence unless the method is restarted (generally every n steps) with direction $d_{t}=-g_{t}$, (see Powell [26], Biggs [3,4]). Powell suggests a restart every n steps or whenever

$$
\left|g_{i+1}^{T} g_{i}\right| \geq 0.2\left|g_{i+1}^{T} g_{i+1}\right| .
$$

Since the step taken in the direction of the negative gradient frequently results in a considerably small reduction in the objective function, Beale [2] derived a restart criterion intended to improve convergence rate. The restart step was taken to be the computed direction $\mathrm{d}_{\mathrm{t}}$ rather than $-g_{t}$ Subsequent non-restart steps are defined by ( $t$ being the index of the latest restart step):

$$
d_{\mathrm{i}+1}=-\mathrm{g}_{\mathrm{i}+1}+\beta_{i} d_{i}+\gamma_{i} d_{t},
$$

where

$$
\beta_{i}=\left(y_{i}{ }^{\mathrm{T}} g_{i+1}\right) /\left(d_{i}{ }^{\mathrm{T}} y_{i}\right)
$$

and
$\gamma_{i}=\left(y_{t}{ }^{\mathrm{T}} g_{i+1}\right) /\left(d_{t}{ }^{\mathrm{T}} y_{t}\right)$,
for $i=t+1, t+2, \ldots \ldots, t+n-1$.
Shanno [28], inspired by Beale's approach [2], proposed

$$
\begin{equation*}
d_{i+1}=-\left[I-\frac{d_{i} y_{i}^{T}}{y_{i}^{T} s_{i}}+\frac{d_{t} y_{t}^{T}}{y_{t}^{T} s_{t}}\right] g_{i+1} \tag{13}
\end{equation*}
$$

where $y_{i}$ is given in (4), $s_{i}$ is as in (7) and $t$ is the index of the last restart. The update matrix uses information from two prior points, namely $x_{i}$ and $x_{t}$ where the information gathered at $\mathrm{X}_{\mathrm{t}}$ is critical and must be exploited. Shanno [28] defined, for $k>t$, the following double update scheme

$$
\begin{equation*}
H_{t}=I-\frac{s_{t} v_{t}^{T}+y_{t} s_{t}^{T}}{y_{t}^{T} s_{t}}+\left[1+\frac{y_{t}^{T} y_{t}}{y_{t}^{T} s_{t}}\right] \frac{s_{t} s_{t}^{T}}{y_{t}^{T} s_{t}} \tag{14}
\end{equation*}
$$

and

$$
\begin{equation*}
H_{i+1}=H_{t}-\frac{s_{i} y_{i}^{T} H_{t}+H_{t} y_{y_{i}} s_{i}^{T}}{y_{i}^{T} s_{i}}+\left[1+\frac{y_{i}^{T} H_{t} y_{i}}{y_{i}^{T} s_{i}}\right] \frac{s_{i} s_{i}^{T}}{y_{i}^{T} s_{i}} \tag{15}
\end{equation*}
$$

The search direction at iteration $i$ is computed using

$$
d_{i+1}=-H_{i+1} g_{i+1}
$$

$$
\begin{aligned}
& d_{i+1}=-H_{i+1} g_{i+1} \\
& =-H_{t} g_{i+1}+\frac{s_{i}^{T} g_{i+1}}{s_{i}{ }^{T} y_{i}} H_{t} y_{i}-\left(\left(1+\frac{y_{i}{ }^{T} H_{t} y_{i}}{s_{i}{ }^{T} y_{i}}\right) \frac{s_{i}^{T} g_{i+1}}{s_{k}{ }^{T} y_{k}}-\frac{y_{i}^{T} H_{t} g_{i+1}}{s_{i}{ }^{T} y_{i}}\right) s_{i}
\end{aligned}
$$

The vector $H_{t} g_{i+1}$ and $H_{t} y_{1}$ are defined by

$$
H_{t}^{\prime} g_{i+1}=g_{i+1}-\frac{v_{t}^{T} g_{i+1}}{v_{t}^{T} y_{t}} y_{i}+\left(\left(1+\frac{y_{t}^{T} y_{t}}{v_{t}^{T} y_{t}}\right) \frac{v_{t}^{T} g_{i+1}}{v_{t}^{T} y_{t}}-\frac{y_{t}^{T} g_{i+1}}{v_{t}^{T} y_{t}}\right) v_{t}
$$

## and

$H_{t}^{\prime} y_{t}=y_{t}-\frac{v_{t}^{T} y_{i}}{v_{t}^{T} y_{t}} y_{t}+\left(\left(1+\frac{y_{t}^{T} y_{t}}{v_{t}^{T} y_{t}}\right) \frac{v_{t}^{T} y_{i}}{v_{t}^{T} y_{t}}-\frac{y_{t}^{T} y_{i}}{v_{t}^{T} y_{t}}\right) v_{t}$.
In implementing this algorithm additional storage is required to store vectors $x_{i+1}, x_{i}, g_{i+1}, g_{i}, d_{i}, d_{t}$, and $y_{t}$ (a total storage still of order n).

Another far more successful search direction, proposed by Shanno, is generated by using update (15) in the computation of the search direction. This yield for $i>t$
$H_{t}^{\prime}=\left[I-\frac{v_{t} y_{t} T+y_{t} v_{t} T}{v_{t}^{T} y_{t}}+\frac{y_{t} y_{t}^{T}}{v_{t}^{T} y_{t}} * \frac{v_{t} v_{t}^{T}}{v_{t}^{T} y_{t}}\right] \eta_{t}+\frac{v_{t} v_{t}^{T}}{v_{t}^{T} y_{t}}$.

Shanno therefore suggested scaling the matrix $\mathrm{H}_{\mathrm{t}}$ with

$$
\eta_{\mathrm{t}}=\left(\mathrm{v}_{\mathrm{i}}^{\mathrm{T}} \mathrm{y}_{\mathrm{i}}\right) /\left(\mathrm{y}_{\mathrm{t}}^{\mathrm{T}} \mathrm{y}_{\mathrm{t}}\right)
$$

but not the matrix $\mathrm{H}_{\mathrm{i}+1}$. In this case the two additional vectors are defined by

$$
H_{t}^{\prime} g_{i+1}=\eta_{t} g_{i+1}-\frac{v_{t}^{T} g_{i+1}}{y_{t}^{T} y_{t}} y_{t}+\left(\frac{2 v_{t}^{T} g_{i+1}}{v_{t}^{T} y_{t}}-\frac{y_{t}^{T} g_{i+1}}{y_{t}^{T} y_{t}}\right)
$$

and
$H_{t}^{\prime} y_{i}=\eta_{t} y_{i}-\frac{v_{t}^{T} y_{i}}{y_{t}^{T} y_{t}} y_{t}+\left(\frac{2 v_{t}^{T} y_{i}}{v_{t}^{T} y_{t}}-\frac{y_{t}^{T} y_{i}}{y_{t}^{T} y_{t}}\right)$.

However, he also tested the application of the Flecher [15] scaling in his numerical trials. In consequence he proposed using only the scaled $H_{t}^{\prime}$ at restart steps, and at each nonrestart step to scale according to the following Flecher scaling criterion:

$$
d_{i+1}^{\prime}=\left[2\left(f_{i+1}-f_{i}\right) / d_{i+1}^{T} g_{i+1}\right] d_{i+1}
$$

The vectors that require retention in storage for this method are $x_{i+1}, x_{i}, g_{i+1}, g_{i}, d_{i}, d_{t}$, and $y_{t}$.

## 3 A new Memoryless Variable Metric CG Algorithm

In this derivation, we start by presenting a new variable metric (VM) update formula that will be used in the derivation of the new memoryless VM CG method. The notion of self-scaling quasi-Newton algorithms was first proposed by Oren [21], and Oren \& Spedicato [22]. The update formula used in this paper is a generalization of Oren's update [21], modified to satisfy

$$
\begin{equation*}
H_{i+1} u_{i}=\sigma_{i} v_{i} \tag{16}
\end{equation*}
$$


The resulting update formula is given by

$$
\begin{equation*}
H_{i+1}=H_{i}+\frac{2 u_{1}^{T} H_{1} H_{i}}{\left(u_{i}^{T} v_{i}\right)^{2}} v_{i} v_{i}^{T}-\frac{t_{1}^{T} H_{1}^{T} H_{1}+H_{1} \psi_{1} v_{T}^{T}}{u_{i}^{T} v_{i}} . \tag{17}
\end{equation*}
$$

The parameter $\sigma_{i}$ is introduced to make the method invariant under multiplication of the objective function by a constant. It is worth mentioning that the standard CG-method can be obtained from (17) if the approximation to the inverse Hessian $H_{i}$ is taken to be the identity matrix and the vectors $u_{i}$ and $v_{i}$ are chosen to be $y_{i}$ and $s_{i}$, respectively. Like in (14), the matrix $H_{t}$ is this given as

$$
\begin{align*}
& H_{t}=I+\frac{2 u_{t}^{T} u_{t}}{\left(u_{t}^{T} v_{t}\right)^{2}} v_{t} v_{t}^{T}-\frac{v_{t} u_{t}^{T}+u_{t} v_{t}^{T}}{u_{t}^{T} v_{t}} . \\
& H_{t}=I+\frac{2 u_{t}^{T} u_{t}}{\left(u_{t}^{T} v_{t}\right)^{2}} v_{t} v_{t}^{T}-\frac{v_{t} u_{t}^{T}+u_{t} v_{t}^{T}}{u_{t}^{T} v_{t}} . \tag{18}
\end{align*}
$$

Consequently,

$$
\begin{equation*}
H_{i+1}=H_{t}+\frac{2 u_{i}^{T} H_{t} u_{i}}{\left(u_{i}^{T} s_{i}\right)^{2}} s_{i} s_{i}^{T}-\frac{s_{i} u_{i}^{T} H_{t}+H_{t} u_{i} T_{i}^{T}}{u_{i}^{T} s_{i}} . \tag{19}
\end{equation*}
$$

The search direction, in this case, is defined by:

$$
\begin{align*}
d_{i+1}= & -H_{i+1} g_{i+1} \\
& =H_{t} g_{i+1}+\frac{v_{i}^{T} g_{i+1}}{u_{i}^{T} v_{i}} H_{t} u_{i}-\frac{2 u_{i}^{T} H_{t} u_{i}-u_{i}^{T} H_{t} g_{i+1}}{u_{i}^{T} v_{i}} v_{i} \tag{20}
\end{align*}
$$

where the two additional vectors that need to be stored to implement this method are defined by

$$
\begin{equation*}
H_{t} g_{i+1}=g_{i+1}-\frac{s_{t}^{T} g_{i+1}}{y_{t}^{T} s_{t}} y_{t}+\frac{\left(2 y_{t}^{T} y_{t}\right)\left(s_{t}^{T} g_{i+1}\right)-y_{t}^{T} g_{i+1}}{y_{t}^{T} s_{t}} s_{i} \tag{21}
\end{equation*}
$$

and

The following theorem reveals that the search direction (20) is a special case of the Beale's 3-term CG method, given as

$$
\begin{equation*}
d_{\mathrm{i}+1}=-\mathrm{g}_{\mathrm{i}+1}+\beta_{i} d_{i}+\gamma_{i} d_{t} \tag{23}
\end{equation*}
$$

where

$$
\beta_{i}=\left(y_{i}^{\mathrm{T}} g_{i+1}\right) /\left(d_{i}^{\mathrm{T}} y_{i}\right)
$$

and

$$
\gamma_{i}=\left(y_{t}^{\mathrm{T}} g_{i+1}\right) /\left(d_{t}^{\mathrm{T}} y_{t}\right)
$$

for $i=t+1, t+2, \ldots \ldots, t+n-1$.
Theorem 1: If $f(x)$ is quadratic and the vectors $u_{i}$ and $v_{i}$ are chosen to be $y_{i}$ and $s_{i}$, respectively, the search direction given by (20) is equivalent to the 3-term search directions generated by Beale's method [2] when the line searches are exact.

Proof. From (20), and since an exact line search is used gives

$$
\begin{aligned}
& s_{i}^{T} g_{i+1}=0 \text {, we obtain } \\
& d_{i}=-H_{t} g_{i+1}+\frac{y_{i}^{T} H_{t} g_{i+1}}{s_{i}^{T} y_{i}} s_{i} .
\end{aligned}
$$

We also note that for a quadratic function
$g_{k+1}=A x_{k+1}+b=A\left(x_{t+1}+\sum_{i=t+1}^{k} v_{i}\right)+b=g_{t+1}+\sum_{i=t+1}^{k} A v_{i}$.
Hence, for ELS and quadratic functions

$$
s_{t}^{T} A s_{k}=0, \text { for } i=t+1, \ldots, \ldots .
$$

Thus,

$$
\begin{equation*}
s_{t}^{T} g_{i+1}=s_{t}^{T} g_{t+1}=0 \tag{24}
\end{equation*}
$$

Now from (21), using (24), we have

$$
\begin{equation*}
H_{t}^{\prime} g_{i+1}=g_{i+1}-\left[y_{t}^{T} g_{i+1} / v_{t}^{T} y_{t}\right] v_{t} \tag{25}
\end{equation*}
$$

Substituting (25) in (23) we get

$$
\begin{equation*}
d_{i+1}=-g_{i+1}+\frac{y_{t}^{T} g_{i+1}}{s_{t}^{T} y_{t}} s_{t}+\frac{y_{i}^{T} g_{i+1}}{v_{i}^{T} y_{k}} s_{i}-\frac{\left(y_{t}^{T} g_{i+1}\right)\left(y_{i}^{T} s_{t}\right)}{\left(s_{i}^{T} y_{i}\right)\left(s_{t}^{T} y_{t}\right)} s_{i} \tag{26}
\end{equation*}
$$

By the conjugacy condition we have

$$
y_{i}^{T} s_{t}=0
$$

Thus, (26) reduces to

$$
\begin{equation*}
d_{i+1}=-g_{i+1}+\frac{y_{t}^{T} g_{i+1}}{s_{t}^{T} y_{t}} s_{t}+\frac{y_{i}^{T} g_{i+1}}{s_{i}^{T} y_{i}} s_{i} \tag{27}
\end{equation*}
$$

The search direction (27) is identical to the search direction of Beale's method (23) (see [2]) and hence the proof is complete.

Usually, conjugate gradient algorithms are periodically restarted. Powell's restarting procedure [26], used in this algorithm, is for testing whether there is very little orthogonality left between the current gradient and the previous one. At step r when

$$
\left\|g_{r+1}^{T} g_{r}\right\| \geq 0.2\left\|g_{r+1}\right\|^{2}
$$

the algorithm may be restarted using (18) with $H_{t}$ set to $I$. For $i=r+1$, (20) is employed in the computation of the search direction.

## 4 Choosing the vectors $u_{i}$ and $v_{i}$

One obvious choice for the vectors is $u_{i}=y_{i}$ and $v_{i}=s_{i}$. This choice defines our first algorithm and for which a variant of the standard Secant equation is satisfied, namely

$$
H_{i+1} y_{i}=\sigma_{i} s_{i},
$$

(MNEWH1)
for

$$
\sigma_{i}=\frac{y_{i}^{T} H_{i} y_{i}}{s_{i}^{T} y_{i}}
$$

The other choice is inspired by the approach of Wei et al. [30]. Assuming that the objective function is smooth, then using the Taylor series for $f(x)$ at the point $x_{i+1}$ gives

$$
\begin{aligned}
& f(x) \cong f_{i+1}+g_{i+1}^{T}\left(x-x_{i+1}\right) \\
& \quad+\frac{1}{2}\left(x-x_{i+1}\right)^{T} G_{i+1}\left(x-x_{i+1}\right)
\end{aligned}
$$

where $G_{i+1}$ denotes the Hessian of $f(x)$ at the point $x_{i+1}$. It follows that

$$
f_{i} \cong f_{i+1}-s_{i}^{T} g_{i+1}+\frac{1}{2} s_{i}^{T} G_{i+1} s_{i} .
$$

Thus,

$$
s_{i}^{T} B_{i+1} s_{i}=2\left(f_{i}-f_{i+1}\right)+s_{i}^{T}\left(g_{i}+g_{i+1}\right)+s_{i}^{T} y_{i}
$$

However, if the following special case Taylor series for $f(x)$ is used

$$
f_{i}(x) \cong f(x)+\frac{1}{2}\left(x-x_{i}\right)^{T} A_{i}\left(x-x_{i}\right)
$$

for $A_{i}$ being a symmetric positive definite matrix, and using the relationship obtained for $s_{i}^{T} B_{i+1} s_{i}$, then the following modified version of the Secant equation is obtained

$$
\begin{equation*}
B_{i+1} s_{i}=\hat{y}_{i} \tag{28}
\end{equation*}
$$

for

$$
\hat{y}_{i}=y_{i}+\frac{\rho_{i}}{\left\|s_{i}\right\|^{2}} s_{i},
$$

where $\rho_{i}=2\left(f_{i}-f_{i+1}\right)+\left(g_{i}+g_{i+1}\right)^{T} s_{i}$.
Adopting this choice in our derivation, we have from (16) and (28)

$$
H_{i+1} \hat{1}_{i}=\sigma_{i} s_{i},
$$

(MNEWH2)
for the choices $u_{i}=\hat{y}_{i}$ and $v_{i}=s_{i}$.
The last choice is based on the modified secant equation derived in $[14,18,19]$. The methods introduced by the authors utilize the step vectors $s_{i}$ and $s_{i-1}$ (along with the corresponding $y_{i}$ and $y_{i-1}$ ) in the construction of a variant to the standard quasi-Newton methods that are based on the classical secant equation. The idea is that previous iteration data is discarded after used once and that exploiting that data in the construction of the Hessian (or its inverse) approximation at each iteration pays off, as indicated by the results presented for the multi-step methods. The inverse Hessian approximation update generally satisfies:

$$
H_{i+1}\left(y_{i}-\mu_{i-1} y_{i-1}\right)=s_{i}-\mu_{i-1} s_{i-1}
$$

(MNEWH3)
or

$$
v_{i}=H_{i+1} u_{i}
$$

where

$$
\mu_{i-1}=\frac{\delta_{i-1}^{2}}{2 \delta_{i-1}+1}
$$

and

$$
\delta=\frac{\left\|s_{i}\right\|}{\left\|s_{i-1}\right\|}
$$

This expression for $\delta$ may be generalized by introducing a scaling factor, $\gamma \geq 0$ (see [18]) that provides a control mechanism for convenient easy switching to the standard
secant equation update method obtained by setting the scalar $\gamma$ to zero. Therefore,

$$
\delta=\gamma \frac{\left\|s_{i}\right\|}{\left\|s_{i-1}\right\|}
$$

## 5 Numerical Results and Conclusion

For the above memoryless QN-algorithms it is necessary to ensure that

$$
\begin{equation*}
\mathrm{u}_{\mathrm{i}}^{\mathrm{T}} \mathrm{v}_{\mathrm{i}}>0 \quad \text { for } i \geq 0, \tag{29}
\end{equation*}
$$

so that the positive definiteness of the update matrix is maintained to ensure that the computed search vector is downhill. However, condition (29) is, in practice, replaced by a stronger line search criteria as follows

$$
\begin{equation*}
\left|s_{\mathrm{i}}{ }^{\mathrm{T}} \mathrm{~g}_{\mathrm{i}+1}\right|<\rho_{1}\left|s_{i}{ }^{\mathrm{T}} g_{i}\right| \tag{30}
\end{equation*}
$$

and

$$
\begin{equation*}
\mathrm{f}_{\mathrm{i}+1}-\mathrm{f}_{\mathrm{i}}<\rho_{2} s_{i}^{\mathrm{T}} g_{i} \tag{31}
\end{equation*}
$$

Conditions (30) and (31) are sufficient to ensure convergence of any descent method [16]. Shanno used $\rho_{1}=0.1$ and $\rho_{2}=0.0001$ and to test his double update algorithms and we use those same choices for our methods.
In order to assess the performance of the new algorithms (MNEWH1, MNEWH2, MNEWH3), those are benchmarked against Shanno's memoryless QN algorithm [28]. The methods are tested on a collection of 30 varied dimensionality test problems with dimensions ranging $2 \leq \mathrm{n} \leq 1000$. The test functions can be found in [13,14,15,18]. A cubic fitting technique line search strategy is used for all methods. The algorithms terminate when the gradient vector magnitude is less than $10^{-5}$. All methods are restarted every n iterations or whenever (12) is satisfied, with

$$
d_{i+1}=\frac{d_{i}^{T} d_{i}}{g_{i+1}^{T} g_{i+1}} d_{i}
$$

Performance of the algorithms is evaluated by considering both the total number of function evaluations (NOF) and the total number of iterations (NOI). The results are reported in Table 1.

Analysis of this table shows that the three derived methods have a clear advantage over Shanno's method. When it comes to function/gradient evaluations, MNEWH3 seems to perform best (as it saves an overall about 28.4\% in NOF). However, it only saves overall about $4.81 \%$ in NOI). When it comes to the number of iterations (NOI), MNEWH2 is the winner (as it saves an overall about $16.8 \%$ in NOF and saves overall about $8.6 \%$ in NOI).

In conclusion, the new double update methods developed here are promising especially when the number of function/gradient evaluations is of significance. The number of extra vectors required is $\mathrm{O}(\mathrm{n})$. Specifically, the number of vectors required to keep in storage seems to be a reasonable tradeoff against the numerical gains incurred.

TABLE I.
NUMERICAL COMPARISON OF THE ALGORITHMS

| function | Size <br> (n) | $\begin{gathered} \text { MSHAN } \\ O^{\text {a }} \\ \hline \end{gathered}$ | $\begin{gathered} \text { MNEWH } \\ \mathbf{1}^{\mathbf{a}} \\ \hline \end{gathered}$ | $\begin{gathered} \text { MNEWH } \\ 2 \\ \hline \end{gathered}$ | $\begin{gathered} \text { MNEWH } \\ 3 \\ \hline \end{gathered}$ |
| :---: | :---: | :---: | :---: | :---: | :---: |
|  |  | NOI(NOF) | NOI(NOF) | NOI(NOF) | NOI(NOF) |
| ROSEN | 2 | 34(170) | 31(105) | 32(144) | 36(141) |
| CUBIC | 2 | 19(128) | 17(90) | 21(111) | 20(112) |
| BEALE | 2 | 10(43) | 10(27) | 11(39) | 12(41) |
| BOX | 2 | 11(61) | 11(57) | 11(58) | 11(57) |
| FREUD | 2 | 10(53) | 10(29) | 9(31) | 11(29) |
| BIGGS | 3 | 12(42) | 17(60) | 16(51) | 17(54) |
| RECIPE | 3 | 5(21) | 5(19) | 4(20) | 5(19) |
| HELICAL | 3 | 29(127) | 46(99) | 33(101) | 31(103) |
| POWL3 | 3 | 14(48) | 16(37) | 15(35) | 15(36) |
| POWELL | 4 | 59(277) | 29(175) | 31(181) | 33(179) |
| WOOD | 4 | 23(83) | 23(51) | 23(55) | 24(51) |
| DIXON | 10 | 23(69) | 23(49) | 23(48) | 23(48) |
| OREN | 10 | 14(52) | 14(60) | 14(58) | 16(55) |
| EXPOWELL | 20 | 42(174) | 40(109) | 41(104) | 39(106) |
| EX-WOOD | 20 | 25(103) | 26(57) | 25(66) | 26(57) |
| NONDIGN | 20 | 27(134) | 24(56) | 25(78) | 27(51) |
| $\begin{aligned} & \hline \text { SUM- } \\ & \text { QUAR } \end{aligned}$ | 25 | 8(31) | 8(38) | 8(34) | 9(30) |
| OREN | 30 | 25(76) | 27(96) | 26(80) | 26(71) |
| TRI-DIGN | 30 | 31 (91) | 31(64) | 30(61) | 31(60) |
| $\begin{gathered} \text { SHALLO } \\ \mathrm{W} \end{gathered}$ | 40 | 8(31) | 8(25) | 7(23) | 6(22) |
| FULL | 40 | 46(134) | 46(95) | 44(94) | 44(91) |
| OREN | 50 | 35(115) | 34 (133) | 34(128) | 33(111) |
| $\begin{gathered} \text { EX- } \\ \text { ROSEN } \end{gathered}$ | 60 | 29(136) | 32(91) | 30(95) | 28(88) |
| EX-WOOD | 60 | 34(125) | 33(82) | 33(82) | 31(78) |
| WOLFE | 80 | 49(147) | 49(99) | 48(101) | 44(90) |
| NONDIGN | 90 | 27(155) | 24 (58) | 27(149) | 22(51) |
| $\begin{gathered} \text { EX- } \\ \text { ROSEN } \end{gathered}$ | 100 | 29 (128) | 30(174) | 30(147) | 29(111) |
| EXPOWELL | 100 | 46(201) | 41(131) | 44(176) | 41(119) |
| EX-WOOD | 100 | 36(140) | 39(191) | 37(180) | 33(130) |
| EXROSEN | $\begin{gathered} 100 \\ 0 \end{gathered}$ | 30(127) | 33(152) | 34(151) | 29(116) |
| $\begin{gathered} \text { TOTAL } \\ \text { NOI(NOF) } \\ \hline \end{gathered}$ |  | 790(3222) | 777(2491) | 722(2681) | 752(2307) |

${ }^{\text {a. }}$ algorithms terminate when the gradient vector magnitude is less than $10^{-5}$

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