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# A recursive formulation of limited memory variable metric methods

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Variable metric methods with limited memory can be efficiently used for large-scale unconstrained optimization in case the sparsity pattern of the Hessian matrix is not known. These methods are usually realized in the line-search framework so that they generate a sequence of points $x_i \in \mathcal{R}^n$, $i \in \mathcal{N}$, by the simple process

$$x_{i+1} = x_i + \alpha_i d_i, \tag{1}$$

where $d_i = -H_i g_i$ is a direction vector, $H_i$ is a positive definite approximation of the inverse Hessian matrix and $\alpha_i > 0$ is a scalar step-size chosen in such a way that

$$F_{i+1} - F_i \leq \varepsilon_1 \, \alpha_i \, d_i^T g_i, \quad d_i^T g_{i+1} \geq \varepsilon_2 \, d_i^T g_i \tag{2}$$

(the weak Wolfe conditions), where $F_i = F(x_i)$, $g_i = \nabla F(x_i)$ and $0 < \varepsilon_1 < 1/2$, $\varepsilon_1 < \varepsilon_2 < 1$. Matrices $H_i$, $i \in N$, are computed either by using a limited number ($m \ll n$) of variable metric updates applied to the scaled unit matrix or by updating low dimension matrices. The first approach, used in [9], is based on the computation of the direction vector $d_i$ using the Strang recurrences [8]. The second approach, used in [1], is based on the matrix expression described below. To simplifying notation, we omit index $i$ and replace index $i + 1$ by $+$.

Variable metric method from the Broyden class use the update

$$
\begin{aligned}
H_+ &= H + UMU^T = H + [d, Hy] \begin{bmatrix} m_1, & m_2 \\ m_2, & m_3 \end{bmatrix} \begin{bmatrix} d \\ Hy \end{bmatrix} \\
&= H + \frac{1}{b}dd^T - \frac{1}{a}Hy(Hy)^T + \frac{\eta}{a}\left(\frac{a}{b}d - Hy\right)\left(\frac{a}{b}d - Hy\right)^T,
\end{aligned} \tag{3}
$$

where $d = x_+ - x$, $y = g_+ - g$, $a = y^T Hy$, $b = y^T d$ and $\eta$ is a free parameter. We need to express $m$ consecutive steps of (3) (with the initial matrix $\gamma I$) in the form $H_+ = \gamma I + \bar{U}\bar{M}\bar{U}^T$, where $\bar{U} \in R^{n \times 2m}$ and $\bar{M} \in R^{2m \times 2m}$. In [1], the authors propose explicit expressions of the matrix $\bar{M}$ for three classic variable metric updates: DFP ($\eta = 0$), BFGS ($\eta = 1$) and the rank one ($\eta = b/(b - a)$). For other values of the parameter $\eta$, such explicit expressions are not known. In this contribution we describe another way, based on recursive construction of the matrix $\bar{M}$, which allows us to realize any member of the Broyden class of the variable metric updates. The following theorem is proved in [7].

**Theorem 1** *Let $H_+$ be a matrix defined by (3) and $H = \gamma I + \bar{U}\bar{M}\bar{U}^T$. Then*

$$H_+ = H_1 + \bar{U}_+ \bar{M}_+ \bar{U}_+^T,$$

*where $\bar{U}_+ = [\bar{U}, d, H_1 y]$ and*

$$
\bar{M}_+ = \begin{bmatrix} \bar{M} + m_3 \, zz^T, & m_2 \, z, & m_3 \, z \\ m_2 \, z^T, & m_1, & m_2 \\ m_3 \, z^T, & m_2, & m_3 \end{bmatrix}. \tag{4}
$$

*Here $m_1 = (1/b)(\eta a/b + 1)$, $m_2 = -\eta/b$, $m_3 = (\eta - 1)/a$ are elements of matrix $M$, $z = \bar{M}\bar{r}$ and $\bar{r} = \bar{U}^T y$.*

If $i \leq m$, the construction of matrix $H_{i+1}$ follows straightforwardly from Theorem 1. Thus we describe the construction of matrix $H_{i+1}$ in case $i > m$. We will assume that $H_{i+1-m} = \gamma_i I$. At the beginning of the $i$-th iteration, we have available the rectangular matrix $\bar{U}_{i-1} = [d_{i-m}, y_{i-m}, \ldots, d_{i-1}, y_{i-1}]$ and the block upper triangular matrix

$$
\bar{R}_{i-1} = \begin{bmatrix}
d_{i-m}^T y_{i-m}, & \cdots & d_{i-m}^T y_{i-1} \\
y_{i-m}^T y_{i-m}, & \cdots & y_{i-m}^T y_{i-1} \\
\cdots\cdots\cdots & \cdots & \cdots\cdots\cdots \\
0, & \cdots & d_{i-1}^T y_{i-1} \\
0, & \cdots & y_{i-1}^T y_{i-1}
\end{bmatrix},
$$

whose every block contains two rows and one column. First we determine matrix $\bar{U}_i = [d_{i-m+1}, y_{i-m+1}, \ldots, d_i, y_i]$ from matrix $\bar{U}_{i-1}$ by deleting the first two columns and adding the last two columns. Similarly easily we obtain matrix $\bar{R}_i$ from matrix $\bar{R}_{i-1}$. Only the last column $\bar{U}_i^T y_i$ of this matrix has to be computed. Furthermore, we compute recursively matrix $\bar{M}_i = \bar{M}_i^i$ in such a way that we set

$$
\bar{M}_{i-m+1}^i = \begin{bmatrix}
m_{i-m+1}^1, & m_{i-m+1}^2 \\
m_{i-m+1}^2, & m_{i-m+1}^3
\end{bmatrix}
$$

(indices 1, 2, 3 are now placed up) and for $i-m+1 \leq j \leq i-1$, compute vector $z_j = \bar{M}_j^i \bar{r}_j$, where $\bar{r}_j$ is $j-i+m$-th column of matrix $\bar{R}_i$, whose every even element is multiplied by number $\gamma_i$ (since $H_{i+1-m} = \gamma_i I$), and set

$$
\bar{M}_{j+1}^i = \begin{bmatrix}
\bar{M}_j^i + m_{j+1}^3 z_j z_j^T, & m_{j+1}^2 z_j, & m_{j+1}^3 z_j \\
m_{j+1}^2 z_j^T, & m_{j+1}^1, & m_{j+1}^2 \\
m_{j+1}^3 z_j^T, & m_{j+1}^2, & m_{j+1}^3
\end{bmatrix}.
$$

Vector $H_{i+1} g_{i+1}$ is computed by the formula

$$
\begin{aligned}
H_{i+1} g_{i+1} = \gamma_i g_{i+1} \quad & + \quad [d_{i-m+1}, \gamma_i y_{i-m+1}, \ldots, d_i, \gamma_i y_i] \, \bar{M}_i \\
& [d_{i-m+1}, \gamma_i y_{i-m+1}, \ldots, d_i, \gamma_i y_i]^T g_{i+1}
\end{aligned}
$$

(even columns of matrix $\bar{U}_i$ are multiplied by number $\gamma_i$). As we can see, approximately $6mn$ operations (addition and multiplication) are consumed in $i$-th iteration. However, approximately $2(m-1)n$ operations can be saved, if we compute and store inner products $d_j^T g_{i+1}$, $y_j^T g_{i+1}$ instead of $d_j^T y_i$, $y_j^T y_i$, $i-m+1 \leq j \leq i$. Then the first $m-1$ inner products $d_j^T y_i$, $y_j^T y_i$, $i-m+1 \leq j \leq i-1$ can be determined from the previously computed inner products by the formulas $d_j^T y_i = d_j^T g_{i+1} - d_j^T g_i$, $y_j^T y_i = y_j^T g_{i+1} - y_j^T g_i$, $i-m+1 \leq j \leq i-1$. Thus it is necessary to compute only two inner products $d_i^T y_i$, $y_i^T y_i$. Inner products $d_j^T g_{i+1}$, $y_j^T g_{i+1}$, $i-m+1 \leq j \leq i$ can be used for the computation of direction vector $s_{i+1}$, so we save $2mn$ operations.

The method described has been tested by using a set of 60 test problems with 1000 variables. This set (Test25) was obtained by merging the sets Test14, Test15, Test18 described in [6], which can be downloaded from `http://www.cs.cas.cz/luksan/test.html` (together with report [6]). The results of the tests are listed in Table 1, where `NIT` is the total number of iterations, `NFV` is the total number of function and gradient evaluations, `NF` is the number of failures and `TIME` is the total CPU time. We have tested the original `LBFGS` subroutine, described in [2], and our realizations of limited memory variable metric methods implemented in the UFO system [5]. In Table 1, `BFGSSTR` denotes the limited memory BFGS method with the Strang recurrences [9] (an analogy of `LBFGS`), `BFGSBNS` denotes the limited memory BFGS method with compact matrices described in [1], `BFGSNEW` denotes the limited memory BFGS method with recursive construction

of matrix $\bar{M}$ described above, `LMVMNEW` denotes the limited memory variable metric method with recursive construction of matrix $\bar{M}$ that use parameter $\eta$ proposed in [4], and `CG` denotes the conjugate gradient method. Note that the first four rows in Table 1 correspond to different implementations of the BFGS method and that our approach gives the best results.

| Method | NIT | NFV | F | TIME |
|:---:|---:|---:|:---:|---:|
| LBFGS | 110406 | 117226 | 2 | 43.38 |
| BFGSSTR | 99125 | 104085 | - | 37.56 |
| BFGSBNS | 91650 | 96235 | - | 36.89 |
| BFGSNEW | 85430 | 89796 | - | 33.50 |
| LMVMNEW | 92877 | 99033 | - | 34.61 |
| CG | 144990 | 222460 | 1 | 60.77 |

Table 1: Test results.

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